



**A PREMIXED ROTATING DETONATION ENGINE:
DESIGN AND EXPERIMENTATION**

Dissertation

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DESIGN AND EXPERIMENTATION**

DISSERTATION

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Ionio Q. Andrus, MS

Major, USAF

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DISSERTATION FOR A PREMIXED ROTATING DETONATION ENGINE:
DESIGN AND EXPERIMENTATION

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Abstract

Desire for a more efficient air breathing engine has shifted research attention to the Rotating Detonation Engine (RDE). Detonation is a more efficient combustion process than deflagration and provides a pressure gain. The RDE detonation cycle occurs in a compact volume to produce a high specific impulse engine. Computational fluid dynamic (CFD) models have predicted higher specific impulse and detonation wave speeds than has been seen in experimental RDE. The CFD models frequently assume premixed reactants and ignore inlet geometries to facilitate rapid computation. An experimental premixed RDE was sought to test if the premixed assumption in CFD was the root cause of the discrepancy between computational and experimental results. Design of a successful premixed RDE employed a feed system that simultaneously arrested flashback into the premixture while it fed the detonation. Flashback arresting feed designs were explored with single injector tests and validated with a fully premixed RDE. A relationship between arresting length and detonation feed requirements was derived and used to design a premixed RDE that fed premixture through feed slots that were 2.5 cm long and 0.5 mm high and operated on ethylene fuel and air oxidizer. The premixed RDE operated within a narrower region of equivalence ratio than a non-premixed RDE. Chemiluminescence video indicated that the premixed RDE experience combustion reactant-product mixing, and supports the theory that mixing delays are the

root cause of slower wave speeds in experimental RDE. Time averaged chemiluminescence results indicate that RDE detonations do not complete the reaction within the detonation wave, and suggest that future CFD studies should assume unmixed reactants, model the full injection geometry, and include a comprehensive chemical mechanism.

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Table of Contents

	Page
Abstract.....	iv
Acknowledgments.....	vi
Table of Contents	vii
List of Figures	xii
List of Tables	xxi
I. Introduction.....	1
1. Motivation	1
2. Background.....	2
3. Research Focus	6
3.1. Overview	6
3.2. Research Objectives.....	7
II. Literature Review.....	10
1. Overview	10
2. Detonation Fundamentals.....	13
2.1. Chapman-Jouguet Detonation	13
2.2. Zel'dovich-Von Neumann-Döring	20
2.3. Sizing Machinery for Detonation	22
3. Historical Rotating Detonation Engine Research	27
3.1. Russia: Zel'dovich and the Premixed Apparatus	27
3.2. United States: Nicholls' Work for AFRL	29
4. Current Research.....	30
4.1. Premixed Rotating Detonation Engines.....	30
4.2. Computational Fluid Dynamics for Rotating Detonation Engines.....	33
4.2.1. Russian Numerical Analysis.....	36
4.2.2. Wolanski's Group	39
4.2.3. Naval Research Laboratory Numerical Modeling	39
4.2.4. Numerical Summary	53
4.3. Experimental Non-Premixed RDE	53
4.3.1. Russian RDE Experiments	53
4.3.2. U.S. Air Force Research Laboratory RDE	55
4.3.2.1. Eight Centimeter Modular RDE (The Pratt Rig)	55
4.3.2.2. The 51 Centimeter Unique RDE (The Boeing Rig)	55
4.3.2.3. Fifteen Centimeter Modular Radial Inflow (Shank's Rig) ...	56

4.3.2.4. Fifteen Centimeter Radial Outflow RDE (Naples' Rig).....	57
5. Quenching Premixed Flame	64
6. Premixed Burner Flame Stability	74
6.1. The Role of Blowoff and Flashback in an RDE	74
6.2. Historical Research	76
6.3. Application Beyond Laminar Flames	80
7. Conclusions	87
III. Arresting Flashback	89
1. Overview	89
2. Premixed Injector Methodology	91
2.1. Premixed Detonation Engine Injector Apparatus	91
2.1.1. Injector Segment Test Section	92
2.1.2. Interface with Detonation	94
2.1.3. Instrumentation	95
2.1.4. Uncertainty	96
2.2. Test Methodology	97
3. Results	98
3.1. Premixed Injector in a PDE Host	99
3.1.1. The Speed of Flashback	99
3.1.2. The Relation between Slot Height, Slot Length, and Quenching..	102
3.1.3. Adjusted Velocity Gradient Comparison with Published Blowoff and Flashback Limits	104
3.2. Premixed Injector Hosted by an RDE	106
3.2.1. The Relationship between Feed Slot Height and Length in an RDE...	107
3.2.2. Adjusted Velocity Gradient Comparison with Published Flashback and Blowoff Limits	109
3.2.3. Comparison of Theoretical Quench Distance and Slot Height.....	113
3.2.4. Cycle Timeline Considerations.....	116
4. Conclusions & Recommendations	120
IV. Construction and Operation of a Premixed RDE.....	123
1. Background.....	123
2. Methodology.....	124
2.1. Test Apparatus.....	125
2.1.1. Baseline RDE Design Parameters.....	126
2.1.2. Mixing Assembly.....	126
2.1.3. Detailed Design of a Premixed RDE Feed System.....	127
2.1.4. Premixed Feed / Flashback Arrestor Design	132
2.1.5. Detonation Channel	134
2.1.6. Ignition of the Premixed RDE	135
2.2. Fuel Selection	135
2.3. Instrumentation	136

3.	Results	140
3.1.	Premixed RDE Operating Modes	140
3.2.	Comparison to Burner Stability	142
3.3.	Operating Map Comparison between a Premixed and Non-Premixed RDE	142
3.4.	Circumferential Velocities	148
4.	Conclusions	152
V.	Multi-Spectral Chemiluminescence	155
1.	Introduction	155
2.	Background.....	156
3.	Methodology.....	158
3.1.	Preliminary Spectrum	158
3.2.	Configuration of the RDE for Optical Access.....	161
3.3.	Conversion of Video to Detonation Phase Angle-Averaged Stills.....	163
3.4.	False-Color Recombination of Multi-Spectral Data.....	170
3.5.	Error and Uncertainty of Phase Angle and Intensity	171
4.	Results and Discussion.....	176
4.1.	Hydroxyl (OH*) Bandpass Image	177
4.2.	Methylidyne (CH) Bandpass Image	181
4.3.	Ethenediylidene or Bicarbon (C-C) Bandpass Imagery.....	184
4.4.	False Color Multi-Spectral Image	186
5.	Conclusions from Multi-Spectral Imagery.....	189
VI.	Conclusions and Recommendations	191
1.	Motivation	191
2.	Objectives and Achievements	191
2.1.	Objective 1	192
2.2.	Objective 2	192
2.3.	Objective 3	194
2.4.	Objective 4	194
3.	Unique Contributions	195
4.	Significance	196
5.	Recommendations for Future Work.....	197
Appendix I	Experimental Analogue of a Premixed Rotating Detonation Engine in Plane Flow .	199
1.	Introduction	200
1.1.	Experimental Setup.....	202
2.	Methodology.....	207
2.1.	Test Control.....	207
2.2.	Test Section Function	208
2.3.	Data Collection	209

2.4. Imagery Processing.....	209
3. Results	214
3.1. Choked Flame in the Detonation Channel	214
3.2. Detonation Decoupling and Shock Velocities.....	217
3.3. Detonation Related Phenomenon	218
3.4. Engineering Design Considerations.....	220
3.5. Feedback	222
3.6. Flashback.....	222
4. Conclusions	223
5. Acknowledgments.....	224
6. References	224
Appendix II Uncertainty Analysis for Mass Flow Rate and Derivatives	226
1. Mass Flow Rates.....	226
1.1. Fuel	226
1.2. Oxidizer (Air)	228
1.2.1. Total Mass Flow Rate Uncertainty Overview	230
1.2.2. Specific Heat Ratio	230
1.2.3. The Uncertainty of P_i	233
1.2.4. The Uncertainty of the Universal Gas Constant.....	233
1.2.5. The Uncertainty of Molecular Weight	233
1.2.6. The Uncertainty of the Pressure Transducer	234
1.2.7. The Uncertainty of the Thermocouple	234
1.2.8. The Uncertainty of Mach Number.....	236
1.2.9. The Uncertainty with the Number of Nozzles.....	237
1.2.10. The Uncertainty of the Nozzle Throat Diameter	237
1.2.11. Total Mass Flow Rate Uncertainty in Detail	237
1.3. Premixture Combined Flow Rates.....	239
1.4. Equivalence Ratio	239
1.5. Mixture Gas Constant (R_{mix}).....	240
1.6. Area from Mass Flow Rate	242
2. Velocity	243
3. Velocity Gradient Estimate Uncertainty	244
Appendix III Improving Detonation Cell Width Prediction Model	253
1. Background.....	253
2. Motivation	254
3. Methodology.....	263
4. Results	264
5. Conclusions and Recommendations	271
Appendix IV Modeling Laminar Flame Speed and Quenching Distance as a Function of Pressure and Equivalence Ratio	273

1. The Predictor Variable	273
2. Modeling Flame Speed as a Function of Pressure and Equivalence Ratio	276
2.1. Ethylene-Air Flame Speed	276
2.2. Hydrogen-Air Flame Speed	279
2.3. Quenching Diameter Estimates	281
2.4. Ethylene-Air Quenching Distances	282
2.5. Hydrogen-Air Flame Speed and Quenching Distances	285
2.6. Ethane-Air Quenching Distance	290
Appendix V Selected Computer Algorithms.....	292
1. Matlab Script LengthEquation.m.....	292
2. Matlab Script Design VelGradCalc.m	294
2.1. Matlab Function get_gas_props.m.....	296
2.1.1. Matlab Function BB_EqnOfState.m.....	316
2.1.2. Matlab Function BWR_EqOState.m	320
2.2. Matlab Function mix_properties.m	325
2.3. Matlab Function StabVelGrad.m.....	329
2.4. Matlab Function get_flame_props.m.....	329
Appendix VI Circumferential Variation in Wave Speed	333
1. Introduction	333
2. Methodology.....	333
3. Results and Discussion.....	338
4. Conclusion.....	348
5. Recommendations.....	349
List of Symbols	350
List of Acronyms.....	354
Bibliography	356
Vita	373

List of Figures

	Page
Figure 1. Cut-away (left) and cross-section (right) of a notional non-premixed RDE showing the a) fuel plenum, b) oxidizer plenum, c) detonation channel, d) oxidizer injection plate, e) centerbody, f) fuel plenum housing, and g) oxidizer plenum housing. Fuel from a) and oxidizer from b) flow into the detonation channel c) where they rapidly mix and sustain detonation that moves circumferentially k) in channel ..3	3
Figure 2. Cross-section of a notional non-premixed RDE showing the a) fuel plenum, b) oxidizer plenum, c) detonation channel, d) oxidizer injection plate, e) centerbody, f) fuel plenum housing, and g) oxidizer plenum housing. Fuel from a) and oxidizer from b) flow into the detonation channel c) where they rapidly mix and sustain detonation	11
Figure 3. The Hugoniot curve for combustion showing the 5 regions and 2 Chapman-Jouguet (CJ) points adapted from Kuo (38, p. 360)	15
Figure 4. Algorithm for Chapman-Jouguet detonation velocity iterative determination as described in Kuo (38, pp. 373-375)	18
Figure 5. Entropy trends for the Hugoniot relations adapted from Kuo (38, p. 367)	19
Figure 6. Illustration of the Zel'dovich, von Neumann, Döring detonation wave structure between the shock front at Location 1 and the combustion products at Location 2, adapted from Kuo (38, p. 362)	21
Figure 7. Von Neumann Spike overlaid on Rayleigh lines for the reactants and products of a detonation as adapted from Kuo (38, p.383)	22
Figure 8. Schlieren image of a hydrogen-air detonation at 1 atm and an equivalence ratio of 1.0. The detonation wave is moving right to left, and the transverse detonation waves are clearly seen as horizontal density gradients extending behind the detonation wave (48).....	23
Figure 9. Diagram of a detonation cell (adapted from Gavrikov et al. (181)).....	24
Figure 10. Detonation cell size in millimeters versus the minimum ignition energy in Joules at $T_0 = 293\text{ K}$ and $P_0 = 1\text{ atm}$, from (49,51–65).....	25
Figure 11. The cross section diagram of Voitsekhovskii's premixed annular detonation apparatus from reference (7)	28
Figure 12. Summary of CFD and experimental wave speeds (2,19,23,28,35–37,74–83)	34

Figure 13. Result of NRL inlet size study (76) using an ideal injection scheme of infinitely small holes evenly distributed across the inlet plenum area	40
Figure 14. Time averaged enthalpy of an RDE flow field split along 20 streamlines from Nordeen et al. (8)	41
Figure 15. Pathlines computed from time averaged streamlines from Nordeen et al. (8).....	42
Figure 16. Slot geometries used for NRL plenum feedback study (75).....	44
Figure 17. Total enthalpy contours and flow streamlines in an RDE with varying mixing rates and initial mixed fractions from Nordeen et al. (22)	46
Figure 18. Temperature (top) and Mach (bottom) contour plots of an RDE flow field simulated with finite injectors and simple mixing from Schwer et al. (84).....	49
Figure 19. Temperature (top) and instantaneous heat release (bottom) of an RDE flowfield modeled with premixed injection by Schwer and Kailasanath (77)	50
Figure 20. Comparison of RDE to PDE gross specific impulse using an integral computational method in a fixed wave frame of reference from Paxson (37)	51
Figure 21. Operating modes for a hydrogen-air non-premixed RDE with multiple waves and different injector-to-channel area ratios from Bykovskii et al. (72)	54
Figure 22. Cross Section of the AFRL modular 15 cm radial outflow RDE, Fotia et al. (104).....	58
Figure 23. Specific impulse and thrust grouped by mass flow rate and global equivalence ratio for a hydrogen-air non-premixed RDE (105).....	59
Figure 24. Experimental and numeric specific impulse results for hydrogen-air RDE data from Fotia et al. (106), Rankin et al. (23) and Schwer et al. (74,76,77,84)	60
Figure 25. Instantaneous radial cross sections of an operating RDE using acetone-PLIF techniques as reported by Rankin et al. (107)	63
Figure 26. Diagram of the laminar flame of thickness δ propagating between two walls of length L into the paper and separated by distance d adapted from Turns (108, p. 285)	65
Figure 27. Vector diagram of the reaction and conduction speeds for laminar flame	69
Figure 28. Estimated quenching distance model for a laminar hydrogen-air mixtures based on data from Lewis and Von Elbe (118) and Yang et al. (155).....	72

Figure 29. Cut-away model of a notional non-premixed RDE showing a differentially small sector of azimuth	75
Figure 30. Two dimensional cross section of notional a) non-premixed and b) premixed RDE flow paths	75
Figure 31. Critical boundary layer velocity gradients for hydrogen-air and ethylene-air fuel mixtures, standard temperature and pressure, data from Grumer et al. (30) and Fine (122,182)	77
Figure 32. Flashback for a hydrogen-air low-swirl burner in confined and unconfined configurations of differing material types adapted from Duan et al. (128) and used by permission from ASME, data from a:(128), b:(183), c:(184), d:(185), and e:(30)	85
Figure 33. Diagram of the premixed injector feed slot segment control variables.....	91
Figure 34. Drafting model of the premixed injector	92
Figure 35. a) D-shaped shim that changes the effective slot length b) test section assembled with a plastic plate and with U and D-shaped shims	93
Figure 36. Assembled injector test apparatus inserted into a PDE host (left) and an AFRL 15 cm RDE host (right)	94
Figure 37. Close-up of the premixed injector connected in the horizontal configuration to the RDE host	95
Figure 38. Flame quenching in a narrow premixed feed channel	100
Figure 39. Flashback occurring in a narrow premixed feed channel	100
Figure 40. Pressure and ion probe data from a flashback into ethylene-air premixture	101
Figure 41. Flashback indication for premixed ethylene-air in slot of varying heights and lengths showing that a narrower channel allows for a quicker termination of flashback	102
Figure 42. Mixture pressure, slot length, slot height, and flashback indication for ethylene-air showing that narrower slots require higher feed pressure and arrest flashback more quickly	103
Figure 43. Adjusted gradient comparison with published premixed flame stability limits from Grumer et al. (30)	104

Figure 44. Relationship between slot height and length for arresting flashback in an RDE-hosted premixed injector	108
Figure 45. Variation of ethylene-air injector feed pressure with slot length, mass flow rate, and slot height.....	109
Figure 46. Injector adjusted velocity gradients for hydrogen-air (left) and ethylene-air (right) premixture flowing into an RDE host and compared with historical data	110
Figure 47. Distribution of the flashback and no-flashback results separated by injector orientation in the RDE Host	112
Figure 48. Idealized pressure trace of a PDE and an RDE highlighting the additional dwell at high pressure of a PDE	113
Figure 49. Comparison of slot height, h , to the theoretical quenching distance, d_Q , calculated with the average feed pressure for ethylene-air (left) and hydrogen-air (right) in the RDE hosted injector	114
Figure 50. Diagram of the detonation cycle timeline.....	116
Figure 51. CAD model of an easily adjustable premixed RDE.....	125
Figure 52. Length calculation using Equation 61 with the inputs shown in the lower left, lines representing the independent variation of single variables indicate the influence of that variable on the quenching length needed to support the assumed cycle.....	128
Figure 53. Adjusted velocity gradient predictions as a function of slot height	130
Figure 54. Interface plane of the premixed RDE showing shim spacing in the feed slots	132
Figure 55. Photograph of assembled frustra stack with inset showing segmented con-annular slot	133
Figure 56. Diagram of a feed slot segment between frustra.....	134
Figure 57. Premixed RDE sensing and control diagram	136
Figure 58. premixed RDE operation with ethylene-air showing detonation mode (a) waveform and (b) spectrum, and acoustic mode (c) waveform and (d) spectrum	141
Figure 59. Velocity gradient observations for the premixed RDE compared with published (30) flashback and blowoff limits for detonation and acoustic operation modes	143

Figure 60. Operating maps for a) non-premixed and b) premixed RDE using ethylene and air	144
Figure 61. Wave speed calculations for (a) non-premixed and (b) premixed RDE operating with ethylene-air.....	145
Figure 62. Time sequence of ethylene air detonation during 1 detonation cycle	146
Figure 63. Collage of two complete laps of the detonation: with highlighting showing the dark band highlighted in yellow ellipses (top) and without highlighting (bottom).....	147
Figure 64. Pathlines and velocity profiles for manually tracked points.....	149
Figure 65. Chapman-Jouguet detonation velocity for ethylene-air, assuming a mixture of reactants and a percentage by mass of pre-combusted products	152
Figure 66. Chemiluminescence from a single cycle of an ethylene-air premixed detonation moving from left to right in the RDE and imaged through a 300 nm to 342 nm bandpass filter corresponding with OH emission.....	155
Figure 67. Pathlines for a detonation wave cycle: two approximate pathlines are drawn as dashed lines that flow from the bottom to the top, wrap around the cycle image right to left, and pass through the rotating wave 2 times before exit; the dark band of products is indicated with arrows at locations (a), (b), and (c)	156
Figure 68. Spectrum of an ethylene-air RDE operating at 0.99 kg/s and $\phi = 1.02$ showing anticipated emission bands and available filter transmission curves.....	159
Figure 69. Premixed RDE configured with a quartz outerbody for optical access and operating at 0.33 kg/s and $\phi = 0.86$	161
Figure 70. Field of view image for the multi-spectral video showing the premixed RDE configured with a quartz outerbody, opaque plates, and 60 degree sector used to time-average the detonation cycle	162
Figure 71. Diagram of the field of view and significant datum lines used to track the detonation wave front in high speed video imagery	163
Figure 72. Linear fit to the cumulative phase angle (top) and residual error to the least squares regression (bottom) as a function of time	166
Figure 73. Data cube collecting 60 degrees of azimuth from 8 frames of video imagery and storing it in the appropriate cycle azimuth for time averaging	168
Figure 74. Color distributions for the false-color recombined multi-spectral imagery	170

Figure 75. Cycle azimuth error is introduced by using the small angle approximation; cycle azimuth error is approximately 1.35° at 30° off azimuth, or about 0.4%	173
Figure 76. Full color imagery of an ethylene-air premixed RDE configured with a quartz outerbody and showing the distinctive blue hues of Swan band emission captured with an exposure of 122 μs, or approximately 1/4 th of a cycle	176
Figure 77. Hydroxyl (OH*) emission from time averaged filtered high speed video of an ethylene-air premixed RDE operating at 0.320 kg/s total mass flow, $\phi = 1.11$	177
Figure 78. Cross section of the average OH intensity at the 270 pixel axial location	179
Figure 79. Methylidyne (CH) emission from time averaged filtered high speed video of an ethylene-air premixed RDE operating at 0.382 kg/s total mass flow, $\phi = 0.992$	181
Figure 80. Residual error for the linear fit of cycle phase rate for the CH image showing variable phase rates and cyclic measurement error, the linear fit removes the cyclic measurement error but not the variable phase rate	182
Figure 81. Cross section of the CH filtered average intensity taken at the 270 pixel and 125 pixel axial location	183
Figure 82. Time averaged emission from ethenediylidene (C ₂), filtered high speed video of an ethylene-air premixed RDE operating at 0.374 kg/s total mass flow, $\phi = 1.03$	185
Figure 83. Cross section plot of the C-C filtered time-averaged image at the 270 pixel axial location	185
Figure 84. Emission of multi-spectral high-speed imagery cycle-averaged from different runs of an ethylene-air RDE with similar conditions, each filtered image was normalized before combination.....	187
Figure 85. Cross sections from the normalized false-color multi-spectral imagery at the axial locations of 270 and 125.....	189
Figure A1.1 Schematic of the linear test section showing fluid streams and ideal detonation mechanics.....	202
Figure A1.2 Detail drawing of the feed nozzle bar. Nozzles were not contoured. Dimensions are in mm	204
Figure A1.3 Diagram showing conical grooves and steel inserts to create a diffuser in the detonation channel	205

Figure A1.4 Diagram of the two schlieren optical paths for this experiment, a) focused schlieren, b) parallel beam schlieren.....	206
Figure A1.5 Test section timeline diagram. Three separate timelines were tied to a central trigger while the test was separated into two phases by the initiation of the second detonation	208
Figure A1.6 Position measurements between sequential images, $\Delta t = 30 \mu s$, from test J were combined with frame rate and length calibration factors to generate velocity measurements	210
Figure A1.7 Illustration of theoretical Chapman-Jouget Detonation and sonic velocities for hydrogen-air combustion as a function of equivalence ratio as computed with NASA's CEA (137).....	212
Figure A1.8 Two frames showing qualitative measurements of a) decoupling of the shock in the detonation channel and b) combustion in the mixing plenum during test H.....	213
Figure A1.9 Compendium of velocity measurements from high speed schlieren video. The data from -0.1 to 0.28 m were collected using a different field of view than data at distances greater than 0.28 m	216
Figure A1. 10 Time sequenced schlieren of shock waves emanating from a combustion front into the cool reactants during test event B.....	218
Figure A1.11 Flame erosion and sidewall fracturing of the polycarbonate mixing plenum sidewall at the sealed joint with the fuel plenum, following test H.....	221
Figure A2.1 Plot of the contribution of the specific heat ratio uncertainty to the total mass flow rate error as a function of the specific heat ratio, and initial uncertainty.....	232
Figure A2.2 Plot of the proportional relationship between the velocity gradient and pressure (left) and slot height (right) from Equations A2.78 and A2.79 respectively	252
Figure A3.1 Photograph of sooted foil showing detonation cell traces (148)	254
Figure A3.2 Sooted foil record of stoichiometric hydrogen and oxygen in a (A) 3.25 x 0.25 inch rectangular and (B) 2 inch circular tube (148)	254
Figure A3.3 Regression model fit to 18 data points available in the Caltech Detonation Database (49).....	257
Figure A3.4 Custom tests completed in JMP (149) testing the viability of the Baseline model given the regression of the data; all tests show statistical significance that the Baseline Model is true given the observations	258

Figure A3.5 Summary of residuals for baseline model as computed by the JMP statistical package (149)	260
Figure A3.6 Test for constant variance of baseline model based on oxidizer	261
Figure A3.7 Plot of all available observed cell widths for ignition energies regardless of equivalence ratio from references from (49,51–65) catalogued in the CalTech detonation database (49) from MS Excel using a power series to project a predictor variable transformation	264
Figure A3.8 Plots of residuals vs row number for four fuel species: ethylene (C_2H_4), propane (C_3H_8), C_4H_{10} (Butane), and hydrogen (H_2) that highlight the non-linear and non-independence of the observed data, the histogram, normal quantile plot, and Shapiro-Wilk-W test show that the data does come from a normal distribution	265
Figure A3.9 Regression model for $E_{initiation}$	268
Figure A3.10 Model Verification: $E_{initiation}$ combined with $Cosh(\phi)$ and Fuel Type only accounts for 57% of $\log(\lambda)$	269
Figure A4.1 Normal quantile plot of the residuals for the initial polynomial fit to ethylene-air laminar flame speeds at elevated pressures	277
Figure A4.2 Plot of a polynomial model to data (151–153) varied by both pressure and mass equivalence ratio	277
Figure A4.3 Residual errors of the ethylene-air flame speed model plotted as a function of the predictor variables percent fuel by volume (left) and initial pressure (right)	278
Figure A4.4 Laminar flame speed model for hydrogen air at a reference condition of 1 atm and 300K with experimental data from (156)	280
Figure A4.5 Residual errors for hydrogen-air flame speed model at reference condition of 300K.....	280
Figure A4.6 Modeled ethylene air flame quenching distance model presented with published experimental data (108,154).....	283
Figure A4.7 A comparison of the failure of the thermal conductivity model to predict hydrogen air quenching distances based on reference conditions.....	285
Figure A4.8 Quenching distance experimental data and linear regression model for a hydrogen-air mixture, data from Lewis and Von Elbe (118) and Yang et al. (155)	287

Figure A4.9 Normal quantile plot for hydrogen-air quenching distance model.....	288
Figure A4.10 Shapiro-Wilk W test for normality of the hydrogen-air quenching distance residuals generated by the JMP (149) software package	289
Figure A4.11 Plot of the predicted natural log of quenching distance with the actual quenching distance for hydrogen air.....	289
Figure A4.12 Experimental data from (118) and model for ethane-air quenching distances	290
Figure A6.1 Diagram of the detonation channel annulus for varying wave speed investigation	334
Figure A6.2 close-ups of the annulus channel showing the barb of the ion probes inserted into the channel (left) and the single 3/8-inch bolt inserted into the detonation channel (right)	335
Figure A6.3 Photograph of the spiral inserted into the base of the detonation channel.....	336
Figure A6.4 Discrete wave speed measurements as a function of azimuth angle measured for 20+ consecutive cycles during 20 separate tests	339
Figure A6.5 Three selected azimuth cycle wave speeds averaged over 25 cycles with standard deviations included	340
Figure A6.6 View of the detonation annulus showing a 1000 m/s detonation wave at the 11 o'clock position and two acoustic waves moving in the opposite direction at 900 m/s and located at the 1 o'clock and 7 o'clock positions.....	345
Figure A6.7 Azimuth wave speeds for (a) clockwise detonation and (b) counter clockwise acoustic waves averaged over 23 detonation cycles from an ethylene-air detonation in an RDE configured with a quartz outer body, 0.65 kg/s total mass flow, and $\phi = 0.98$	346
Figure A6.8 Periodogram of the variation of the (a) detonation wave speed and (b) counter rotating acoustic waves with time for an ethylene-air detonation in an RDE configured with a quartz outer body, 0.65 kg/s total mass flow, and $\phi = 0.98$	347

List of Tables

	Page
Table 1. Description of CFD and experimental detonation wave speed results	35
Table 2. Numerical RDE simulation wave speeds for hydrocarbon fuels, Schwer et al. (78).....	44
Table 3. Test conditions for CFD and experimental specific thrust comparison data from Fotia et al. (106), Rankin et al. (23) and Schwer et al. (74,76,77,84).....	60
Table 4. Design parameters for premixed RDE.....	126
Table 5. Uncertainties for wavefront phase angle with a 95% confidence level.....	175
Table 6. Summary of time averaged image conditions	177
Table A1.1 Test section configurations.....	206
Table A1.2 Summary of test conditions and results	215
Table A2.1 Measurement property uncertainty for gaseous fuel.....	228
Table A2.2 Measurement uncertainty values for gaseous oxidizer	229
Table A3.1 Summary of fit and parameter estimates for an improved cell width prediction using E_{init} and equivalence ratio.....	266
Table A3.2 Description of beta terms for Equation A3.16.....	271
Table A3.3 Description of beta terms for Equation A3.17.....	271
Table A4.1 Summary of fit for the ethylene-air flame speed model	278
Table A4.2 Summary of fit for the hydrogen-air flame speed model	281
Table A4.3 Summary of fit for the ethylene-air flame speed model	287
Table A4.4 Parameter estimates for the hydrogen-air quenching distance model	288
Table A4.5 Summary of fit for the ethane-air quenching distance model	291
Table A6.1 Summary of results and experimental treatments for the azimuthal wave speed review	342

A PREMIXED ROTATING DETONATION ENGINE: DESIGN AND EXPERIMENTATION

I. Introduction

1. Motivation

In 2012, a call from the U.S. Air Force's (USAF) headquarters notified units needing to re-program funds to submit their requests as soon as possible. At the time, the Evolved Expendable Launch Vehicle (EELV) program office at Los Angeles Air Force Base (AFB), CA was struggling to fund the development of a rocket adapter capable of carrying two satellites simultaneously into orbit. With a relatively miniscule research and development budget, the office sought approval to move the \$20 million needed to kick-start the effort from the rocket procurement allocation. This maneuver, called reprogramming money, requires special approval from an often doubtful Washington bureaucracy and is also known to come with one very large risk. With the operational Air Force in the midst of a war, fuel consumption had exceeded the approved allocation and the Air Force was looking for money to pay the bill. Instead of being re-programmed for development of rocket parts, the EELV money was re-directed by Washington to pay the USAF fuel bill. Subsequently, the dual launch capability that could have saved billions of dollars over the ensuing decade never got off the ground.

This thinly veiled solicitation for expendable funds was not isolated to space acquisition nor to 2012 and highlighted how fuel efficiencies affect the entire USAF. Improving fuel efficiency is critical to meet core flying activities and frees resources for

every other military mission. Modern technological advances have pushed conventional turbine engine efficiencies to the limits of practicality, so achieving the next improvement will require non-conventional adaptations to the engine.

Recognizing the need to reduce fuel consumption, the Detonation Engine Research Facility (DERF) at the Air Force Research Laboratory's Turbine Engine Combustion Branch (AFRL/RQTC) initiated research in 2009 on a novel device (1,2) known as a Rotating Detonation Engine (RDE) that combusts fuel with lower entropy generation and provides a pressure gain across a nearly constant volume combustion process. These engines utilize the inherently more efficient process of detonation (3) rather than the less efficient conventional deflagration process. Current RDE research was inspired by the theoretical and experimental efforts described briefly below and in Chapter II. Differences between the wave speed of numerical simulations and experimental results indicated that in-situ mixing of may be affecting experimental RDE operation and detonation reaction. The research described in Chapters III, IV and V is centered on designing, operating, and understanding a premixed RDE that removes the time delay of diffusion mixing and provides an experimentally generated data set that permits a comparison of how mixing influences RDE operation.

2. Background

A brief overview of detonation is given here to fully introduce the motivation for studying the influence of mixing on RDE operation. In 1940, Zel'dovich (3) proposed that detonation was an inherently more efficient combustion process than deflagration. The Zel'dovich-von Neumann-Döring model (4-6) describes detonation as a combustion

zone that is closely coupled to a pressure wave, providing a nearly constant volume combustion, and producing a pressure rise across the combustion front. The speed of detonation makes it a difficult process to harness. In 1959, Voitsekhovskii et al. (7) envisioned, built, and operated a novel engine that maintained a constant detonation within an annular channel; a device that would now be referred to as an RDE. The channel walls provided the necessary confinement to guide the detonation circumferentially around the annulus while the gaseous reactants flowed axially and fed the process.

A modern RDE looks similar to the notional RDE shown in Figure 1 and is formed by nesting one cylinder, referred to as a centerbody, inside a larger cylinder referred to as the outerbody. The annular channel formed between the centerbody and the

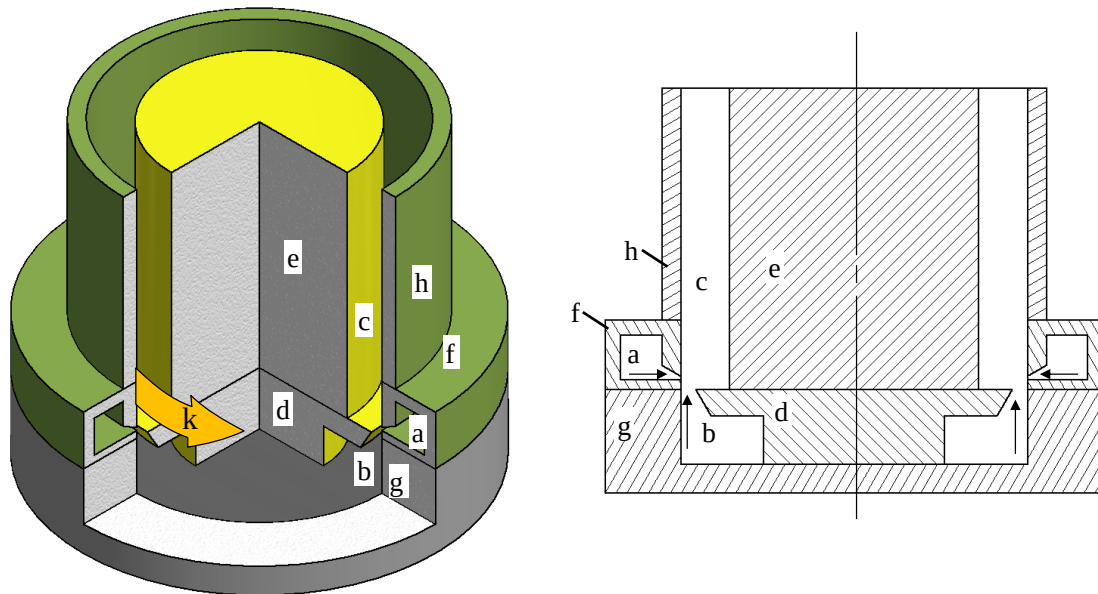


Figure 1. Cut-away (left) and cross-section (right) of a notional non-premixed RDE showing the a) fuel plenum, b) oxidizer plenum, c) detonation channel, d) oxidizer injection plate, e) centerbody, f) fuel plenum housing, and g) oxidizer plenum housing. Fuel from a) and oxidizer from b) flow into the detonation channel c) where they rapidly mix and sustain detonation that moves circumferentially k) in channel

outerbody is called the detonation channel. Fuel and oxidizer are injected into one end of the annular channel through some sort of plenum. In a non-premixed RDE, the fuel and oxidizer are injected separately, while in a premixed RDE they are mixed upstream of the plenum and injected as a mixture into the detonation channel. Once ignited, a detonation will progress circumferentially around the annulus of the channel, consuming the reactants as they enter. If the reactants are injected quickly enough, the detonation will have a constant volume of detonable mixture and will continue uninterrupted indefinitely until the flow of reactants is modified or halted.

The pressure gain in an RDE sets it apart from conventional combustors which experience a pressure loss through deflagration. Thermodynamic cycle analysis (8,9) has predicted that integrated pressure gain combustors can improve overall system efficiency. Achieving improved cycle efficiencies was a goal of the pioneering efforts of Voitsekhovskii (7,10), who operated a captive premixed acetylene-oxygen system exhausted to a vacuum chamber, and Nicholls (11–13), who operated a non-premixed cycle RDE vented to atmospheric conditions. These early efforts enjoyed limited success, but the practical problems associated with igniting and sustaining detonation in Nicholl's device could not be solved at the time. While Voitsekhovskii overcame startup problems, his device was intended as an instrument to study detonation rather than provide propulsion. Subsequently, the startup problems minimized the progress in Russia and halted it almost completely in the United States for 50 years.

Survey reviews of current research (14,15) identified several topics critical to RDE development that need to be studied further. For example, the fundamental mechanisms that initiate a sustained detonation were not well understood by 2014.

Further research into the conditions necessary to start the RDE must occur before reliable operation can become part of an RDE design. The survey papers also identified that a computational and experimental flow fields shows qualitative agreement but reported minor quantitative differences in specific thrust and major differences in detonation wave speed. These differences may indicate deficiencies in computational models or poor implementation of experimental hardware. Answering the questions of what caused the difference between CFD and experimental results and how to ensure a repeatable startup of an RDE will ensure that operational RDE may be designed.

Since RDE development is still relatively new, there is a lot to learn about their design, construction and operation. Development of experimental RDEs at AFRL to date (2,16) has shown that the RDE envelope of operation is influenced by mass flow rate through the system, thermal loading of the components, equivalence ratio, and air and fuel injection schemes. How design choices influence RDE operation and the transition from deflagration to detonation (DDT) are poorly understood. Experimental studies (1,2,16) have also noted that the detonation appeared to be moving in the annulus at speeds slower than described by the Chapman-Jouguet (CJ) detonation theory (17,18). Russo (19) cited Falempin (20) as having theorized that poor mixing is the cause of detonation wave speeds slower than Chapman-Jouguet predictions. In the pursuit of understanding the design trade space for RDEs, numerical models have been constructed to describe the influence of channel size, injection areas, equivalence ratios, and mass flow rates upon RDE performance (21).

The CFD modelers prefer to assume premixed fuel-oxidizer (21,22) to speed calculations, whereas experimental RDE operate without premixing fuel and oxidizer.

This has resulted in separate bodies of results with different physical mechanisms being compared. A comparison of partially premixed computational results from the Naval Research Laboratory (22) with the non-premixed hydroxyl (OH^*) chemiluminescence visualizations of Rankin et al. (23) shows good agreement on detonation wave shapes and the existence of standoff but disagreement on wave speeds. The differences in mixing characteristics between the CFD and experimental RDE are assumed to be the basis for the difference in wave speeds. Ideally, the experimental configurations and numerical models match exactly – a goal that requires experimental premixing or CFD modeled with the complexity of the full chemistry, viscous, and compressible flow.

Construction of a premixed experimental RDE has always been problematic. The published discussion of a successful premixed RDE (7) describes an apparatus that was vacuum driven and had issues with unstart and flashback. Other groups (1,24,25) have tried and failed to operate a premixed RDE, constantly suffering flashback into the feed plenum that starves the detonation cycle of detonable mixture and destroying equipment. Development and construction of a premixed feed system that halts flashback into the premixed fuel and oxidizer is the key to building a successful premixed RDE. Only after constructing a premixed RDE that arrests flashback can a true comparison of experimental results be made to the premixed CFD simulations.

3. Research Focus

3.1. Overview

This dissertation demonstrates the first-ever successful air breathing, premixed RDE. Flashback was overcome by feeding the RDE with long narrow feed slots that

attenuated the detonation wave and quenched the chemical reaction, enabling operation of a premixed ethylene-air RDE. Injector technology was tested with an incremental approach before building a premixed RDE was because, as Thomas et al. (1) reported, premixed RDE operation is risky. The premixed RDE described in (1) featured a porous metal feed plate, which was destroyed when flashback occurred, and required repairs before it could be used again. Early experiments associated with the research for this dissertation (reported in (26), and included as Appendix I) were also destroyed. St. George et al.(24) attempted to partially premix using a novel hybrid fuel injection and metal foam approach that resulted in similar test failures. A close examination of these studies indicated that each attempted to circumvent the detailed modeling of quenching distances at high pressure and construct a feed system with very small holes.

3.2. Research Objectives

The research that led to successful premixed operation had four objectives:

1. Discover the flow conditions that halt flashback into a premixed feed system exposed to a transient detonation.
 - a. Provide experimental results and formulae indicating how quenching distance and velocity gradient should be applied.
2. Characterize the correlations between flashback in a premixed flow exposed to a transient detonation front and traditional burner stability parameters such as: quenching distance and critical boundary layer velocity gradient as functions of the temperature, pressure, equivalence ratio, mass flow rate, and fuel.
 - a. Provide experimental data varied by mass flow rate/ equivalence ratio/ fuel type compared to flashback limits and detonation conditions.
3. Explore the ability of traditional burner stability design principles to effectively arrest flashback in a premixed rotating detonation engine.

- a. Build a flashback map for premixed RDE using mass flow rate, equivalence ratio, quenching distances, and adjusted flashback velocity gradient.
 - b. Demonstrate slot heights that prevent flashback.
- 4. Experimentally characterize the operation of a premixed rotating detonation engine.
 - a. Build a premixed RDE operating map based on mass flow rate and equivalence ratio.
 - b. Understand the differences between experimental premixed RDE results and CFD simulations.
 - c. Understand the differences between experimental premixed and non-premixed RDE.

The success of this effort was reported in two papers by the author (27,28) and expanded in Chapters III, IV, and V of this document. The critical difference for achieving success in this work where others failed was accurate modeling of the quenching distances at elevated pressure and employing a feed system that arrested flashback with the principles of friction flow. Furthermore, this research showed that quenching of a detonation could be described in terms of critical velocity gradients from burner stability theory.

Achieving these objectives moved the United States Air Force toward more efficient engine technology by showing that mixing plays only a minor role in RDE operation. Experimental results indicated that the premixed feed system design needed multiple narrow slots and was constrained by feed and detonation pressures. Experimentation also demonstrated that current CFD models need to include combustion equations for the low pressure deflagration between passages of the detonation wave. The resulting validation of CFD studies and information regarding RDEs answered some of

the fundamental questions of how mixing affects RDE operation and why experimental RDEs differ from computational models. This improved understanding of the RDE operation moves the technology closer to implementation of a more efficient engine, which is a solution that either directly or indirectly affects the entire United States Air Force, including the EELV program.

II. Literature Review

1. Overview

This chapter reviews the existing body of work that describes arresting flashback in premixed flame, computational and experimental RDE, and burner stability. It directly addresses the first research objective, “Discover the flow conditions that halt flashback into a premixed feed system exposed to a transient detonation.” It also describes the fundamental principles used to complete research Objectives 2 and 3: characterize, design, and demonstrate a premixed injection system. Finally, this chapter provides selected summaries of current computational and experimental results that serve as a comparison baseline to complete Objective 4, “Experimentally characterize the operation of a premixed rotating detonation engine.” It steps beyond a simple survey of the existing theory and results by developing a method to adjust burner stability diagrams for detonation flashback conditions.

The design and operation of a premixed RDE required an understanding of the detonation phenomenon, flame quenching, compressible flow, and burner stability theory. Each of these principles highlighted a different aspect of arresting flashback into the premixed feed system. The detonation phenomenon has been studied for decades, and enjoys the well-established models theorized by Chapman (17) and Jouguet (18) and by Zel’dovich (29), von Neumann (5), and Döring (6). Flame quenching is also fairly well established and serves as one of the fundamental principles of premixed combustion systems. Burner stability research carried out in the 1950s (30–32) provided engineering

parameters to design safe and reliable premixed burner systems now used in homes throughout the world. Compressible flow is also well understood (33), with analytical solutions to many of the problems and applications sought by engineers. Separately, none of these principles holds the key to achieving safe operation of a premixed RDE, but together they describe how to design a feed system that will continuously supply reactants and arrest flashback for a premixed detonation engine.

The construction of a premixed rotating detonation engine enables direct comparison with computational results and with non-premixed RDE. Several groups have studied RDE using CFD models (34–37) where the fuel and oxidizer were already assumed to be premixed. Current experimental RDE operate by injecting fuel and oxidizer in separate streams (1,2) with a configuration similar to the notional diagram shown in Figure 2. The RDE operated at the DERF inject fuel into the oxidizer stream at

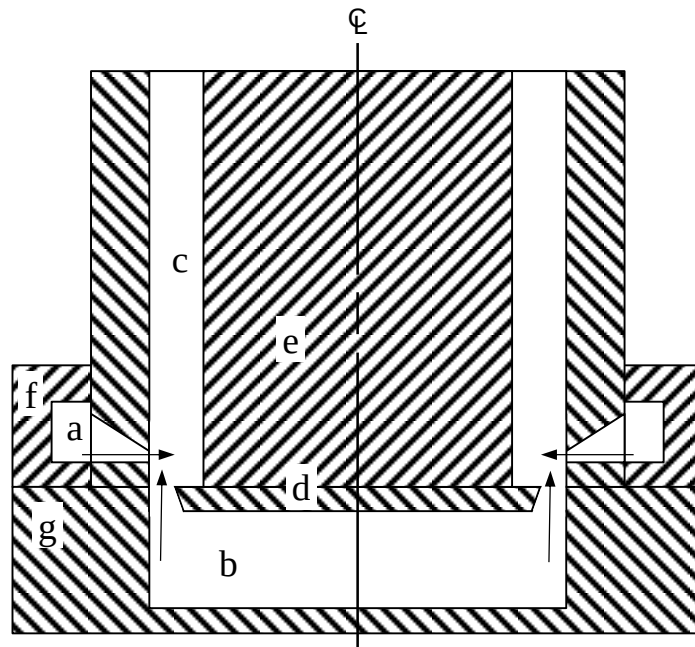


Figure 2. Cross-section of a notional non-premixed RDE showing the a) fuel plenum, b) oxidizer plenum, c) detonation channel, d) oxidizer injection plate, e) centerbody, f) fuel plenum housing, and g) oxidizer plenum housing. Fuel from a) and oxidizer from b) flow into the detonation channel c) where they rapidly mix and sustain detonation

the detonation channel inlet, and mixing occurs almost immediately due to the high diffusion rates of the gaseous fuels and the turbulence induced by injecting the fuel jets into the cross-flowing air. Liquid fuels, particularly the heavier hydrocarbons that the US Air Force employs, diffuse much more slowly (38, pp. 671, 681-682). It is anticipated that successful detonation requires these heavier hydrocarbons to be mixed well before the injection point. However, Nordeen et al. (22) performed a CFD study on mixing effects and concluded that degree of mixedness does not significantly impact the wave speed nor does it decrease the efficiency of an RDE. The wave speeds reported by Nordeen et al. (22) showed only a small decrease as mixing delays were introduced. Notably, the CFD used a two dimensional simplification of an RDE, as if the annulus of an RDE had been un-wrapped and laid flat. Additionally, the assumption of an ideal injection system that used infinitely small injectors distributed evenly across a feed plate avoided the vorticity and turbulence created in the finite injection architecture of experimental RDE. These two assumptions included in the CFD model cannot be matched in an experimental RDE, and will be discussed in further detail in Section 4.2 of this chapter. The experimental wave speeds for both a non-premixed and premixed experimental RDE are compared in Chapter IV.

Mixing the oxidizer and fuel before injection presents a hazard due to the potential for flashback into the mixing chamber and subsequent explosive termination of the equipment (1,24,26). Arresting flashback from the detonation into the premixed plenum is the fundamental problem of designing a premixed RDE. In deflagration systems, thermal quenching and flame stability prevent flashback and are discussed in Sections 5 and 6 of this chapter. Thermal quenching and flame stability theory and

principles guided design choices that overcame the risks and hazards associated with premixing. The experimental results from application of these principles are shown in Chapter III.

2. Detonation Fundamentals

The first step in understanding a detonation combustion cycle is to understand detonation itself. Over the past century, two predominant models were developed by Chapman (17) and Jouguet (18) (CJ) and by Zel'dovich (29), Von Neumann (5), and Döring (6) (ZND) to predict the detonation conditions. These models provide a one-dimensional perspective of an intrinsically three dimensional phenomena. Significant experimental data has enabled empirical relationships to be formed between detonation cell size, ignition energy, and minimum detonation chamber cross section sizes.

2.1. Chapman-Jouguet Detonation

A simple zero-dimensional model of detonation formed by Chapman and Jouguet describes the change in properties across a detonation wave front. Kuo (38, pp. 361-379) showed a complete derivation that highlights the form of the energy conservation equation known as the Hugoniot relation:

$$\frac{\gamma}{\gamma - 1} \left(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1} \right) - \frac{1}{2} (p_2 - p_1) \left(\frac{1}{\rho_1} + \frac{1}{\rho_2} \right) = q \quad (1)$$

where p is the pressure, ρ is density, and γ is the ratio of specific heat. The thermal release q is defined by the change in enthalpy of formation, h^o , between Station 1 and 2:

$$q \equiv h_1^o - h_2^o \quad (2)$$

The left hand side of Equation 1 is controlled by the right hand side. In practice, the heat release term is a function of the fuel-oxidizer chemistry, and Equation 1 becomes a function of only pressure and density. Plotting Equation 1 for constant heat release from initial pressure p_1 and density ρ_1 yields the Hugoniot curve shown in Figure 3. The curve represents all possible solutions of $\{p_2, \rho_2\}$ under the perfect gas assumption for a combusting mixture whose start point is at $\{p_1, \rho_1\}$ and whose per unit mass heat release, q , is constant. The line itself is a hyperbola which asymptotes to the pressure and specific volume axes. Lines extending from the origin are tangent at exactly one point on each leg of the Hugoniot curve. These points have the special name referred to as CJ points which will be described in subsequent paragraphs.

Kuo (38, pp. 359-360) showed that the Hugoniot relation of Equation 1 may be derived from the Rayleigh-line relation:

$$\rho_1^2 u_1^2 = \frac{p_2 - p_1}{\frac{1}{\rho_1} - \frac{1}{\rho_2}} = \dot{m}^2 \quad (3)$$

where ρ is density, u is velocity, p is pressure, and $\dot{m}$ is the mass flow rate of fluid between State 1 and State 2.

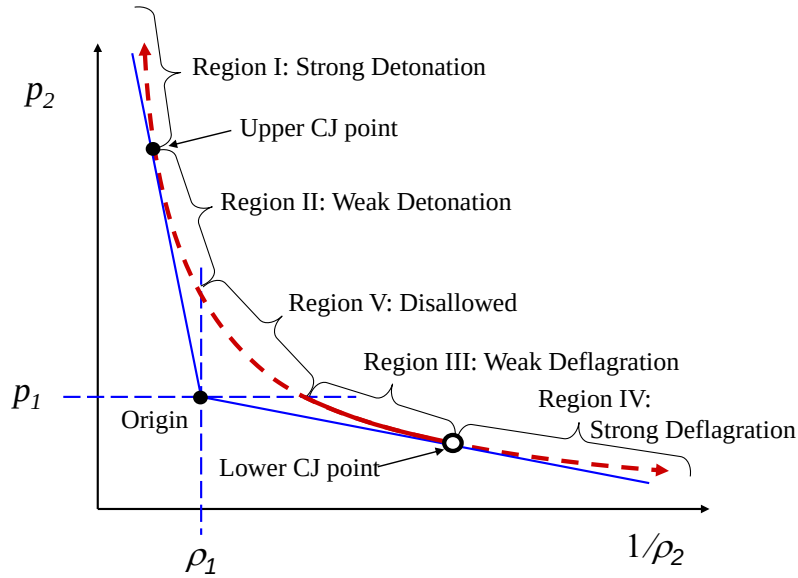


Figure 3. The Hugoniot curve for combustion showing the 5 regions and 2 Chapman-Jouguet (CJ) points adapted from Kuo (38, p. 360)

Kuo (38, pp. 357-363) also explains that while the Hugoniot curve represents all possible mathematical solutions to the Hugoniot relation, not all regions are physically accessible. The curve may be divided into 5 regions and 2 key points described here with the assumption that the entire mixture undergoes a single combustion process:

Region I: Strong Detonation. The detonation wave in this region is moving slower than the speed of sound in the burned gases, allowing disturbances of rarefaction to be communicated to the detonation wave. Rarefaction decreases the strength of the combustion wave in this region and drives it back to the upper CJ point. Detonation in this region is seldom seen (38, p. 363), requiring over-driven shock waves and very strong confinement.

Upper Chapman Jouguet Point: At this point, the detonation travels at the speed of sound relative to the burned gases. Most experimental detonations fall at this point on the Hugoniot curve. This is also the local minima of entropy generation.

Region II: Weak Detonation. The detonation is moving slower than the speed of sound relative to the burned gases, and pressure waves can coalesce to drive the combustion in this region up the Hugoniot curve toward the upper CJ point. Detonation in this region is rarely observed (38, p. 363) and requires extremely fast chemical kinetics.

Region III: Weak Deflagration. The most often observed solution for deflagration (38, p. 364), the gas velocity is accelerated through the deflagration wave (but not pushed supersonic), and experiences a slight pressure drop.

Lower Chapman Jouguet Point: The maximum deflagration wave speed is predicted here, with the deflagration wave moving at Mach 1. Deflagration at this point is not seen experimentally (38, p.364), and entropy is at a local maximum.

Region IV: Strong Deflagration. Never observed experimentally (38, p. 364), since gas flow relative to the deflagration front must shift from subsonic to supersonic.

Region V: Prohibited. In this region, $p_2 > p_1$ and $\rho_2 > \rho_1$, implying through the Rayleigh line relation of Equation 3 that the velocity of the detonation is imaginary, and there is no physical solution.

Within an RDE, the combusting mixture may fall into Regions I, II, III, or at either CJ point depending on the portion of the cycle and location within the channel. Discussion of the results in Chapter IV will identify that deflagration and detonation may co-exist within the RDE detonation channel making a classification of the combustion relative to the Rayleigh chart ambiguous when considering the combustion process as a

whole single process rather than multiple processes. The descriptions above suggest that determination of the combustion region is based on the speed of sound adjacent to the combustion zone. The speed of sound is a thermochemical property of the gas mixture, and analytical derivations are described in most thermodynamic texts, such as Çengel and Boles (39), that allow a good estimation from the fluid properties of specific heat ratio, temperature, and specific gas constant. Determination of the speed of sound in the burned gases of a detonation engine can be difficult due to the short duration of the detonation event, comparatively long response times of thermocouples, and detonation waves which tend to break sensors.

Calculation of the velocity of the detonation wave with the Chapman-Jouguet theory is not trivial (38, pp. 373-381) and requires iteration. Figure 4 displays the flow chart for a determining scheme to find the Chapman-Jouguet detonation velocity. The equations require calculation of the species in the reactants, species in the products, and the resulting energies. Gordon and McBride (40,41) used a Newton-Raphson iteration

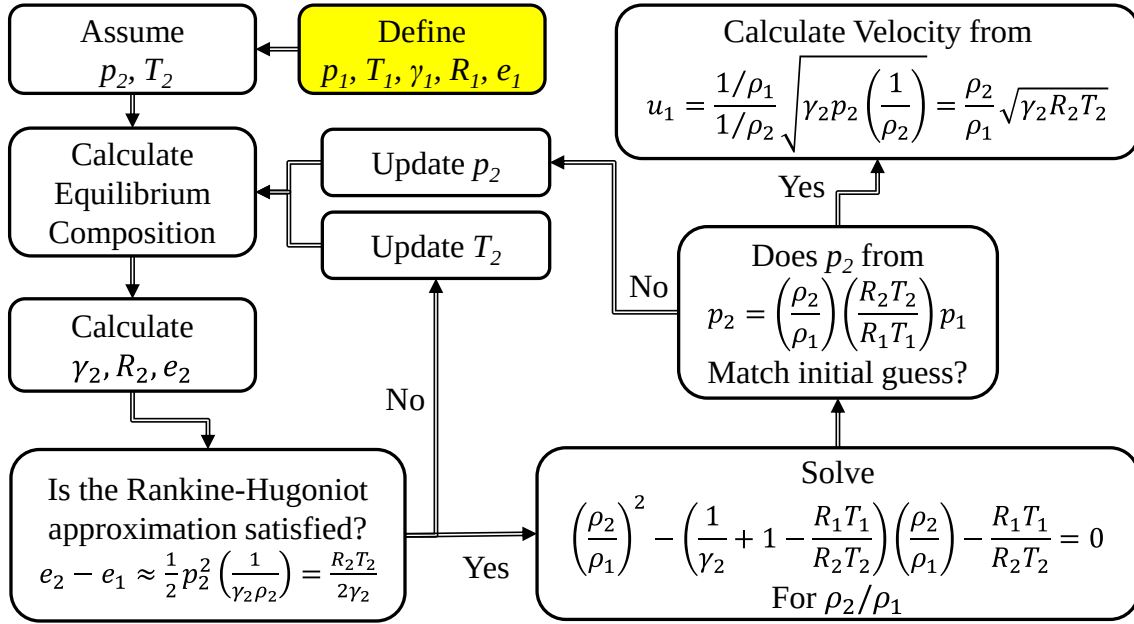


Figure 4. Algorithm for Chapman-Jouguet detonation velocity iterative determination as described in Kuo (38, pp. 373-375)

method within the NASA CEA code to accurately predict Chapman-Jouguet velocities with fewer iterations. The CEA code was used in this effort when predictions of detonation wave speeds were required. The Chapman-Jouguet model is an energy balance across the detonation wave. As such, it is one-dimensional and cannot predict what happens when the mixture is not homogeneous. In a real gas mixture where there is significant variation of species in the region of detonation, the Chapman Jouguet theory will not capture the off-nominal conditions and will predict detonation properties from an ideally mixed mixture. An additional box was added in Figure 4 beyond what Kuo described to highlight that the entire calculation is based on a good understanding of the initial conditions. If reactants are partially burned before detonation, then the initial conditions should reflect the increase in temperature, variation in pressure, and presence of combustion products.

In general, the CJ theory is useful because it balances the energy between the unburned and burned gases. Kuo (38, pp. 365-367) showed that CJ theory predicts attainable regions of combustion and identifies combustion at the upper CJ point as the minimum entropy generator, as illustrated in Figure 5. Entropy is a key indicator of thermodynamic performance. The main draw-back to Chapman-Jouguet theory is that it does not explain the detonation structure. Detonation structure is important because it, in turn, defines the geometry of detonation hardware.

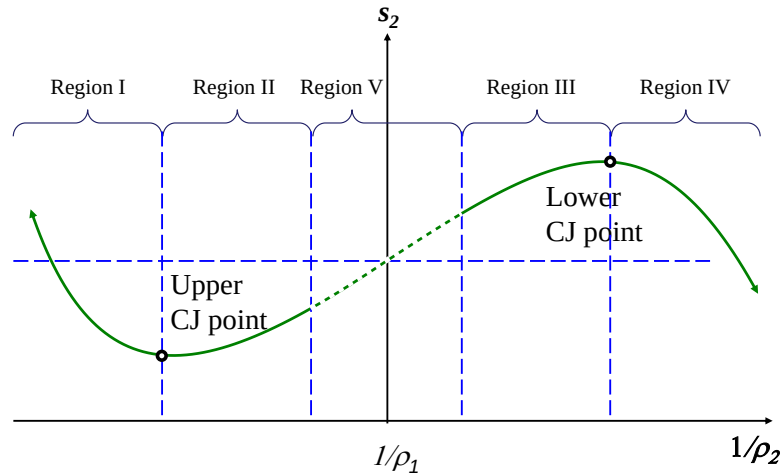


Figure 5. Entropy trends for the Hugoniot relations adapted from Kuo (38, p. 367)

For pulsed detonation engines, Heiser and Pratt (42) proposed a one-dimensional thermodynamic model that is generally accepted as the ideal detonation thermodynamic cycle. Their analysis failed to account for the irreversible losses that occur when the gases expand through a nozzle, as noted by Dyer and Kaemming (43), who proposed an appropriate modification that maintains conservation of energy by accounting for irreversible expansion through the nozzle. This correction reduces the estimated work available to the detonation cycle, thereby presenting a better quantity for efficiency

calculations. When possible, the Heiser-Pratt model with the Dyer-Kaemming correction should be used to calculate the ideal detonation cycle. For an RDE, the thermodynamic model and subsequent efficiency calculations become significantly more complicated because the detonation combustion is mixed with some deflagration and portions of the flow experience expansion waves as well. As will be discussed in Section 2.2 of this chapter, Nordeen et al. (8) analyzed the numerical solutions to an RDE flow field to show that the ZND detonation thermodynamic cycle could be modified to provide an optimistic one-dimensional model for a rotating detonation engine. Both the PDE and the RDE thermodynamic cycles are more closely approximated by the ZND detonation model than the CJ model.

2.2. Zel'dovich-Von Neumann-Döring

Zel'dovich, von Neumann, and Döring (5,6,29) each extended the one-dimensional view of detonation from the CJ theory (17,18). They postulated that there was a defined structure to the detonation wave that drives the thermal properties shown in Figure 6. The structure consisted of a leading shock and a trailing combustion wave. The leading shock preheated and compressed the reactants to the point where combustion reactions could occur. The reaction rate is modeled to start slowly and progress with increasing rapidity until all products are consumed. Zel'dovich, von Neumann, and Döring delineated between the initial compression performed by the shock and the trailing combustion which progressed like deflagration at high temperature and pressure.

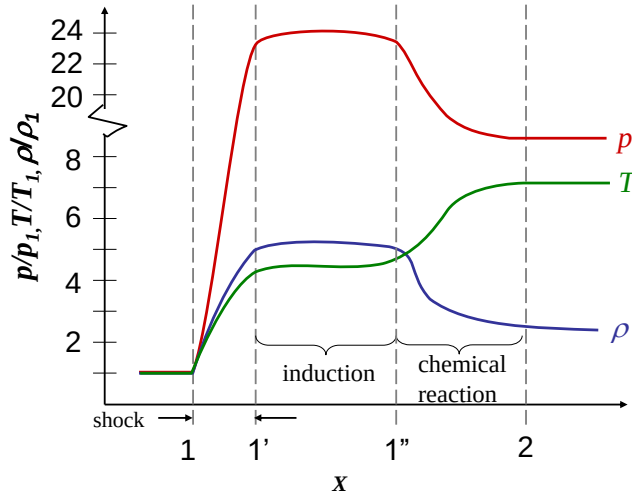


Figure 6. Illustration of the Zel'dovich, von Neumann, Döring detonation wave structure between the shock front at Location 1 and the combustion products at Location 2, adapted from Kuo (38. p. 362)

The pressure and density gradients at the leading edge of the shock produce a rise in pressure and temperature referred to as the von Neumann spike which has been verified experimentally (refer to Kuo (38, p. 383) for a complete reference list).

Figure 7 shows the progression of a gas mixture from the initial pressure and density, through the initial pressure and temperature rise of the von Neumann spike, and back to the Upper CJ point. Generally, the von Neumann spike is not measured directly, but its effects drive the schlieren techniques and the high-speed thermocouple data collection used.

The ZND model has proven very useful to understanding and modeling detonation combustion. The analysis of a simulated RDE flowfield by Nordeen et al. (8) showed that the ZND thermodynamic model was a good approximation. As described in Section 4.2.3, the annular flowfield of an RDE was divided into lanes defined by streamlines. Each lane that passed through the detonation experienced a slightly different cycle. Using a ZND approximation, and calculating additional losses for those portions of

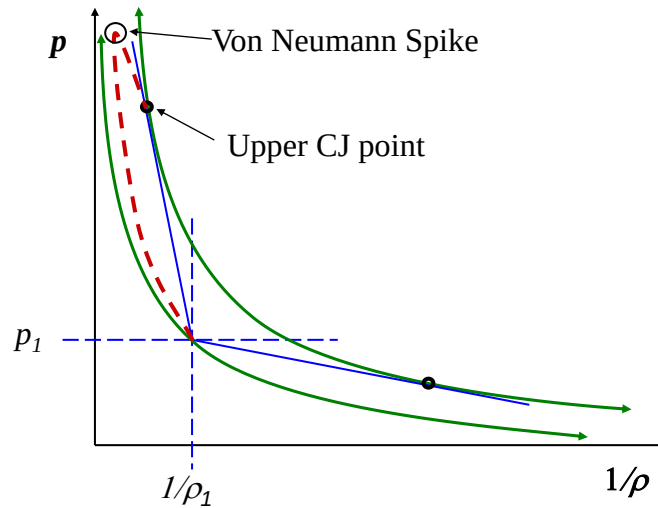


Figure 7. Von Neumann Spike overlaid on Rayleigh lines for the reactants and products of a detonation as adapted from Kuo (38, p.383)

the flow that expanded or experienced an oblique shock, they were able to calculate specific thrust with a one dimensional model. They recognized that a small portion of the flow does not pass through the shock, and that by ignoring it, they have a slightly optimistic calculation. This implies that performance modeling for an RDE may be computed using sets of algebraic equations, obviating the need for full CFD analysis.

Kaemming et al. (44) and Shah (9) used a similar approach of splitting the flow along stream-lanes to generate a computational model for RDE combustion. They did not restrict themselves to a single model and instead used computational solvers to calculate thermodynamic efficiencies and exhaust properties. Both Nordeen and Kaemming's models predict pressure gain across the combustor and a moderate improvement in combustion efficiency for RDE when compared to the Rankine cycle.

2.3. Sizing Machinery for Detonation

Detonation has a very distinct three-dimensional structure. The multi-dimensionality of detonation was noted as early as 1926 by Campbell and Woodhead

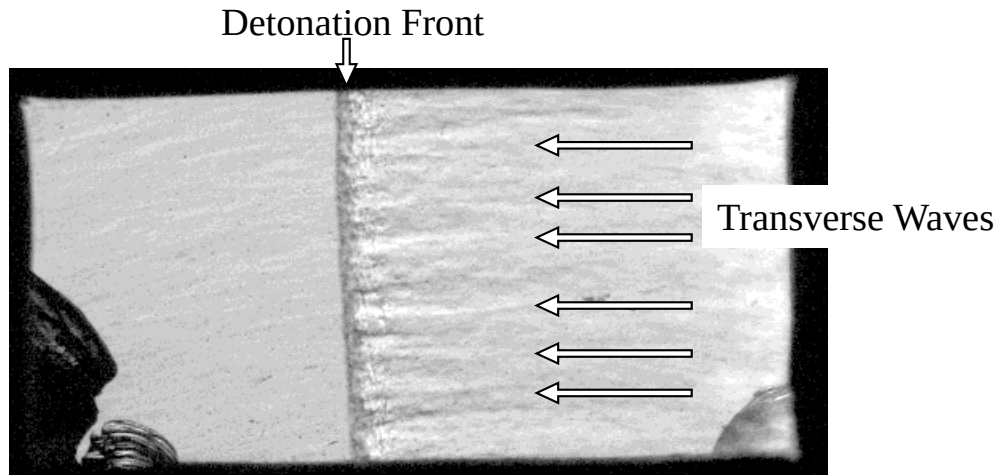


Figure 8. Schlieren image of a hydrogen-air detonation at 1 atm and an equivalence ratio of 1.0. The detonation wave is moving right to left, and the transverse detonation waves are clearly seen as horizontal density gradients extending behind the detonation wave (48)

(45,46) who studied spinning detonations in lean mixtures. Later, Denisov and Troshin (47) used sooted foils to record transverse waves in the detonation. These transverse waves travel at right angles to the detonation wave, creating triple points where two transverse waves meet with the detonation shock wave. Babbie and Stevens (48) captured an image, shown in Figure 8, of the transverse waves using high speed schlieren. The detonation wave is moving from right to left, and the transverse waves are seen as horizontal density gradients extending to the right of the detonation front. The triple-points exist within the detonation wave while also moving perpendicular to the direction of the detonation wave movement.

Historically, cell width was measured from triple-point traces left on a sooted foil record. When traversing over a sooted foil, triple-points remove the soot, and leave a characteristic fish-scale pattern. Where the triple-points meet, a triple-point junction occurs, as shown in Figure 9. Triple-point junctions are easily identified, and their

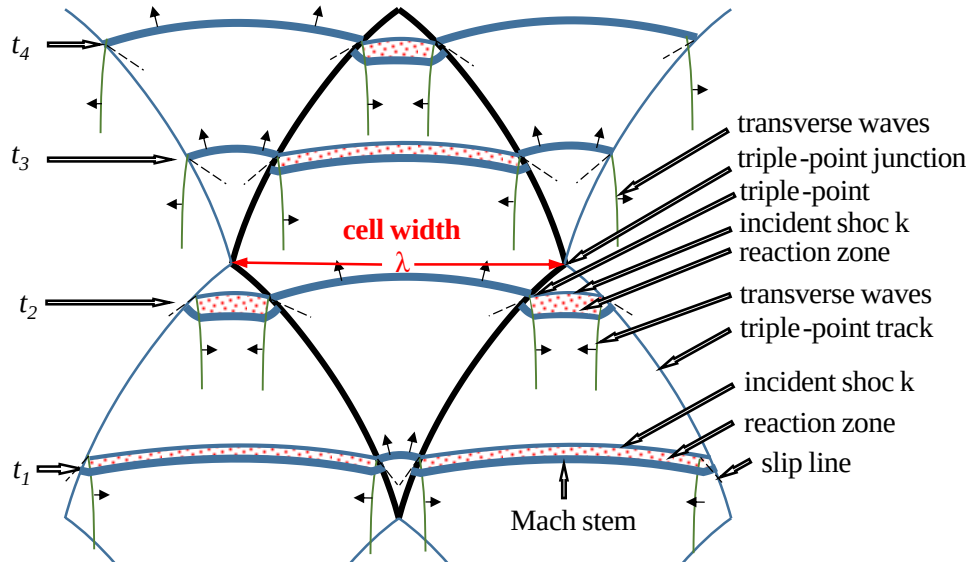


Figure 9. Diagram of a detonation cell (adapted from Gavrikov et al. (182))

spacing is used to quantify the detonation cell width. Cell width, λ , is the distance between two adjacent triple points, measured perpendicular to the direction of the detonation motion.

Enough data has been collected to loosely characterize a detonation cell width with regard to the equivalence ratio, pressure, initial temperature, and fuel-oxidizer mixture (49, pp. 7-69), although the detonation research community has not agreed on a single unified model. From these studies, a relationship between the minimum initiation energy of the detonation and the cell size has been proposed (50, pp. 25-26):

$$E_{initiation} = 3.375 \lambda^3 \quad (4)$$

where λ is the cell width in mm, and $E_{initiation}$ is the initiation energy in Joules. As described in Appendix II, this relationship has been found to be statistically representative for all stoichiometric hydrocarbon-fuel/ oxidizer combinations tested. But the model is more robust than stoichiometric conditions. Figure 10 shows the combined plot of Equation 4 with a subset of the data contained in the detonation database (49)

from references (49,51–65). All mixture initiation energies lie within one order of magnitude to the line, and the relationship is statistically valid for all equivalence ratios, not just stoichiometric conditions. Using the inverse function of Equation 4, the ignition energy gives a good estimate of the cell size, which may then be used to size detonation hardware (66). Obviously, when employing Equation 4 for design, extra margin must be made for those fuels (such as hydrogen) or fuel-oxidizer mixtures (such as rich ethylene-air) that show the greatest deviation from the model line.

Detonation hardware must leave large enough spacing that the detonation can self-propagate. In experiments with oxy-acetylene systems, Mitrofanov and Soloukhin (67) found that a detonation transitioning from a tube would de-couple for some mixture conditions. Sustained detonation required a minimum number of transverse waves, or cells to maintain propagation in the larger space. This relationship between cell size and

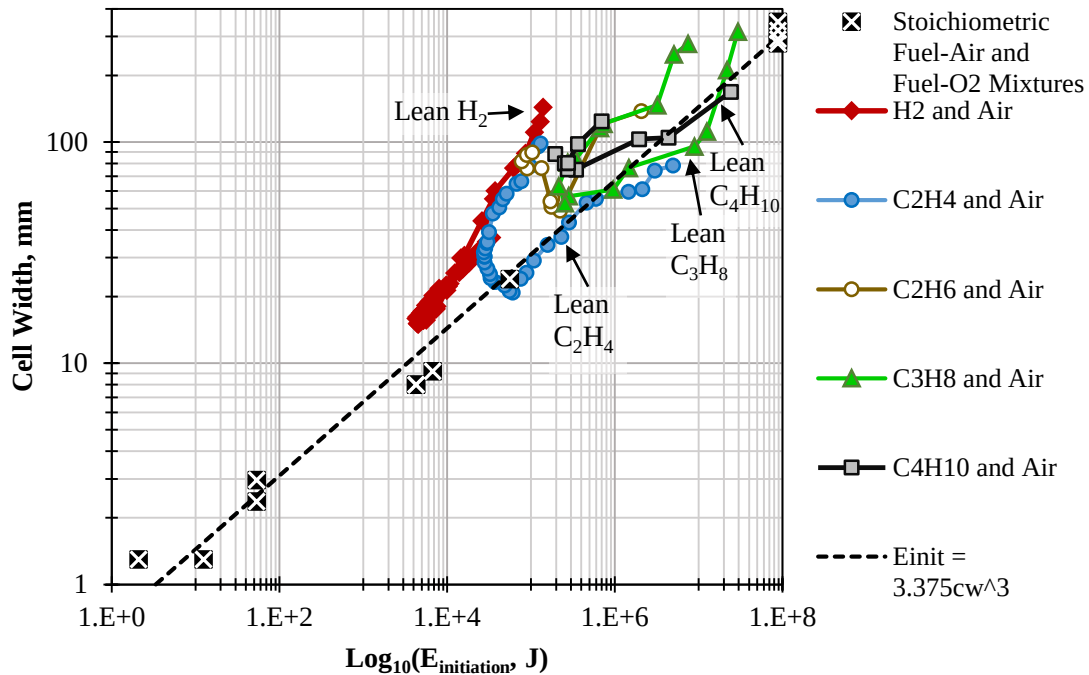


Figure 10. Detonation cell size in millimeters versus the minimum ignition energy in Joules at $T_0 = 293$ K and $P_0 = 1$ atm, from (49,51–65)

self-sustaining detonation is called the critical diameter, d_c . The mathematical relation for detonation exiting two different geometries was summarized by Kuo (38, p. 404) with Equations 5 and 6.

$$d_c = 13\lambda \quad \text{for circular tubes} \quad (5)$$

$$d_c = 10\lambda \quad \text{for planar channels} \quad (6)$$

When detonations propagate through a tube or planar channel sized smaller than the critical diameter, the detonation transitions from a multi-head detonation to a single-head spinning detonation which relies on the walls of the confinement to maintain stability of the detonation structure. There is a lower limit to the tube size where even spin detonation no longer propagates that is referred to as the limiting diameter, d^* . The accepted relationship for the limiting diameter in a smooth walled circular tube was first reported by Kogarko and Zel'dovich (68) (as reported by Kuo (38, p. 406)) as:

$$d^* = \frac{\lambda}{\pi} \quad (7)$$

where λ is the detonation cell width. When a mixture exists inside a tube or channel smaller than the limiting diameter, the mixture will theoretically not maintain a detonation; instead a detonation will transition to a deflagration. Deflagration occurs in channels much smaller than the limiting diameter, and this provides an opportunity for halting flashback. Design of a feed system that employs feed channels smaller than the limiting diameter turns a detonation arrest problem into a deflagration arrest problem that can be addressed with premixed flame quenching and blow-off theories.

3. Historical Rotating Detonation Engine Research

The Rotating Detonation Engine is a relatively new engine concept, having just over 6 decades of limited research. A premixed RDE was first achieved in Russia by Voitsekhovskii et al. (7,10,69) but was designed as a self-contained combustor in a vacuum driven flow with no practical application. The apparatus met the scientific objective of studying detonation waves, and the experiment has not been repeated. A further description of the historic Russian efforts is found in Section 3.1 of this chapter. The success was enough to provide insight into detonation cell structures and to inspire Nicholls et al. (70) with the idea of utilizing the continuous detonation in an annulus as a rocket engine, described more fully in Section 3.2 of this chapter. Nicholl's research led to a non-premixed RDE design. However, the non-premixed RDE had difficulty maintaining the detonation after startup, and an assumed requirement to control the directionality of the detonation ended research for several decades in the United States. The RDE research that has occurred over the past one to two decades will be discussed in Section 4 of this chapter.

3.1. Russia: Zel'dovich and the Premixed Apparatus

The first continuously operating RDE experiment used premixed fuel and oxidizer (7,10,69) and was performed by B. V. Voitsekhovskii in Russia at the beginning of the Cold War. The test apparatus was constructed to flow pressurized reactants (oxygen and acetylene) radially outward from a central feed hole and into a detonation channel and then capture products in a vacuum collection system. The detonation traveled circumferentially in a channel at the perimeter of the feed system as shown in Figure 11.

- 1 Annular Channel
- 2 Disk Made of Plastic Glass
- 3 Erosion Made in 3-4 Seconds by a Maintained Detonation
- 4 Steel Plate

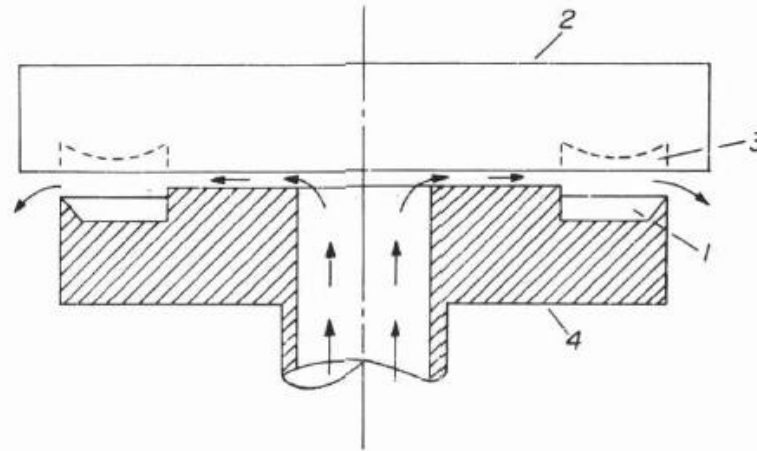


Figure 11. The cross section diagram of Voitsekhovskii's premixed annular detonation apparatus from reference (7)

The detonation traveled perpendicular to the reactant flow and initially had problems with flashback into the feed system on startup. The rotating detonation was started by igniting a charge at one point of the annular channel, and the detonation would progress in both directions around the annular detonation channel until both detonation heads collided at the location 180 degrees from initiation. When these two detonation heads met, the combined over-pressure was sufficient to push the detonation back into the feed reservoir. Avoiding backfire was recognized as a “considerable technical difficulty,” and was overcome “by selecting a specially shaped supply nozzle and by establishing the correct pressure regime.” No details other than the schematic in Figure 11 were given regarding the design.

The next technical challenge Voitsekhovskii overcame was detonation unstart when a dual-headed detonation consumed all available reactants, and the detonation was

starved. By placing a fast acting (explosively activated) shutter near the initiator, the branch of detonation progressing toward the shutter was reflected, while the remaining branch was left free to propagate around the detonation channel. The explosive actuation of the shutter moved the reflector out of the channel before the detonation had traveled all the way around, allowing it to continue and the RDE to operate.

Key observations from this work continue to be noted in modern RDE research. First, multiple modes of detonation were seen in Voitsekhovskii's apparatus and are similar to single wave, multiple wave, and multiple counter-rotating wave operation in modern RDE. The blue-green emission from the chemical reaction (vs. the normally observed yellow combustion emission) is indicative of a low-sooting combustion. Detonation Mach numbers were calculated to be between 1 and 2 relative to the detonation products, which is lower than Chapman-Jouguet predictions and has also been noted in modern RDE research. Finally, agreement with limits described by detonation theory, such as limits of operability due to equivalence ratio and channel width, was seen. Continuing experimental efforts with premixed RDE experimentation will be described in Section 4.1, and premixed CFD research is described in Section 4.2. Continued Russian experimental efforts with non-premixed RDE are described in Section 4.3, along with efforts by the rest of the world.

3.2. United States: Nicholls' Work for AFRL

Nicholls et al. (70,12,13) studied the feasibility of utilizing RDE for rocket propulsion. They explored non-premixed detonations in an annular channel where the products flow axially instead of radially. Mixing the reactants in the detonation chamber

avoided the back-fire issue. A frangible diaphragm was inserted in the channel next to an ignition source in an attempt to avoid detonation unstart immediately after initiation. The frangible diaphragm was designed to withstand the 200 μ s initiation from the igniter and then burst when the initial detonation completed one rotation. It was found that the diaphragm reduced the initial detonation pressure wave by 75%, resulting in unstart after one rotation. Directionality was an assumed requirement that is not addressed in modern experimental RDE where transition from deflagration to detonation (71) occurs regardless of ignition effects, even when the ignition source is a detonation. At the conclusion of Nicholl's work, mixing geometry and turbulence were suspected as the root causes of the inability to maintain a detonation within the channel, but this has not been confirmed by modern experimental results described in Section 4.3.

4. Current Research

Significant RDE research is ongoing, or has recently occurred, in the United States at the DERF, the Naval Research Laboratory (NRL), NASA, the Department of Energy, the University of Cincinnati, Purdue, Aerojet, and at General Electric. Research is also occurring in Japan, Russia, and Poland. Published works by these groups are described in this section and provide the dialogue of scientific observation, questions, answers, and discovery that will move RDE technology forward.

4.1. Premixed Rotating Detonation Engines

Although there is a strong desire in the pressure-gain research community to see a premixed RDE function, very little published work is currently available. Most premixed RDE attempts have resulted in failure (1,24,26) and some will be briefly described here.

Voitsekhovskii (10) was the first to operate a premixed RDE. His work spurred the continued research on non-premixed RDE in the former Soviet Union (71,72) using both oxygen and air as oxidizers. The current group at the Lavrent'ev Institute of Hydrodynamics has even attained non-premixed detonation with propane and kerosene (73). The original premixed apparatus was vacuum driven and self-contained. As a result, it allowed for characterization of the rotating detonation but did not achieve a practical form for inclusion in propulsion systems.

At the DERF, Thomas et al. (1) attempted a premixed RDE, but flashback into the mixing system bent the hardware and ended the experiment. They had attempted to separate the detonation channel from the premixture plenum using porous metal, and they theorized that the combustion had progressed around the edges of the foam block where small gaps existed between the block and the receptacle. After the failure, their attempts to run premixed ceased.

Other groups have attempted to leverage the quenching diameter inherent in metal foams and grids to operate premixed RDE. A metal foam is a porous piece of metal in a similar way that a sponge is porous. Metal foams present a physical barrier, provide structure, and allow fluids to move across them. They are attractive because they are commercially manufactured, present a lot of surface area to the flow passing through them to potentially quench the combustion, and approximate an ideal injection system that distributes infinitely small holes across the entire injection area.

The Naval Postgraduate School (NPS) (25) attempted to use layered wire mesh to quench hydrogen-air flames. The injector failed immediately after ignition with vaporization of the nickel metal mesh. They sought a hydrogen-air premixed RDE to

compare results with CFD studies and particularly sought a metal foam injector because of the similarity to an idealized fuel injection system that was employed in those studies. A close relationship between NPS and the NRL has resulted in a large body of CFD results for premixed RDE that will be described in Section 4.2.3.

At the University of Cincinnati, St. George et al. (24) recently published experiments performed with a partially premixed ethylene-hydrogen-air RDE. They placed the metal foam in the premixed plenum, approximately two inches upstream of the injection of ethylene-air premixture into the detonation channel. Hydrogen was injected at the premixed plenum injection point. Their research showed hydrogen injection stabilized RDE operation. They reported that the hydrogen injection did not always prevent flashback, and thermal cycling and heating of the foam from flashback events caused fracturing and rendered it unusable. The instability issues (flashback) during ethylene-air only operation caused them to recommend against premixing. It is possible that the hydrogen injection scheme may have caused a significant shear layer at the feed plenum that in turn created a flashback-resistant injection scheme that provided greater stability to the operation than the hydrogen fuel chemistry. Tests to confirm this have not occurred and are not planned, so this remains an open area for investigation.

Based on these results, metal foams do not prevent flashback. Although the foam employs extremely small holes, the high feed pressures required to force the gas through may be pushing the theoretical quenching distance so small that the flame propagates through the foam and into the plenum. Another possible explanation is that the distribution of the holes in the plenum may be allowing recirculation zones to form which hold the flame next to the foam. The aggregate structure of the foam may be limiting heat

transfer away from these flame eddies, and it subsequently vaporizes until the reaction breaches the premixed plenum and destroys the equipment.

As part of the work for this dissertation, a planar detonation motor serving as a two-dimensional analogue to an RDE was constructed to test the ability of 120 step expansion nozzles to avoid flashback (26). A hydrogen-air mixture was fed through the nozzles into the optically accessible linear detonation channel. High-speed schlieren video showed anchoring of flames at the feed nozzles, decoupling of the detonation in the channel, and flashback occurring when the pressure waves pushed the reaction through the holes. The complete paper describing the effort may be found in Appendix I. Although the effort ultimately failed to prevent flashback or maintain a detonation within the channel, it provided insight into the flashback process. It was noted that the expansion nozzles frequently disallowed deflagration from burning upstream until a subsequent detonation pushed the reaction back into the plenum. This showed that quenching calculations must be based on the overpressure of the detonation wave and not the time-averaged flow conditions. It also allowed for the observation that the detonation immediately de-coupled when pushed through the 0.4 mm throats of the feed nozzle. These key insights led to investigating longer and narrower feed geometries (27) which eventually proved successful at arresting flashback in an RDE (28), and are described in greater detail in Chapters III. and IV. of this dissertation.

4.2.Computational Fluid Dynamics for Rotating Detonation Engines

A premixed rotating detonation is needed to verify some of the initial conclusions reached through CFD studies. In an attempt to understand the key physics of a rotating

detonation engine, the research community has turned to CFD. Computational fluid dynamic models and simulations provide unparalleled access to the flow properties when the simulations are correct, allowing interrogation of the physical properties of the fluid at every point in the flow. When the simulations are inaccurate, they are at least meaningless and at worst misleading. Verification of CFD results involves grid or mesh convergence and comparison to accepted models and experimental data. A summary comparison between the wavespeeds measured experimentally and predicted numerically is shown in Figure 12 (2,19,23,28,35–37,74–83). A brief description of each data set is included in Table 1, and the papers from which they come are discussed in Sections 4.2, 4.3, and in Chapter IV. While the numerical results exist almost entirely between 80 and 100 percent of V_{CJ} , the experimental results are mostly below 80 percent of V_{CJ} predictions. Until the underlying causes of the discrepancy in wave speeds can be

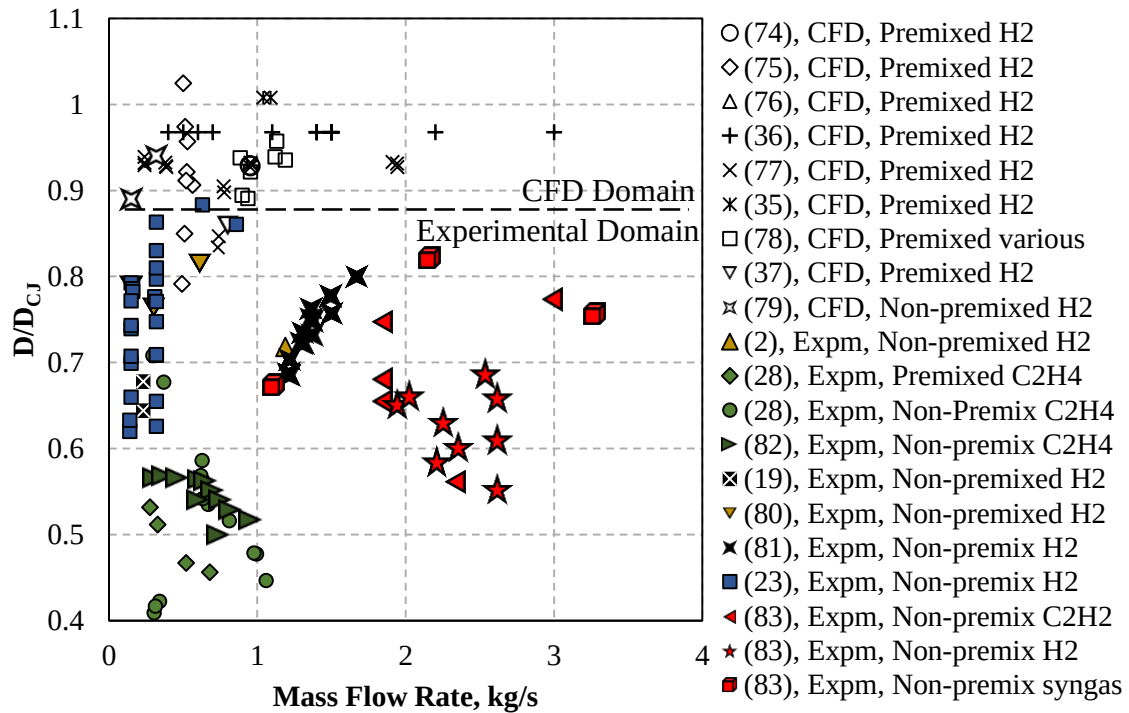


Figure 12. Summary of CFD and experimental wave speeds (2,19,23,28,35–37,74–83)

understood, the experimental and CFD community will be suspect of the other's results. In other words, the models and simulation only provide increased understanding to the degree that they can be verified.

The CFD community commonly employs several simplifications or assumptions that are central to the difference between CFD and experimental work. The number of

Table 1. Description of CFD and experimental detonation wave speed results

Sym bol	Reference / Year	Research Group	Numeric/ Experiment	Fuel/ Oxidizer	ϕ	Pre- mix?	RDE d _{in} , cm	Finite Injector?
○	(74)/2014	NRL	Numeric	hydrogen/air	1.0	Yes	8	No/3D
◇	(75)/2013	NRL	Numeric	hydrogen/air	1.0	Yes	8	Yes/2D
△	(76)/2011	NRL	Numeric	hydrogen/air	1.0	Yes	13	No/2D,3D
+	(36)/2010	NRL	Numeric	hydrogen/air	1.0	Yes	13	No/2D,3D
×	(77)/2015	NRL	Numeric	hydrogen/air	1.0	Yes	8	Yes*/2D
✱	(35)/2009	Yi et al.	Numeric	hydrogen/air	1.0	Yes	13	No/ 3D
□	(78)/2013	NRL	Numeric	hydrogen, ethylene, ethane, and propane / air and oxygen	1.0	Yes	8	No/ 2D
▽	(37)/2014	NASA	Numeric	hydrogen/air	1.03	Yes	-	No/2D
✕	(79)/2016	UTRC	Numeric	hydrogen/air	0.99- 1.01	No	15	Yes/3D
▲	(2)/2012	AFRL	Experiment	hydrogen/air	1.29	No	15	Yes
◆	(28)/2016	AFRL	Experiment	ethylene/air	0.97- 1.04	Yes	15	Yes
●	(28)/2016	AFRL	Experiment	ethylene/air	0.99- 1.03	No	15	Yes
►	(82)/2015	AFRL	Experiment	ethylene/air	0.95- 1.09	No	15	Yes
⊠	(19)/2011	AFRL	Experiment	hydrogen/air	1.63- 1.75	No	8	Yes
▼	(80)/2015	AFRL	Experiment	hydrogen/air	1	No	15	Yes
✱	(81)/2012	AFRL	Experiment	hydrogen/air	0.92- 1.37	No	15	Yes
■	(23)/2015	AFRL	Experiment	hydrogen/air	0.71- 1.31	No	15	Yes
◀	(83)/2015	LIH-S	Experiment	acetylene/air	1.25- 1.35	No	30	Yes
★	(83)/2015	LIH-S	Experiment	hydrogen/air	0.8- 1.6	No	30	Yes
▣	(83)/2015	LIH-S	Experiment	syngas/air	0.89- 1.36	No	30	Yes

* NRL both finite and ideally distributed injectors were used. Wave speeds dropped for the finite injector model results

equations required to accurately model the fluid movement, species, energy, thermodynamics, etc. creates a very computationally intensive model. Furthermore, due to the sharp pressure gradients associated with detonation, the grid or mesh must be extremely refined. The result is that the models or simulations must be simplified to complete in a reasonable amount of time. Simplifications often made for RDE CFD are 1) the detonation channel is assumed to be two dimensional, 2) fuel and oxidizer are assumed to be premixed, 3) geometry is abbreviated by excluding the feed system, and 4) chemical reaction models are reduced. Chemistry is simplified in two ways; first, the number of reactions is limited by removing those which are deemed insignificant to the global mechanism, and second, reactions may be limited only to those at high pressure so that most deflagration is excluded. As seen in Table 1, not all assumptions are applied uniformly to all investigations. Recently, several groups (79,84) have progressed to modeling a separate stream non-premixed RDE to include the reactant feed systems.

The following is a summary of some of the numerical studies associated with RDE. The descriptions below are more inclusive than Figure 12 and Table 1 which were limited to those studies that reported both wavespeed and mass flow rates. The summaries are categorized by the research group without attempting to catalogue them chronologically.

4.2.1. Russian Numerical Analysis

A two-dimensional model of an oxygen-hydrogen RDE was constructed by Zhdan et al. (34) It extended the numerical analysis done previously using 1-D equations and allowed calculation of the detonation wave structure without inputs from experimental

solutions. It employed the two-dimensional Navier-Stokes equations, one equation for tracking the molecular species of the reactants and products, one equation for tracking the molecular weight of the products, and the Arrhenius relationship for a global hydrogen-oxygen reaction of

$$t_{ind} = \frac{K_a M_{O_2}}{\rho v_{O_2}} \exp\left(\frac{\epsilon_a}{RT}\right) \quad (8)$$

Here t_{ind} is the chemistry induced delay of reaction in the induction zone, K_a is the pre exponential factor, M_{O_2} is the molecular weight of oxygen, v_{O_2} is the mass fraction of oxygen, ρ is the density of the mixture in the induction zone, ϵ_a is the activation energy, R is the universal gas constant, and T is the temperature of the mixture. This single step reaction captures the combustion associated with the detonation well but does not accurately capture any deflagration occurring in the channel. Their injection system was modeled as a uniform flow across the computational boundary without finite injectors and, consequently, contains no information about eddies where flames may hold. Parametric studies were performed varying the annulus diameter to length, the manifold feed pressure to stagnation pressure, and expansion associated with a diverging annulus cross section. Their model reported mean specific impulses of approximately 2500 m/s and zero mean rotation of the flow. It also reported detonation wave speeds between 2210 m/s and 2330 m/s in oxygen-air. They reported that the detonation structure compared well with experimental work performed previously. The study was focused on rocket engine application and served as an initial model for future CFD studies performed by Yi et al. (35) and by the Naval Research Laboratory (NRL) (36).

Zhdan et al.(85) further expanded the Russian research by adapting the numeric model to handle non-stoichiometric mixtures. This involved manually modifying Equation 8 with the chemical reaction constants for the predetermined equivalence ratios. A grid refinement study indicated that the detonation wave speed was very sensitive to the degree of refinements (predicted faster wave speeds with increasing grid refinement). Disliking the fine grid due to the longer computational times, they opted to use the medium grid and assert that the detonation wave speed in the models must deviate no more than 2% to be acceptable (85, p. 72). They reported wave speeds increasing from 2030 m/s at an equivalence ratio of 0.5 to 2810 m/s at an equivalence ratio of 2.0. Mean specific impulses were reported between 3592 1/s at an equivalence ratio of 0.5 to 1478 1/s at an equivalence ratio of 2.0. They also predicted that a minimum annulus circumference would increase as the mixture became richer.

Comparisons of the experimental non-premixed RDE data to these numerical calculations (86–88) showed a discrepancy: Experimental wave speeds were roughly 80% of V_{CJ} predictions while the numerical model wave speeds were within 2%. This discrepancy between wave speed results found with premixed computational RDE and non-premixed experimental RDE continues within the research community. The difference between computational and experimental wave speeds did not appear to surprise the Russians, who had noted experimental wave speeds slower than Chapman-Jouguet predictions since at least 1969 (89, p. 272).

4.2.2. Wolanski's Group

Yi et al.(35) leveraged the Russian numeric efforts and modeled a premixed hydrogen-air detonation engine in three dimensions. The numeric RDE was based on the experimental RDE invented by Wolanski et al. (90) for a 13 cm inner diameter, 15 cm outer diameter RDE. The feed system was assumed to be a homogenous distribution of infinitely small holes, whose area when summed would equal some fraction of the total RDE detonation chamber cross section. Employing the idealized injection scheme of evenly distributed infinitely small holes allowed them to control flow rates and velocities with an area ratio and a choked flow mechanism. Combustion chemistry focused only on the reactions associated with detonation, using a one-step Arrhenius reaction similar to Equation 41 but which underestimated any deflagration that might be occurring within the RDE. Detonation wave speeds from this simulation were calculated at approximately 1975 m/s, which agreed well with predictions from NASA's CEA code. The wave speed and specific thrust were found to be similar for both one wave and two wave operation modes. This study is the first reported three dimensional CFD for an RDE.

4.2.3. Naval Research Laboratory Numerical Modeling

The Naval Research Laboratory presented their first RDE numeric model (21,36) in 2010. They used the Euler equations based on previous work (91) with pulsed detonation engine numerical models and similar to those shown by Zhdan et al.(34) and Yi et al.(35) The NRL study modeled a hydrogen-air mixture in a two dimensional 43 cm circumference RDE. Inlet geometries were idealized with the assumption of infinitely small feed holes evenly distributed across 20% of the channel cross section, similar to the

Russian studies and with the same drawbacks. Their study identified that the RDE contains multiple combustion cycles that included detonation, deflagration, and portions of the combusted product which experience an oblique shock. They identified that the flow and combustion cycles may be split along streamlines and that detonation is the predominant combustion cycle. The model did not predict transition from 1 to 2 wave, and displayed a detonation wave extending three-quarters of the detonation channel height. This tall refill zone was taller than seen experimentally and is at the lower limit of the experimental Bykovskii RDE sizing relations (72) that indicate the channel height needs to be approximately one and a half to twice the refill height. They also identified that the zone of deflagration that appears between the fresh reactants and the detonated products was a source of losses for thermodynamic efficiency.

The NRL group numerically studied performance (76) response to inlet sizing, annulus diameter, annulus length, and annulus width with a 14 cm hydrogen-air RDE. The inlet, annulus diameter, and annulus length studies were performed on a two dimensional grid as before, but the model was modified to a three dimensional geometry

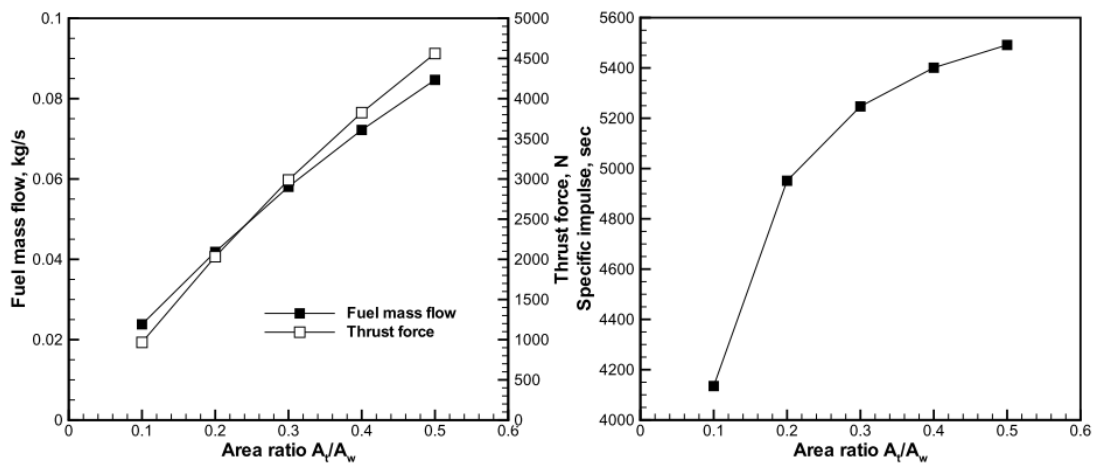


Figure 13. Result of NRL inlet size study (76) using an ideal injection scheme of infinitely small holes evenly distributed across the inlet plenum area

to achieve the annulus width study. Inlet areas were idealized and varied as indicated in Figure 13. Increasing the inlet area improved performance by allowing greater total mass flow rates at similar feed pressures. Another finding was that while the average specific thrust did not vary with increasing annulus width, the time-dependent specific thrust showed an increased cyclic amplitude (figure not shown).

In addition to performance and sizing, the NRL group also developed the basis for thermodynamic cycle analysis (8) in 2011. They took the numerical analysis of a 14 cm RDE operating with hydrogen-air and split it along streamlines as shown in Figure 14. They found that a one dimensional Zeldovich-Von Neumann-Döring detonation cycle was only slightly more optimistic than the fluid in the simulation that passed through the shock wave (streamlines 1-4 and 11-20). They were also able to take the streamlines from the detonation wave centered CFD in Figure 14 and create pathlines in the laboratory frame of reference, as shown in Figure 15. Whereas streamlines show the lines of fluid velocity at a given instant in time, the pathlines represent the physical movement that a fluid particle takes as it exits the combustor. Figure 15 showed circumferential flow

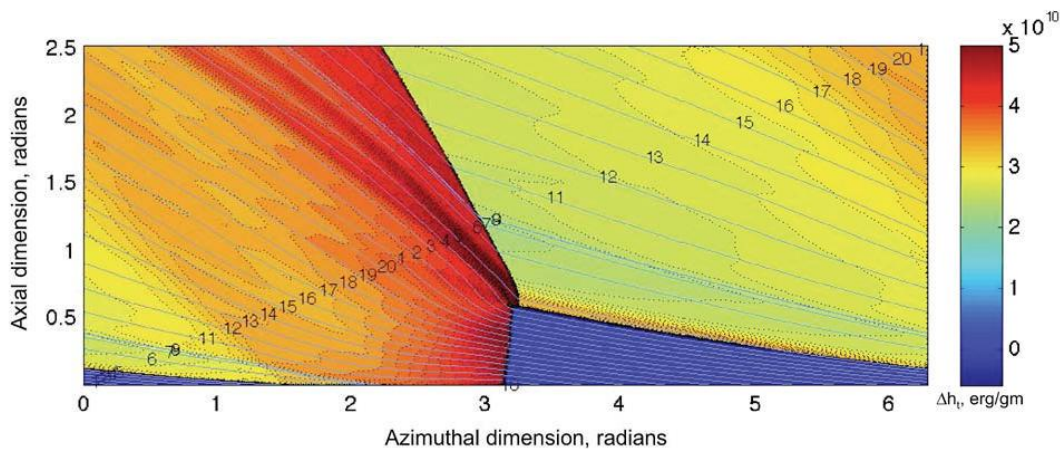


Figure 14. Time averaged enthalpy of an RDE flow field split along 20 streamlines from Nordeen et al. (8)

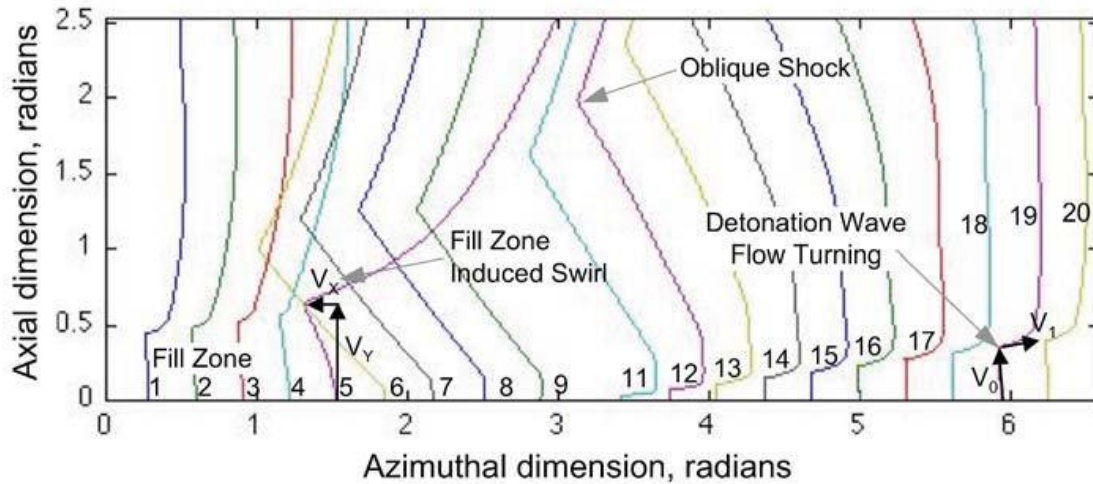


Figure 15. Pathlines computed from time averaged streamlines from Nordeen et al. (8)

reversal within a detonation cycle and cycle averaged circumferential swirl of zero at the RDE exit.

The NRL group modeled finite injector (92) and exhaust (93) effects in 2012. They took the RDE3D model used in the previous studies and coupled it with a second model located either at the exhaust or the feed end of the detonation annulus. They concluded that modeling the exhaust plume had very little impact on the performance measurements, but that injectors have a large effect on temperature and pressure profiles within the RDE due to a very different flow field within the channel. They noted that mass flow into the plenum through the finite injectors was not seen, but that no assessment could be made about combustion reaching the plenum since their plenum model could not account for thermal or radical quenching of a reacting flow. The analysis indicated that moving from the ideal injection scenario of infinitely small holes distributed homogenously at the inlet plane to an even and regular distribution of finite feed holes or slots destabilized the detonation wave. Furthermore, they predicted that increasing the area of each injector will allow larger pressure variation within the plenum

and increase the probability that the detonation wave instabilities will interrupt the detonation cycle. The finite injection simulations still assumed premixed reactants were fed into the channel, and it is not understood or observed how these conclusions apply directly to the current non-premixed experimental RDE.

In 2013, the NRL used their numerical models to evaluate performance based on hydrocarbon fuels (78), inlet geometries that limit feedback pressure (75), and how mixing affects the detonation flowfield (22). For the hydrocarbon fuel study, they moved from a 2- γ model where the specific heat ratio of the gases was set based on whether the gas in the cell was products or reactants, to a temperature dependent model of the specific heat in the gas based on temperature curve fits of the gases. For the 2- γ model, the heat release had been scaled down so that the detonation wave speed matched the Chapman-Jouguet predictions. With the new model, wave speeds very close to Chapman-Jouguet predictions were achieved, as illustrated with the comparison shown in Table 2. The model assumed frozen chemistry after combustion and does not capture deflagration reactions, so results will be slightly optimistic. The chemiluminescence studies of Chapter V will show that these assumptions are invalid. A two dimensional approximation of an RDE was used for the inlet geometry simulations, with an inner diameter of 8.0 cm and outer diameter of 10.0 cm, resulting in a mean azimuthal length of 28.3 cm. Variations of the specific thrusts between fuels shown in Table 2 were attributed to differences in chemistry rather than differences in flow field. It should also be noted that the ideal specific thrust for the detonation cycle was calculated using Heiser and Pratt's analysis (42), presumably without conserving energy by correcting for nozzle expansion losses as described by Dyer and Kaemming (43). NRL concluded that the

detonation cycle presented by Heiser and Pratt is still a good baseline for comparison of the expected RDE performance. This conclusion should be revisited with revised assumptions for handling deflagration and chemical reaction mechanisms.

Building upon the previous year's injector study, and leveraging the 9 cm geometry from the hydrocarbon study, NRL increased the injectors' geometric complexity to see if they could limit the pressure feeding into the mixture plenum (75). Geometries included slanted straight slots, cavity slots, expanding nozzle slots, and diode slots. The former three geometries are shown in Figure 16. The injector plate was designed with 50 equally spaced injectors with a throat area of either 1.13 mm or 2.26

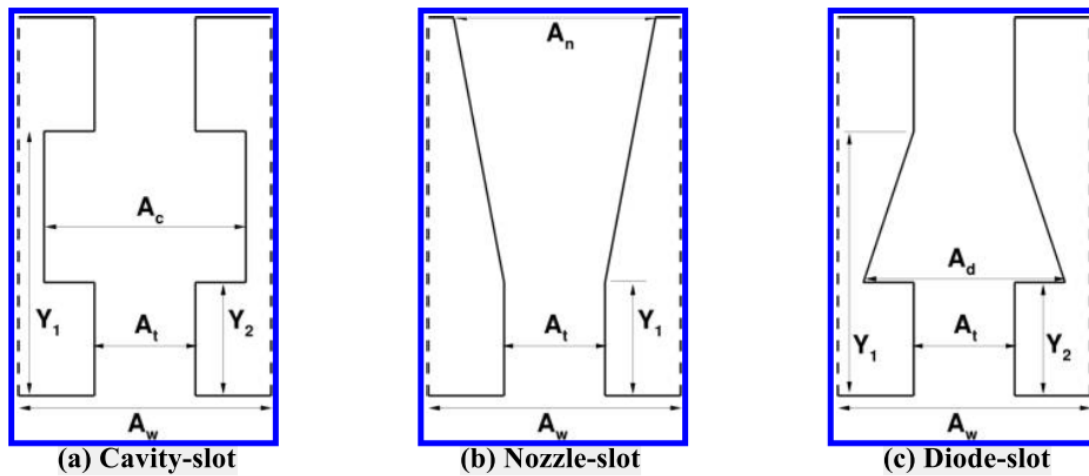


Figure 16. Slot geometries used for NRL plenum feedback study (75).

Table 2. Numerical RDE simulation wave speeds for hydrocarbon fuels, Schwer et al. (78).

Fuel Mixture	D_{CEA2} , m/s	Wave Speed		Ideal (42)	Isp_f	
		D_{NRL} , m/s	D_{CEA2}/D_{NRL}		NRL	Ratio
Hydrogen/oxygen	2936	2836	0.9659			
Hydrogen/air	1969	1964	0.9975	4860	4369	0.899
Ethylene/oxygen	2374	2382	1.003	700	596	0.852
Ethylene/air	1824	1821	0.9984	1990	1751	0.880
Ethane/oxygen	2247	2257	0.9956	920	808	0.878
Ethane/air	1710	1710	1.000	2540	2260±23	0.89±0.01
Propane/oxygen	2357	2354	0.9987	1070	939	0.878
Propane/air	1799	1797	0.9989	2080	1851±19	0.89±0.01

mm, depending on whether the simulation was intended to run with a total feed throat to channel cross section area ratio of 0.2 or 0.4. The choice of increasing the area of each injector instead of increasing the number of injectors may have been a desire to facilitate the study, minimizing the time required to create grids and execute simulations. They found that all geometries successfully attenuated the pressure feedback into the plenum but did not eliminate it. Each slot injector was approximately the same, indicating that increasing complexity will increase costs without benefitting flashback resistance. The report did not address flame holding and did not include low-pressure deflagration combustion equations. It was noted that the detonation cycle not only caused an overpressure in the feed slots associated with the detonation front but also an under-pressure associated with the expansion portion of the cycle. The simulation did perform combustion calculations in the feed slots, so lack of combustion in the feed system was an input and not a result. Although not explicitly stated, the equations and CFD grid are assumed to be appropriate for compressible flow but likely did not address friction flow.

The final NRL study published in 2013 dealt with how incomplete mixing in the flow field affects the detonation front (22) in an RDE. For this study, a hydrogen-air RDE was modeled, and the geometry is presumed to be for a 14 cm RDE. Mixing was not modeled directly since it would have required further grid refinement, resulting in increased computational complexity not commensurate with a first attempt to look at mixing effects. Instead, an additional equation was used to estimate sub-scale diffusive mixing of fuel-oxidizer and of reactants-products. A degree-of-mixedness quantity was tracked and adjusted for each cell in the CFD grid, with a boundary condition established at the inlet. This approach alleviated the CFD team from modeling the various fuel and

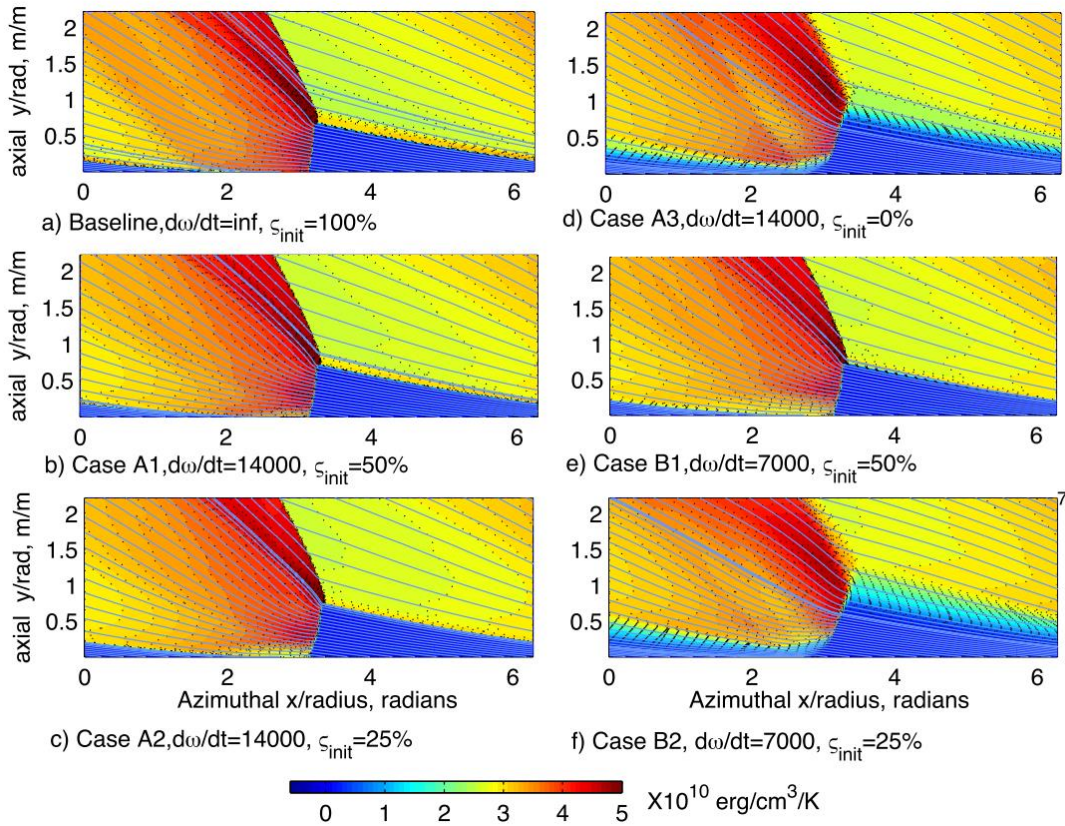


Figure 17. Total enthalpy contours and flow streamlines in an RDE with varying mixing rates and initial mixed fractions from Nordeen et al. (22)

oxidizer inlets, constructing a three dimensional grid, applying correct equations for turbulent flows, and adding multiple equations for diffusion mixing. The approach also provided top-level understanding of how mixing affects the detonation shape and standoff. The study indicated that as a system experiences a slower mixing rate or less initial mixing the detonation should lift off of the injection area and lean forward as shown in Figure 17. When mixing was slow enough, the lower edge of the detonation became rounded and a trailing oblique shock formed (most noticeable in panel d and f). Notably, the wave speeds and specific thrust were unaffected by the mixing effects within this simulation. This is counter-intuitive since wave speeds are known to be affected by mixture ratios. This may be a result of how heat release within a given cell is handled, the

fact that the simulation is two dimensional, or a combination of both factors. The lift-off, rounding, and trailing shocks are qualitatively comparable to detonation fronts seen in experimental (23,82) RDE.

In 2014, the NRL modeled RDE exhaust geometries similar to the converging or diverging nozzles seen on many experimental RDE (94). The study controlled two key ratios for a design of experiments approach to RDE: exit to detonation channel area and mean exit to detonation channel radius. The study showed that fluid swirl within the RDE was significant and decreases with a diverging exit nozzle. The second conclusion from the study was that specific impulse increases with reduced area ratio, a finding that is opposed to that of Zhdan (34, pp. 457-458).

Also in 2014, the NRL moved to a new RDE code called Propel (74). This new code allowed better parallel computing and hybrid structured-unstructured grid meshing. The result is that the simulations now compute seven times faster and with better resolution, a necessary step to enable modeling of three-dimensional diffusively mixed RDE. For the successful simulations, the Propel code was within 4 percent of the I_{sp_f} predictions of the previous code and within approximately 10% of the thrust predictions. The close agreement between models reassured the NRL team with an indication that accuracy was maintained. The propel code appeared to track the trailing shocks (referred to as feedback waves) better than the old code for simulations with a converging exit nozzle. These trailing shocks were seen to interrupt the flowfield in the simulation, and it transitioned out of a detonation cycle. This is similar to experimental RDE that will often fail to maintain detonation when small changes are made to the geometry, but no direct comparison between the simulation and experimentation can be made at this time.

The NRL (22) took the next step toward simulating the experimental RDE in 2015 by modeling equivalence ratios within the RDE numerical models with Equation 9:

$$\phi^* = \frac{2 \left(\frac{f}{o} \right)}{\frac{f}{o} + \left(\frac{f}{o} \right)_{stoich}} \quad (9)$$

where f is the mass of the fuel, o is the mass of the oxidizer, $\left(\frac{f}{o} \right)_{stoich}$ is the stoichiometric fuel-to-oxidizer ratio, and ϕ^* is the adjusted equivalence ratio. The adjusted equivalence ratio is used so that the range of possible values extends from 0 to 2 instead of from 0 to ∞ . The finite range of the adjusted equivalence ratio avoided the computational issue of representing infinity, facilitating post processing with a numerically stable set of results. Also, a stoichiometrically balanced mixture was indicated by $\phi^* = 1$ just like the unadjusted equivalence ratio. The models were used for PDE simulations to verify that the chemistry constants were accurate and then put into an RDE simulation that featured cold, separate-stream fuel and oxidizer injection. The cold flow simulations indicated regions of poor mixing near the injection plane where flame might anchor throughout the RDE cycle. Also, a two dimensional simulation with finite injectors but simple (not separate stream) mixing was performed as described in (22). The two dimensional simulation results, shown in Figure 18, showed a flow field with significantly more turbulence and variation than previous simulations. The finite injection geometry was presumably the root cause of the turbulence in the flow.

Also in 2015, Schwer et al.(77) added the low-pressure physics associated with deflagration to their model. The 9 cm nominal diameter RDE was modeled with both premixed (results shown in Figure 19) and non-premixed (not shown) injection schemes.

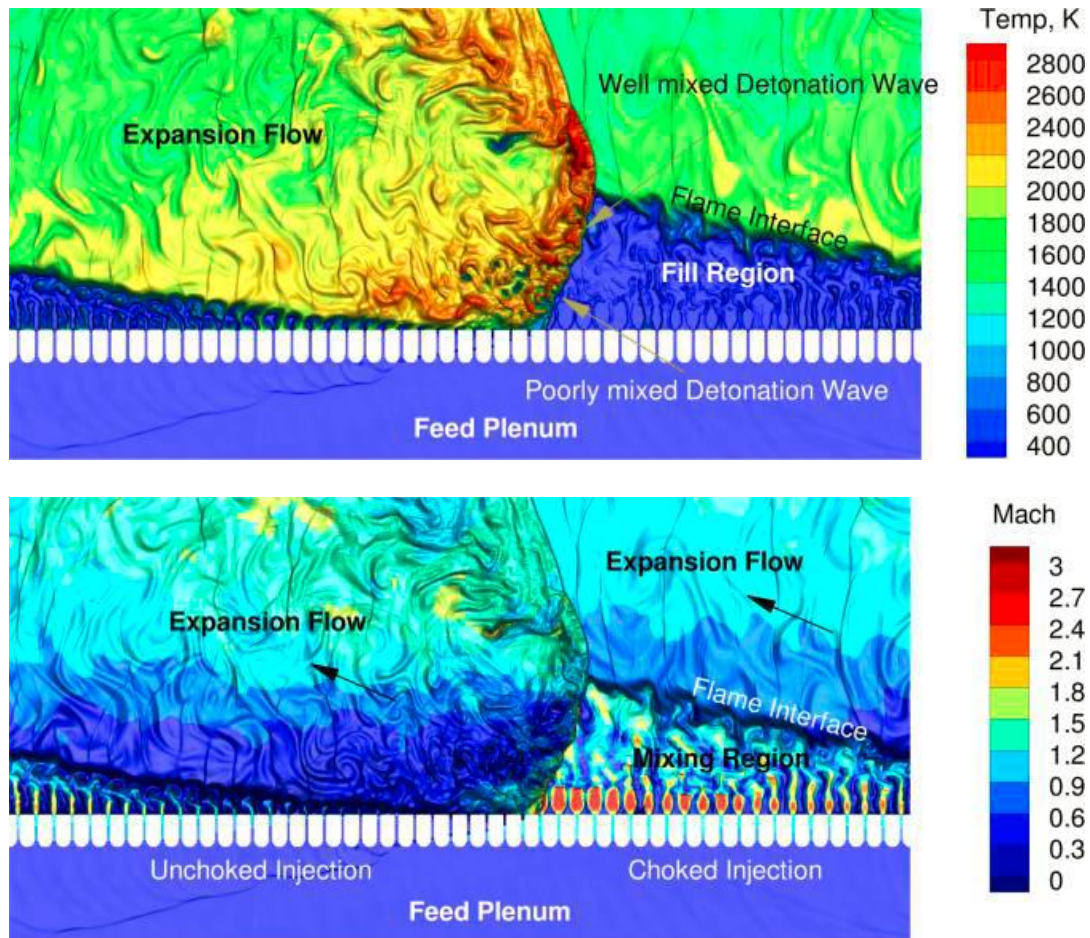


Figure 18. Temperature (top) and Mach (bottom) contour plots of an RDE flow field simulated with finite injectors and simple mixing from Schwer et al. (84)

The addition of the low pressure combustion terms allowed them to more accurately capture the anchored flames and heated reactants that reside within an RDE that has premixed reactants.

The refresh zone noted in Figure 19 is very similar to that of the flow in the premixed RDE that will be described in Section 3 of Chapter IV. Schwer et al. concluded that these low-pressure reactions are significant and need to be included in CFD studies; a conclusion that will be supported with the experimental work that is the subject of this dissertation. They also noted that when a finite injector was used, detonation wave speed predictions dropped by 5% for premixed reactants and 10% for non-premixed reactants.

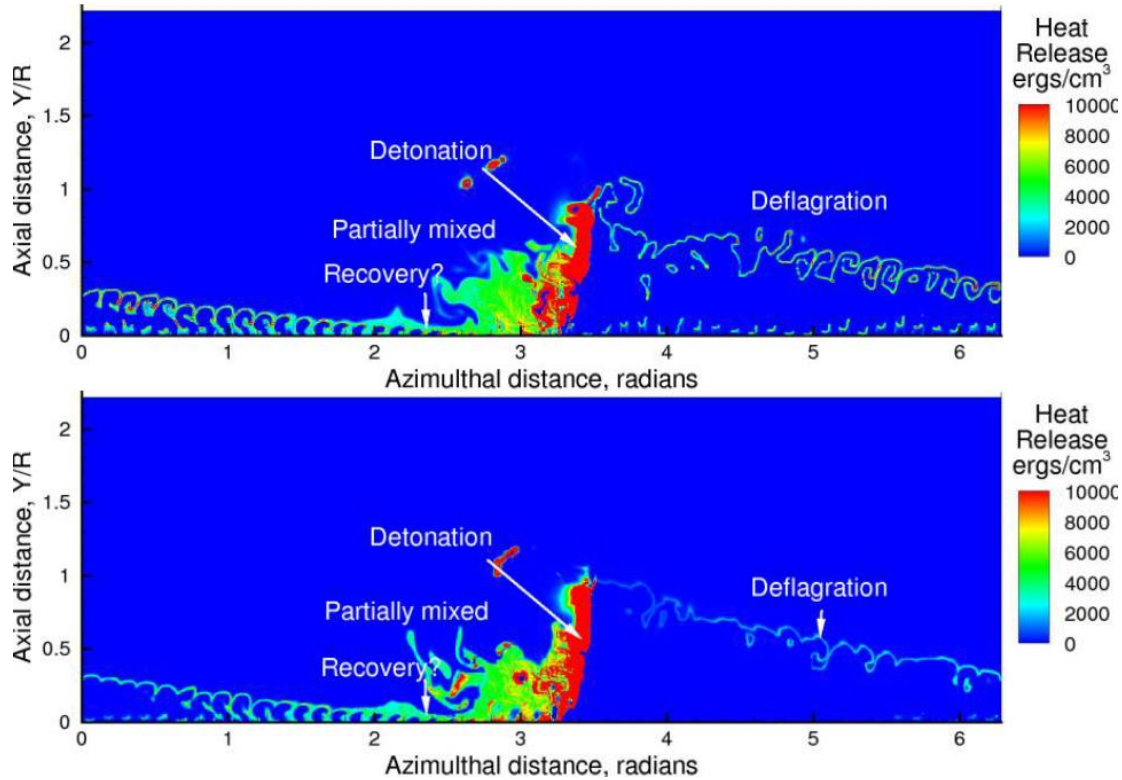


Figure 19. Temperature (top) and instantaneous heat release (bottom) of an RDE flowfield modeled with premixed injection by Schwer and Kailasanath (77)

Paxson (37) took a completely different numerical approach. Instead of reverting to the run-of-the-mill CFD that attempts to time resolve the unsteady movement of the detonation through geometrically referenced cells, he employed a 2nd order Runge-Kutta solver to numerically integrate the Euler formulation of the Navier-Stokes equation in time on a ‘wave frame of reference’ grid. The grid was relatively coarse with 80 cells x 200 cells but captured much of the detail seen in NRLs early work. The solver employed Roe’s approximate Riemann solver (95) to calculate the flux between cells. This numerical approach is shown to be stable for problems where shock and expansion waves dominate the flow (96, pp. 198-234, 632-633). Paxson’s addition of constraints (such as chemical reactivity suppression in the refill and inlet area changes) superimposed on the grid accurately captured key physics within the RDE, and have established a path for

incorporating wall heat transfer and friction effects. The recursive iteration required to achieve a solution is still faster than the large grid finite element or finite volume solvers otherwise employed. His model did capture pre-combustion before the fluid passed through the detonation but also assumed premixed fuel and oxidizer. Inlet geometry was assumed to be an ideal isentropic feed slot, and recirculation zones were not modeled. Turbulence was also not modeled.

Paxson used his code to compare the performance of an RDE with that of a PDE for similar high-speed applications and found that his simulation predicted comparable performance, as shown in Figure 20. His model also predicted increased specific thrust for a larger feed throat area. The initial model appears to be very promising, and further refinements should provide a useful tool for performing parametric studies in the design phase of the RDE development.

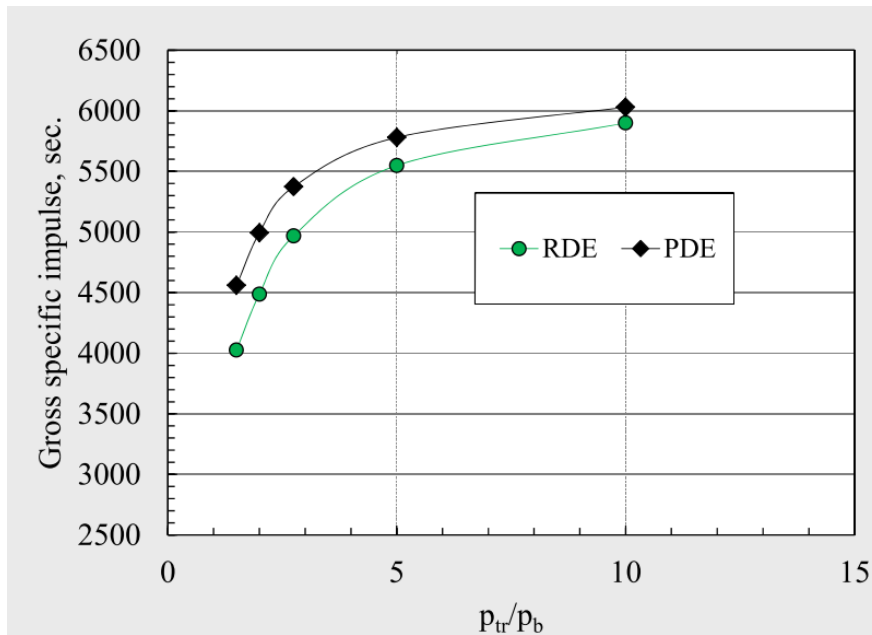


Figure 20. Comparison of RDE to PDE gross specific impulse using an integral computational method in a fixed wave frame of reference from Paxson (37)

After implementation of the improvements, Paxson performed a comparison study (97) to the experimental RDE results reported by Rankin et al. (98). The numeric simulation matched the experimental results both qualitatively and quantitatively. The wave forms seen in the temperature contours compared favorably with those of chemiluminescent RDE flows. Static pressure profiles from the numeric study matched those of the experimental within 10%, with the largest deviation at the inlet where recirculation zones are known to exist, but required highly refined three dimensional grids and small time steps to accurately model. Wave speeds between the experimental and numerical simulation agreed within approximately 5%, but the simulation results were still closer to CJ than experimental.

In 2016, Cocks et al. (79) reported on a high-fidelity CFD simulation of a non-premixed RDE. Their simulation included viscous boundary layer treatments, separate injections, and plenum modeling. Their simulation showed variation in the fuel mixing across the detonation channel during detonation that resulted in a detonation front that was narrower than the channel width. Reported wave speeds at 89% and 94% of V_{CJ} were faster than was seen experimentally. These results required a grid of 93 million cells, a time step of 3×10^{-8} s, and used the computational resources of the NASA High End Computing Program and the Oak Ridge Leadership Computing Facility super computer cluster. Available time limited the number of runs, produced results for two cases, and disallowed a grid convergence study. The unique opportunity to leverage available time on a supercomputer is generally unavailable to most researchers and may not be available again until interest in RDE technology increases significantly.

4.2.4. Numerical Summary

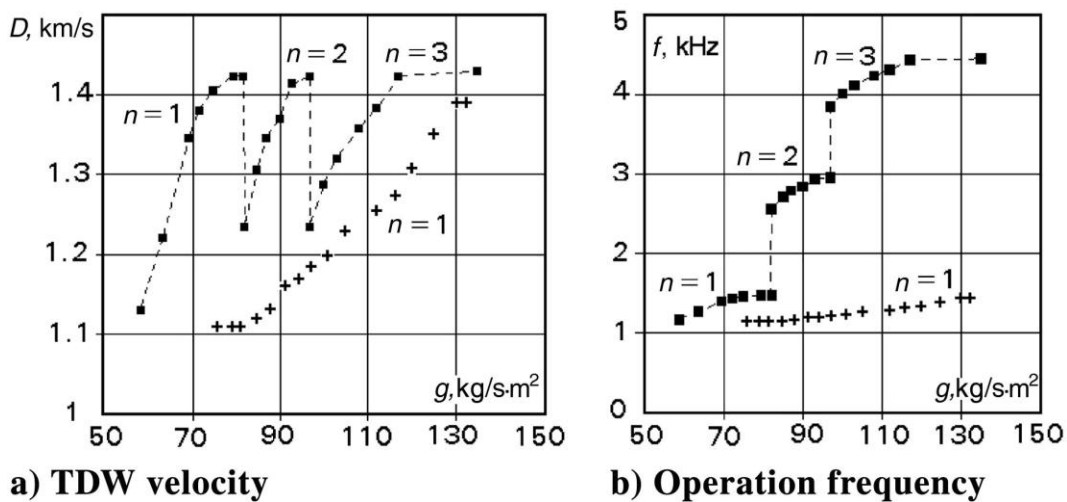
Through efforts to model RDE numerically in two and three dimensions, good insight exists into key design principles associated with sizing inlets, setting feed pressures, selecting channel diameter and length, and expanding the flow as it exits the combustor. Numeric models are slowly building capability to shift from a hydrogen fuel focus, employ complex reaction models, capture the intricacies of finite injection geometries, and to operate with separate fuel and oxidizer streams. With increased capability will come a significantly increased computational cost that limits the quantity of variations. Most of the simplified numeric calculations predict detonation velocities approximately 20% faster than experimental data. It has been proposed that the mode of fuel and oxidizer mixing is a primary contributor to the differences between experimental and computational results. Premixed RDE have experienced flashback that resulted in test article destruction until this work and placed the burden for direct comparison of experimental and computational results on the shoulders of the computational community. Direct comparison with the existing body of premixed numeric results requires construction of a premixed experimental RDE.

4.3. Experimental Non-Premixed RDE

4.3.1. Russian RDE Experiments

In 1969, a survey paper by Voitsekhovskii et al. (89, p. 272) noted the attempt to operate and understand a heterogeneous RDE, which is interpreted to be a non-premixed RDE. He had seen the work of Nicholls et al. (70) and Cullen et al. (13) who had been working on a non-premixed RDE as a rocket engine in the United States before the

program was shut down. A careful reading of (70) identifies that the research became stuck in the paradigm of controlling which direction the detonation wave propagated. The program designed a system that forced detonation in one direction but also halted the detonation after one lap. The Russians were eventually able to work outside the paradigm enough to actually build several successful non-premixed RDE as described in a survey paper by Bykovskii et al. (72). Reported operation of an RDE using hydrogen, propane, and kerosene with oxygen experienced wave speeds between 42 and 95 percent of Chapman-Jouguet estimates. As seen in Figure 21, they noted an increasing wave speed with increasing mass flow rate through the system. Sustained operation required increased mass flow when they went from to a wider feed slot for the oxidizer, and it maintained a single detonation wave instead of breaking into multiple detonation waves. Classic thermodynamic theory (39) suggests that the wider injection slot slowed the flow velocity. The slower velocity in turn likely changed the range and mode of operation because it led to lower turbulence levels, slower harmonic structures, and slower mixing.



a) TDW velocity **b) Operation frequency**
Figure 21. Operating modes for a hydrogen-air non-premixed RDE with multiple waves and different injector-to-channel area ratios from Bykovskii et al. (72)

4.3.2. U.S. Air Force Research Laboratory RDE

4.3.2.1. Eight Centimeter Modular RDE (The Pratt Rig)

Thomas et al. (1) described a modular 8 cm RDE that was originally designed by Pratt & Whitney Seattle Aerosciences Center to operate on ethylene-oxygen and modified to operate on hydrogen-air at the DERF. The design leveraged the relationships between cell size and detonation engine geometry (99,100) to design the detonation channel dimensions. Subsequent testing at the DERF by Russo et al. (16,19) showed operation with standard air between equivalence ratios of 1.63 and 1.75 with a total mass flow through the system of 0.23 kg/s. With an oxygen-nitrogen mixture that was 23% oxygen by mass, the RDE operated between $\phi = 0.85$ and $\phi = 1.6$ with total mass flow rates between 0.28 kg/s and 0.40 kg/s. Detonation wave speeds were found to vary during the detonation run and were reported below 80% of V_{CJ} predictions. Detonation wave direction was noted to reverse randomly. Russo et al. (16) concluded that fuel-oxidizer mixing had a significant influence on the range of equivalence ratio and mass flow rates where operation occurred.

4.3.2.2. The 51 Centimeter Unique RDE (The Boeing Rig)

Dyer et al. (101) reported that a 51 cm RDE device was designed by Boeing Aerospace and tested with both hydrogen-air and ethylene-oxygen-enriched-air at the DERF. This RDE overcame the technical challenges of ignition, sustained detonation, and supporting multiple detonation waves. They found that successful hydrogen-air detonation occurred at different mass flow rates between 1.5 kg/s to 4.1 kg/s for three different channel back-pressurization conditions. Modifications to the original design

improved fuel-oxidizer mixing and allowed the rig to operate on an ethylene-oxygen-enriched-air mixture. The oxygen-nitrogen mixture used as an oxidizer was found to be 24.8% oxygen by mass, a more heavily oxygenated mixture than air. Limits of operation for the ethylene-oxygen-enriched-air were between $\phi = 1.0$ and $\phi = 1.4$ with total mass flow rates between 1.4 kg/s and 3.5 kg/s. They concluded that better mixing, interpreted by the author as a reduced mixing timescale, was necessary to achieve successful RDE operation with hydrocarbons in air.

4.3.2.3. Fifteen Centimeter Modular Radial Inflow (Shank's Rig)

Shank et al. (2,81) described the construction and operation of a 15 cm diameter RDE in 2011 that flowed air radially inward across gaseous fuel jets. The RDE was designed to have modular components that would allow multiple configurations of the detonation channel and non-premixed reactant feed systems. An operating map showed this RDE operated between $\phi = 0.94$ and $\phi = 1.45$ with mass flow rates between 1.1 kg/s and 1.7 kg/s. A high speed camera recorded video of the detonation cycle within the annulus and detonation wave speed was found to vary. Although the detonation had a very consistent time-averaged wave speed, the detonation wave was found to vary based on location within the detonation annulus. After a review of the geometry, it was concluded that the port for the detonation initiator was likely reflecting a shock wave that then changed the detonation wave propagation.

Naples et al. (102) configured the Shank rig with a quartz outerbody used to study the detonation wave mechanics using the chemiluminescence from the hydrogen-oxygen reaction. Angles of the detonation wave, oblique shock, and expansion wave were

measured for hydrogen-air operation at an equivalence ratio of approximately 1.26 between 1.23 kg/s and 1.55 kg/s mass flow. The results were reported for comparison with and validation of CFD simulations. Two key drawbacks were noted with the Shank rig during this study: difficulty changing the air and fuel injection schemes and optical obscuration of the bottom of the detonation channel. To overcome these drawbacks a new RDE was designed and will be discussed next.

4.3.2.4. Fifteen Centimeter Radial Outflow RDE (Naples' Rig)

Based on the drawbacks of the AFRL 15 cm radial inflow RDE, a new radial outflow RDE was designed and constructed to support an annular ejector study by Naples et al. (103) and chemiluminescence studies of Rankin et al. (23). This new RDE maintained similar detonation channel geometry with the 15 cm radial inflow device that allowed reuse of some of the hardware and provided sizing similarity when comparing results. Fotia et al. (104) depicted the cross section of the underlying RDE, as shown in Figure 22. Naples et al. (103) briefly described the geometry and showed that the RDE operated with equivalence ratios of 0.7 to 1.2 for air mass flow rates of 0.152 kg/s. When the mass flow rate was reduced to 0.076 kg/s, the operating region shifted to equivalence ratios of 0.7 to 1.2. This ability to operate the RDE over a wider range of equivalence ratios and at lower mass flow rates has made it the preferred RDE for much of the research that followed at AFRL and served as the basis for which the premixed RDE was designed.

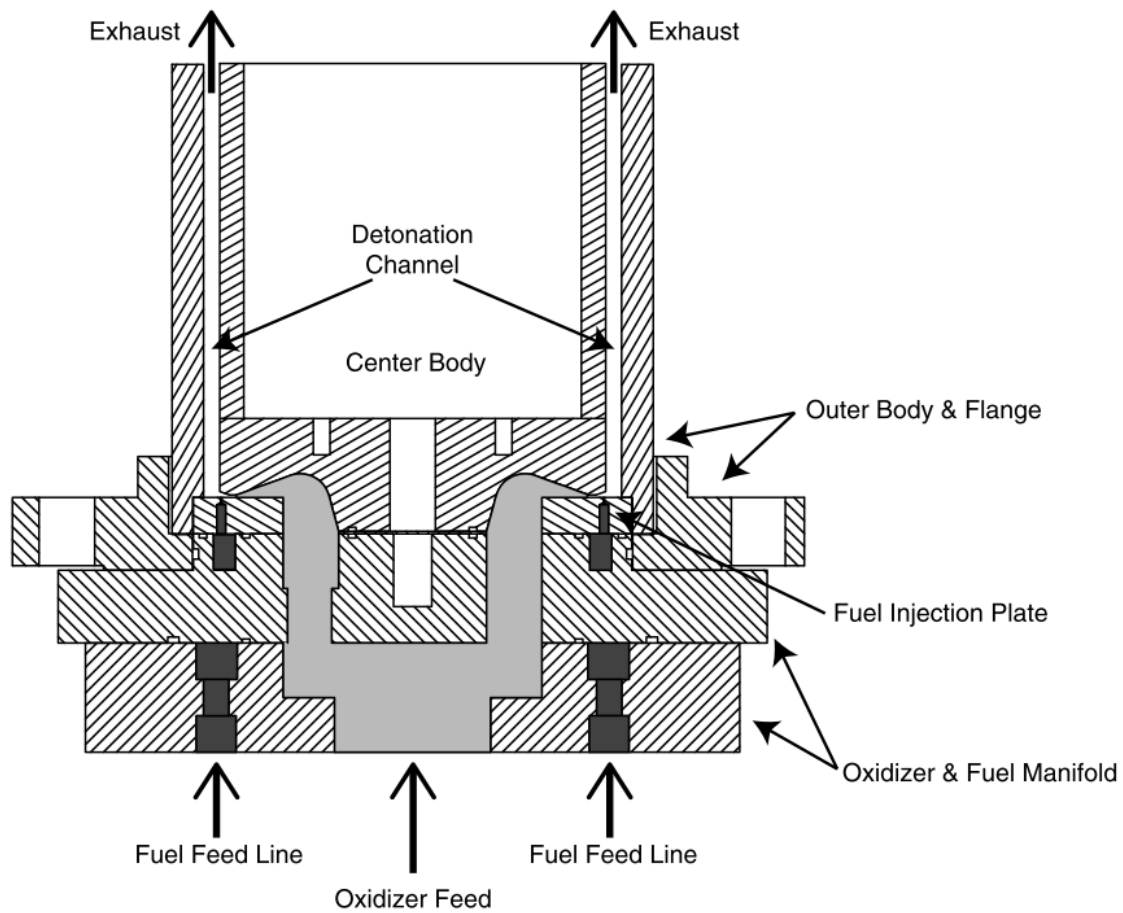


Figure 22. Cross Section of the AFRL modular 15 cm radial outflow RDE, Fotia et al. (104)

Rankin et al. (23) characterized the AFRL 15 cm radial outflow RDE varying mass flow rates, air injection area, fuel injection schemes, and equivalence ratios. The characterization indicated that the number of detonation waves was likely to increase from one to two when either the mass flow increased or when the number of fuel injection points was reduced from 120 to 80. Another conclusion was that counter-rotating detonation waves were likely caused by poor mixing.

Rankin et al. (23) reported static pressure profiles for varying mass flow rates. The steel outerbody of the RDE was instrumented with a rake of capillary tube attenuated pressure (CTAP) sensors. The signals were converted to pressures and showed that the

highest average pressure existed at the bottom of the detonation channel. As mass flow rate increased, the average static pressure at each location in the channel also increased. From the standpoint of attempting to inject premixed fuel and air, the most difficult injection location was assumed to be the bottom of the channel which experiences the highest pressures with transient combustion.

The hydrogen-air performance reported by Fotia et al. (105) showed that specific impulse and thrust could be described as functions of mass flow rate. Figure 23 is one of the summary plots showing that specific impulse and specific thrust increase with mass flow rate and vary with equivalence ratio. They concluded that there was a trade space between inlet stagnation pressure and fuel combustion efficiency and that the trade space was navigated with changes in the detonation engine inlet expansion ratio, exit nozzle

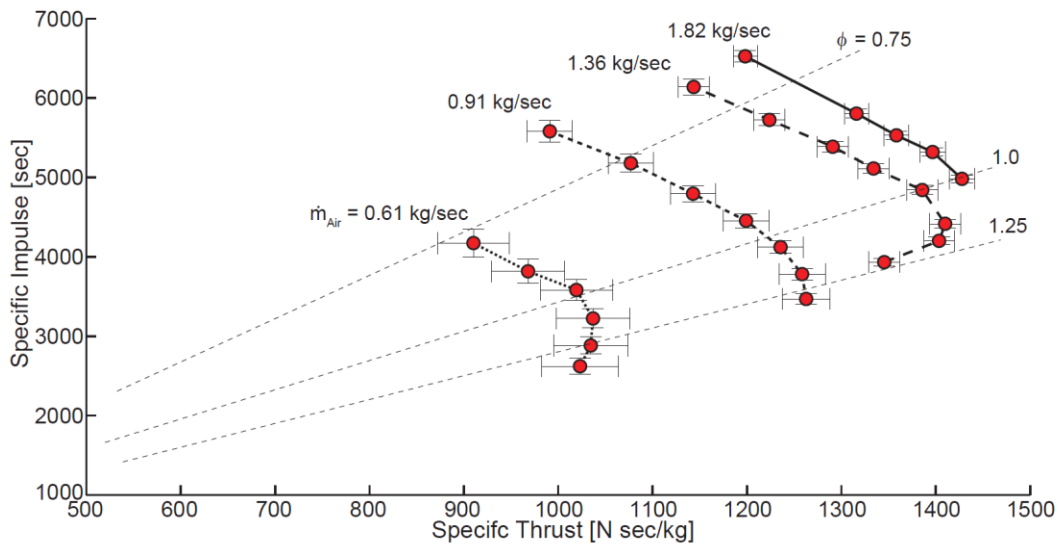


Figure 23. Specific impulse and thrust grouped by mass flow rate and global equivalence ratio for a hydrogen-air non-premixed RDE (105)

constriction ratio, and mass flux through the system. Figure 24 presents specific impulse data from Fotia et al. (106), Rankin et al. (23) and various CFD studies by Schwer et al. (74,76,77,84). As described in Table 3, the data points from the CFD studies were selected to match mass fuel-oxidizer mixture and flow rates as closely as possible. Consequently, the exit treatments and engine size were not matched precisely for the

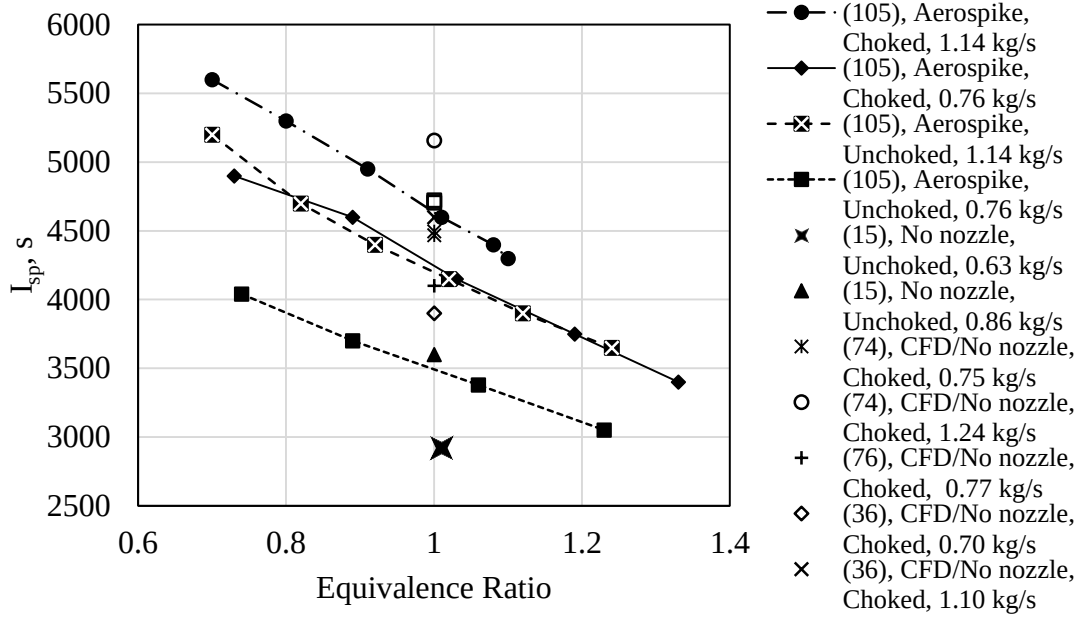


Figure 24. Experimental and numeric specific impulse results for hydrogen-air RDE data from Fotia et al. (106), Rankin et al. (23) and Schwer et al. (74,76,77,84)

Table 3. Test conditions for CFD and experimental specific thrust comparison data from Fotia et al. (106), Rankin et al. (23) and Schwer et al. (74,76,77,84)

Symbol	$\dot{m}$, kg/s	d_{in} , cm	Source	Data set	fuel/ox	Conditions
—●—	1.14	15	(105)/2016	AFRL7	H ₂ /air	experimental, choked
—◆—	0.76	15	(105)/2016	AFRL7	H ₂ /air	aerospike nozzle
-x-	1.14	15	(105)/2016	AFRL7	H ₂ /air	experimental, unchoked
-■-	0.76	15	(105)/2016	AFRL7	H ₂ /air	aerospike nozzle
×	0.62	15	(23)/2015	AFRL6	H ₂ /air	experimental, unchoked, no nozzle
▲	0.89	15	(23)/ 2015	AFRL6	H ₂ /air	
×	0.75	8	(74)/2014	NRL3	H ₂ /air	2-Dimensional CFD,
○	1.24	8	(74)/2014	NRL3	H ₂ /air	no nozzle, flow choked at
+	0.77	13	(76)/2011	NRL5	H ₂ /air	exit for a portion of the
◇	0.70	13	(36)/2010	NRL7	H ₂ /air	cycle
×	1.10	13	(36)/2010	NRL7	H ₂ /air	
□	0.77	8	(77)/2015	NRL8	H ₂ /air	

comparison, and, although the impact of those effects on specific impulse are assumed to be negligible, they have not been definitively characterized.

With those assumptions noted, it can be seen that CFD results show about 10% higher I_{sp} than the unchoked or un-nozzled experimental results. The addition of a choked aerospoke nozzle reduced recirculation zones, allowed for more efficient expansion at the channel exit, and resulted in an increase in the experimentally measured specific impulse. The difference between numerical predicted and experimentally measured specific impulse parallels the wave speed discrepancy, shown in Figure 12.

Cho et al. (82) published chemiluminescence of non-premixed ethylene-air in the AFRL 15 cm radial outflow RDE. Configured with a quartz outerbody, an image intensifier and a high speed camera recorded the hydroxyl spontaneous emissions. Hydroxyl is such a short-lived chemical within the combustion process that it was used as a marker for the detonation wave. Their imagery showed that as mass flow increases the detonation wave grows and fills more of the channel. It also indicated that the combustion zone does not fill the entire cavity cross-section and that there is some stand-off of the detonation wave. It is not known if the standoff of the detonation wave is a result of incomplete mixing in the base of the channel.

The DERF is currently investing resources to move RDE technology toward a viable air-breathing propulsion system. Efforts include an experimental exploration of non-premixed RDE operation (23,104) using thrust measurements and chemiluminescence studies. Naples et al. (106) recently performed studies to characterize the operation of an RDE as a combustor for a turbine engine and demonstrated that the technology provides a viable replacement for traditional burners. Although uncertainties

in the mass flow measurements may prevent a rigorous comparison to existing turbine engines, the demonstration of this technology embedded in the system and operating without failure is significant. Future work will reduce the experimental error to show unambiguously the increase in performance from using a detonation combustion cycle.

Rankin et al. (107) performed planar laser induced fluorescence (PLIF) in a hydrogen-air non-premixed RDE and showed that mixing during detonation varies stochastically and is non-uniform. In Figure 25, small amounts of acetone were mixed well upstream with hydrogen fuel and illuminated with a planar laser sheet to optically pump the acetone to an excited state. The fluorescence produced by the de-excitation of the acetone was amplified with a photo-intensifier and captured on a high speed camera at a detonation channel cross section. The acetone concentration appears as the black-red-yellow-white contour with white being the highest concentration. High acetone concentration is associated with high hydrogen concentration. The irregularity in the mixing from frame to frame, most notably in the 100-135-190 degree sequence, was attributed to the stochastic nature of detonation and the inherent delay that comes with the acetone-PLIF method. More specifically, each frame was collected from a different detonation cycle since the RDE operates at a frequency of 1,000 Hz – 2,000 Hz, and the PLIF laser operates with a 10 Hz, 30 ns pulse. The mismatch in timing meant that hundreds of laps passed unrecorded between PLIF images, and multiple runs were canvassed in search of images at each of the respective detonation cycle phase angles for Figure 25.

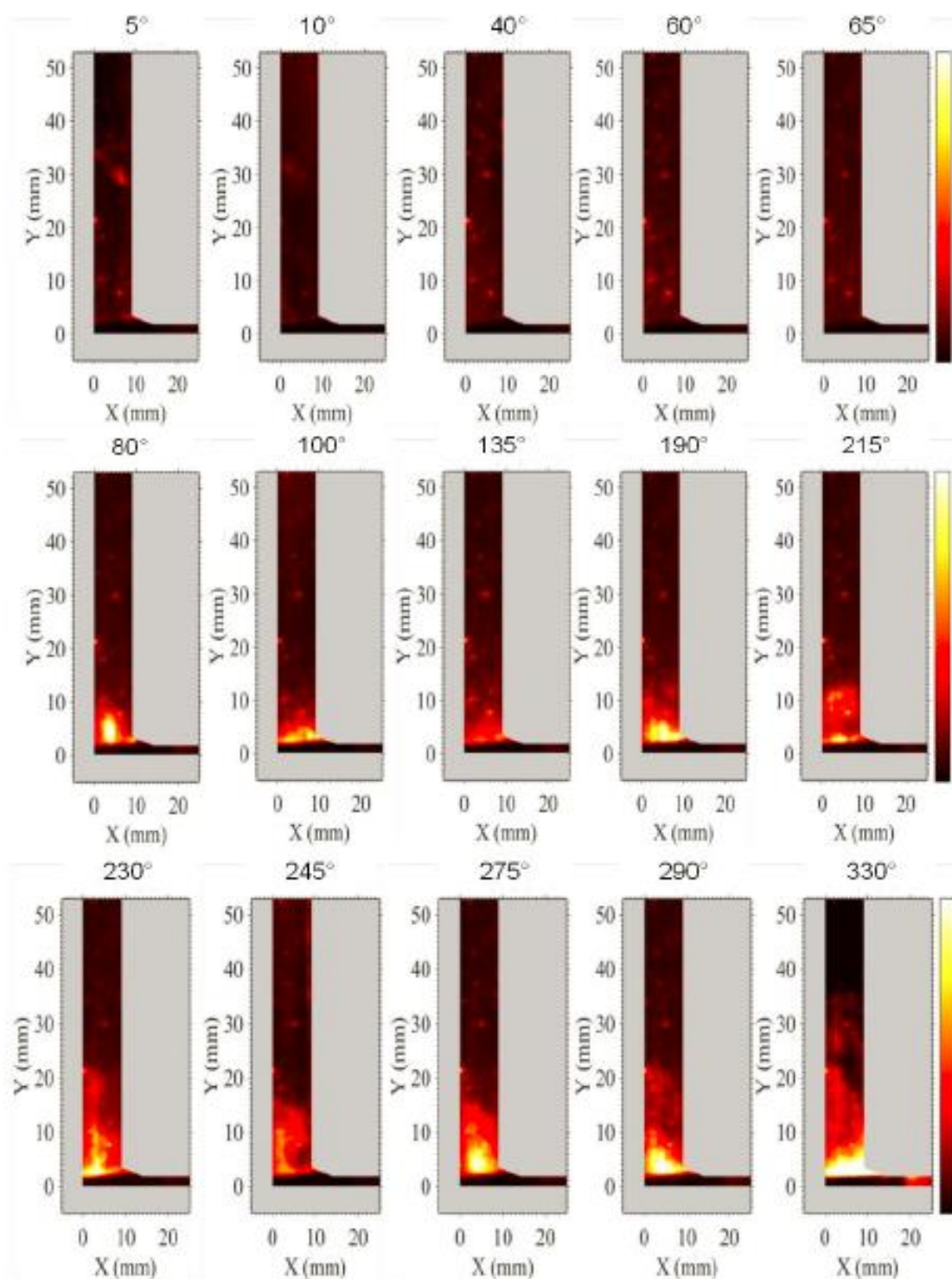


Figure 25. Instantaneous radial cross sections of an operating RDE using acetone-PLIF techniques as reported by Rankin et al. (107)

The PLIF images show mixed reactants with a constant variation of fuel-oxidizer ratios. This author's interpretation of Rankin's data anticipated that when the detonation front arrives, those portions of the mixture near a stoichiometric ratio will react very easily because they exist at the minimum ignition energy. As the stoichiometric portion reacts, it quickly releases energy which continues to drive the detonation forward. Other regions, either rich or lean, will absorb some of the compression energy from the shock wave before it attains a state of ignition and reacts. These rich and lean regions will also release less energy from the reaction than a stoichiometric mixture. This variation of mixture within the detonation zone represents a distinctly three-dimensional issue that may be contributing to the differences in wave speed and specific thrust that exist between computational and experimental results.

5. Quenching Premixed Flame

It is possible to thermally quench a deflagration flame by passing it through two closely spaced plates or a small hole. The maximum distance between two plates where a combustion reaction is just quenched as it reaches the plane where the reactants exit the channel is termed the quenching distance. For a hole, the term is quenching diameter. If the spacing between two plates exceeds the quenching distance, the flame will continue into the channel.

The quenching distance theory provides a mathematical model that supports conventional premixed feed system design. Under steady-state conditions, a premixed burner can be designed to quench flashback. Since a premixed RDE presents a continuous and cyclic pressure and temperature variation to the feed system, the feed

system must be designed to avoid flashback during most of the cycle, tolerate brief reversals, and quench or tolerate combustion until positive flow can re-establish. Under these transient and cyclic conditions, quenching distance theory informs the design process, but it does not completely define it.

Thus, quenching distance is an important design parameter. Turns (108, pp. 283-288) presented quenching distance by balancing heat generated within a flame front, as diagramed in Figure 26, with heat absorbed through conduction into the wall of a slot (radiation and convection are ignored).

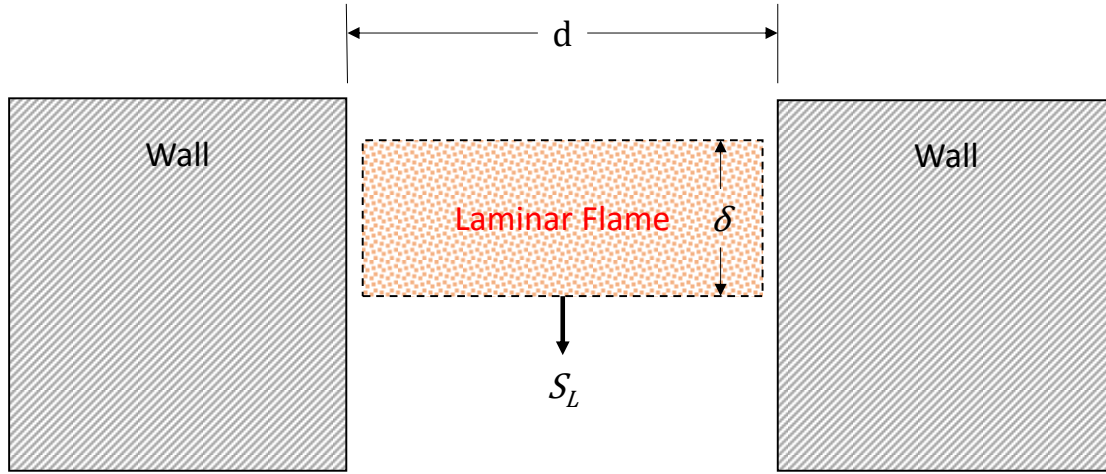


Figure 26. Diagram of the laminar flame of thickness δ propagating between two walls of length L into the paper and separated by distance d adapted from Turns (108, p. 285)

$$\dot{Q}'''V = \dot{Q}_{cond} \quad (10)$$

Where $\dot{Q}'''$ is heat generation within the volume V of the flame front, and $\dot{Q}_{cond}$ is the heat conducted from the burning gas by the wall. Using Fourier's Law, the heat conduction may be written as

$$\dot{Q}_{cond} = kA \frac{dT}{dx} \quad (11)$$

where k is the thermal conductivity of the gas, A is the area of the wall exposed to the flame, dT is the temperature difference between the gas and the wall, and dx is the finite distance measured from the wall toward the center of the flame. If a linear temperature gradient is assumed between the edge and the center of the flame located at $x = d/2$, the conductive term becomes:

$$\dot{Q}_{cond} = -kA \left(\frac{T_b - T_u}{\frac{d}{2}} \right) \quad (12)$$

Where d is the distance separating the sidewalls, T_b is the temperature of the burned gases, and T_u is the temperature of the unburned gases. The heat generation term may be written in terms of the chemical kinetics as

$$\dot{Q}''' = \bar{\dot{m}}_F''' \Delta h_c \quad (13)$$

where $\bar{\dot{m}}_F'''$ is the reaction rate and Δh_c is the enthalpy of combustion. Substituting Equations 11 and 12 back into Equation 9, the heat balance becomes

$$\bar{\dot{m}}_F''' \Delta h_c \mathbb{V} = -kA \left(\frac{T_b - T_u}{\frac{d}{2}} \right) \quad (14)$$

Which may algebraically be solved for $\mathbb{V}/A$:

$$\frac{\mathbb{V}}{A} = -\frac{k}{\bar{\dot{m}}_F''' \Delta h_c} \left(\frac{T_b - T_u}{\frac{d}{2}} \right) \quad (15)$$

Turns (108:283-288) assumed that the flame was laminar with thickness δ and length L along the slot of width d . The surface area exposed to the edge of the flame is

$$A = 2\delta L \quad (16)$$

and the volume of the flame front is

$$\mathbb{V} = \delta L d \quad (17)$$

so that the ratio ($\mathbb{V}/A$) reduces to $d/2$, the distance from the centerline to the sidewall.

The heat transfer equation solved for slot width becomes

$$d^2 = -2k \left(\frac{T_b - T_u}{\frac{1}{2} \dot{m}_F''' \Delta h_c} \right) \quad (18)$$

If considering a tube instead of a slot, the surface area exposed to the edge of the flame is

$$A = \delta \pi d \quad (19)$$

and the combusting volume of the flame front is

$$\mathbb{V} = \delta \pi \frac{d^2}{4} \quad (20)$$

So that the value ($\mathbb{V}/A$) reduces to $d/4$. This result predicts that a slot must be half the diameter of a tube for effective quenching. The previous work for predicting quenching diameters for lean mixtures based on chemical kinetics (109–111) calculated that the ratio of tube diameter to slot distance was $\frac{d_{tube}}{d_{slit}} = 1.64$, and is backed up by experimentation (112,113, p. 84).

Turns (108, pp. 261-269) followed the simplified approach of Spalding (114), and derived the laminar flame speed as:

$$S_L = \left(-2\alpha(\nu + 1) \frac{\bar{m}_F'''}{\rho_u} \right)^{\frac{1}{2}} \quad (21)$$

where S_L is the laminar flame speed, α is the thermal diffusivity of the gas, $\bar{m}_F'''$ is the reaction rate of the fuel, ρ_u is the density of the unburned gases, ν is the mole fraction of the fuel in the unburned mixture. From Equation 21, Turns showed that Δh_c could be written as:

$$\Delta h_c = (\nu + 1)c_p(T_b - T_u) \quad (22)$$

where ν is the mole fraction of fuel in the unburned mixture, c_p is the specific heat of the mixture,. The temperature T_b is for the flame temperature and T_u is the uncombusted mixture. Writing the heat of combustion in terms of the laminar flame speed, S_L , allows us to remove the dependence on mole fraction:

$$\Delta h_c = S_L^2 \frac{\rho_u c_p (T_b - T_u)}{-2\alpha \bar{m}_F'''} \quad (23)$$

which may then be substituted into Equation 15:

$$d^2 = -k \left(\frac{T_b - T_u}{\bar{m}_F'''} \cdot \frac{-2\alpha \bar{m}_F'''}{S_L^2 \rho_u c_p (T_b - T_u)} \right) \quad (24)$$

which simplifies to:

$$d = \sqrt{\frac{2\alpha^2}{S_L^2}} = \frac{\alpha}{S_L} \sqrt{2} \quad (25)$$

Recall that the relation between laminar flame speed, S_L , and flame thickness, δ , is:

$$\delta = \frac{2\alpha}{S_L} \quad (26)$$

so that the relation for quenching distance in a slot becomes:

$$d = \delta \frac{1}{\sqrt{2}} \quad (27)$$

This could be re-arranged to create a non-dimensional number such that,

$$\sqrt{b} = \sqrt{2} = \frac{\delta}{d} = \frac{S_L}{\left(\frac{\alpha}{d}\right)} \quad (28)$$

where b is termed by Turns to be an arbitrary constant (108, p. 285) which is much larger than 2. This constant is the source of non-linearity in the flames assumed temperature profile.

The non-dimensional ratio of flame thickness to quenching distance δ/S_L becomes more informative when the ratio of the flame velocity S_L and thermal velocity α/d is considered. The assumptions laid out at the beginning of the derivation assumed that the laminar flame moves axially along the channel, and that the temperature profile is linear from the center to the edge of the flame. The thermal velocity vector has two

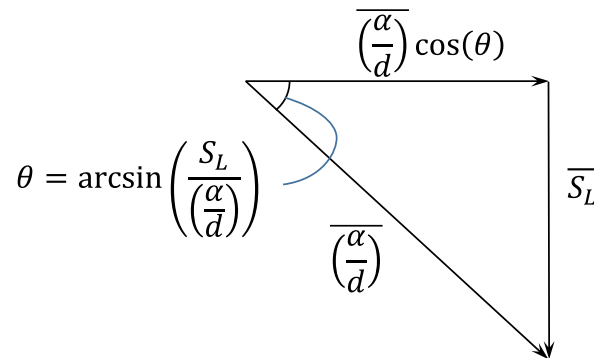


Figure 27. Vector diagram of the reaction and conduction speeds for laminar flame

components: it travels axially along the gap with the flame front and moves the heat transversely into the side wall as shown in Figure 27. The non-dimensional ratio can be used to determine the combined vector angle of flame quenching. If $b = 2$, taking the $\arcsin(1/\sqrt{2})$ yields an angle of 45 degrees, indicating that the conduction rate into the wall and flame speed are equally balanced. If they are balanced, then the flame is able to move the reaction forward as fast as it is being quenched, thus $b = 2$ represents the minimum value for b that avoids quenching. Experimentation has found that the coefficient b must be greater than 2 for sufficient quenching. This is the same as stating that the rate of heat conduction into the side wall and orthogonal to the flame velocity must be greater than the laminar flame speed (i.e. $(\alpha/d > S_L)$). This derivation assumed that convection was negligible and ignored radiant energy effects. Refining the model to account for the energy flux due to radiance and convection may close the gap between the theoretical and experimental values but is not a focus of this research. The pursuit of a functional theory that universally predicts thermal quenching is not trivial, Glassman (115, p. 170) noted that the variation in side-wall conductivity due to material type and condition has created an obstacle to developing a reliable formulation for quenching distance beyond the empirical data collection.

Since flame speed is inversely proportional to the pressure of the reactants, it can also be shown that the quenching diameter can be related to pressure, P , as:

$$d \propto \frac{1}{P} \quad (29)$$

This relation was demonstrated experimentally (116,117) for hydrocarbon-air mixtures. The theoretical quenching distance for a combustible mixture with known experimental properties can be calculated using the engineering relationship derived in Appendix IV:

$$d_Q = d_{Q_{ref}} \frac{\frac{\alpha}{S_L}}{\left(\frac{\alpha}{S_L}\right)_{ref}} \quad (30)$$

where d_Q is the theoretical quenching distance, $d_{Q_{ref}}$ is an experimentally measured quenching distance taken at reference conditions, α is the thermal diffusivity of the reactant mixture, and S_L is the laminar flame speed. Using the relation of Equation 30, quenching distance can be estimated for fuels such as ethylene and ethane with a single data point and accurate models for both flame speed and thermal diffusivity. For ethylene, thermal diffusivity was calculated using the *get_gas_props* function included in Appendix V, while flame speed in air was calculated using the following equation:

$$S_{L_{C_2H_4}} = 47.71 + 259.8\dot{V}_f - 47.45E3(\dot{V}_f - 0.07054)^2 + 10.25E6(\dot{V}_f - 0.07054)^4 - 24.77 \log_{10}(P) \quad (31)$$

where S_L is the flame speed of the subscripted fuel in cm/s, $\dot{V}_f$ is the volumetric flow rate of the fuel by percentage, and P is the static pressure of the reactants in atm. Both flame speed and thermal diffusivity were calculated at the reference conditions and the experimental conditions to generate the mixture's theoretical quenching distance.

For hydrogen, quenching distances should be modeled from empirically collected data since flame speed follows a very different curve than the thermal diffusivity. A least squares fit linear model for hydrogen quenching is:

$$\begin{aligned} \ln(d_{Q_{H_2 \text{ air}}}) = & 2.826173 - 0.342564\dot{V}_f \\ & + 0.0127657\dot{V}_f^2 - 0.000205\dot{V}_f^3 \\ & + 1.2987 \cdot 10^{-6}\dot{V}_f^4 - 2.178311 \log_{10}(P) \end{aligned} \quad (32)$$

where $d_{Q_{H_2}}$ is the quenching distance for hydrogen-air combustion in mm, $\dot{V}_f$ is the volumetric flow rate of the fuel by percentage, and P is the static pressure of the mixture in atm.

The underlying data is plotted in Figure 28 with the model as described in Appendix IV. The plot shows that for hydrogen-air flames, the quenching distance

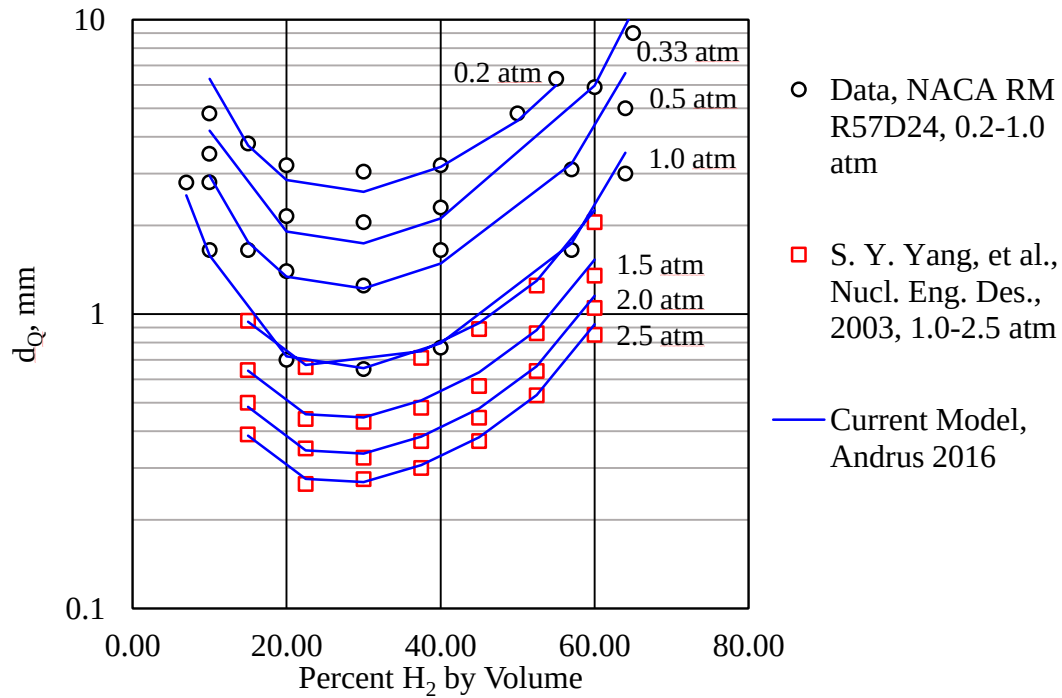


Figure 28. Estimated quenching distance model for a laminar hydrogen-air mixtures based on data from Lewis and Von Elbe (118) and Yang et al. (156)

becomes smaller than can be manufactured using electrostatic discharge machining or laser cutting with feed pressures greater than two atm and equivalence ratios near one.

Manufacturing a feed system with features near the quenching distance at elevated pressures is problematic. Even with today's modern manufacturing methods, fabricating holes with diameters less than 0.2 mm (0.008") and longer than 20 mm is nearly impossible. It is possible, however, to easily create slots down to 0.02 mm (0.001") through the use of laminate construction techniques. For an RDE feed system, features at these small sizes invoke a trade-off between quenching distance and driving pressure. The small features increase the surface area compared to the volume, resulting in a significant pressure loss through the channel or hole.

At the atomic level, heat transfer in a gas is a kinetic transfer of energy from one molecule to another. This is illustrated by argon or CO₂ diluent in a combustion mixture acting as an insulator when compared with helium or nitrogen (113, pp. 83-126, 118–120). It was hypothesized that the larger mass of the argon and CO₂ was more effective at preventing radicals from reaching the side wall where they are quenched, terminating the reaction chain.

Thermal quenching theory does not have the complete solution to describe the quenching phenomenon. The results of a study of propane-oxygen-inert quenching (121) found that "the best agreement between observed and predicted ratios of quenching distances was obtained with the thermal equation plus the assumption that the reaction of active particles and fuel is rate-controlling." (113, p. 90)

One final note on thermal quenching, Fine (122) performed further studies of turbulent flashback with hydrogen-air flames. He experimentally verified the relationship

between quenching distance and reactant pressure for sub-atmospheric hydrogen-air flames. Additionally, his results indicated that as turbulence increases, the quenching distance shrinks, making Figure 28 the best case scenario. He was also looking at flame stability analysis, a constant companion to quenching distance, and found that the reduced quenching distance required higher velocity gradients to avoid flashback. Quenching distances are experimentally determined by halting the flow of reactant through the channel. When the reactants are flowing, the engineering limits for blowoff and flashback are measured instead.

6. Premixed Burner Flame Stability

6.1. The Role of Blowoff and Flashback in an RDE

The principles of flashback and blowoff are part of premixed flame stability. Anticipating how blowoff and flashback affect RDE operation is critical to successfully designing a premixed RDE. These phenomena are heavily influenced by how the RDE combustion occurs. The RDE operates on a uniquely dynamic style where temperature and pressure at a given location varies at a very high rate (thousands of Hertz) and the amplitude varies by a factor of 10 or 20. Consider a differentially small azimuth from the RDE shown in Figure 29. In this small wedge of the RDE, the circumferential activity of the RDE is lost, leaving only axial and radial dimensions, as shown in Figure 30. From this perspective the flow path is so narrow, flows are approximately one dimensional and will only vary with time. The RDE sector operates in a uniquely dynamic cycle where reactants pulse into the chamber, instantaneously detonate, and the expanding products temporarily halt the flow of reactants. Although fuel and oxidizer are being fed into the

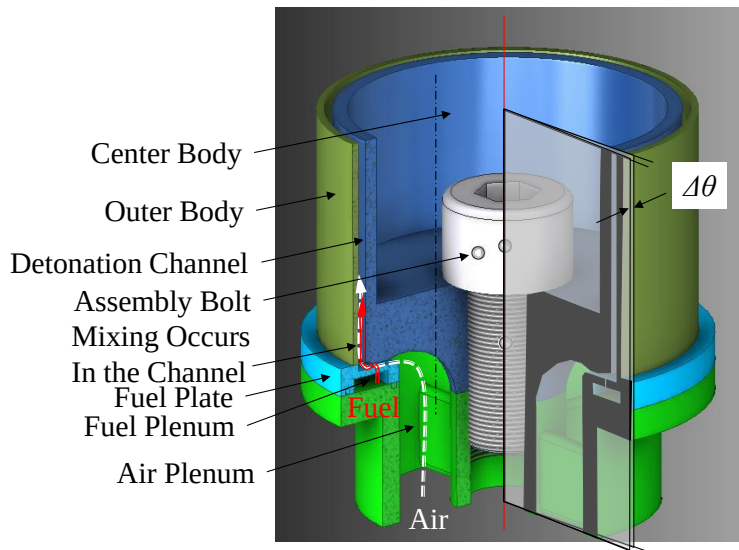


Figure 29. Cut-away model of a notional non-premixed RDE showing a differentially small sector of azimuth

detonation channel continuously, each sector experiences a very cyclic flow. The detonation wave appears and disappears from the sector, almost instantaneously changing cool reactants into hot products at high temperature. These post-detonation products have momentarily stagnated the flow of reactants which may continue to deflagrate. Then

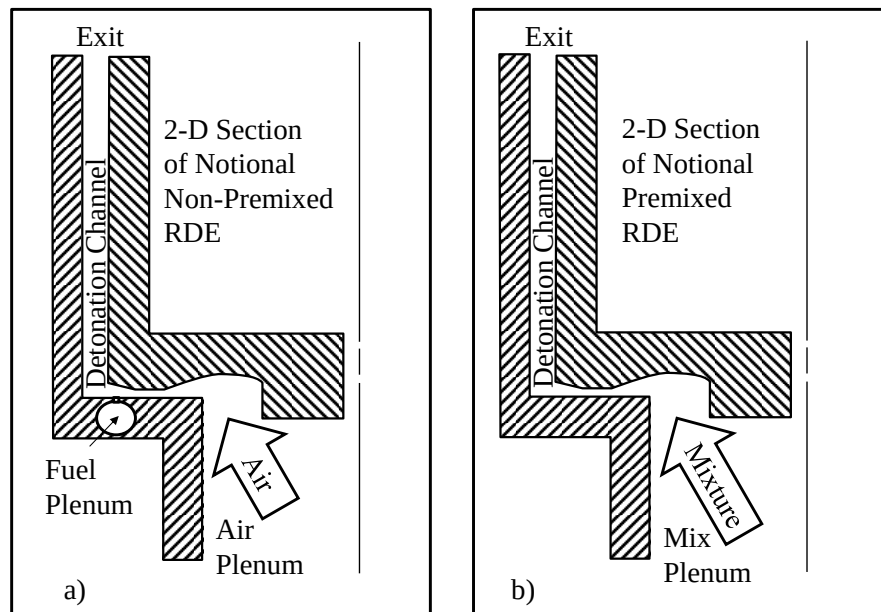


Figure 30. Two dimensional cross section of notional a) non-premixed and b) premixed RDE flow paths

pressure and temperature of the products drop as they expand toward the exit. If the feed plenum arrests the combustion from progressing into the feed system, and the reactant flow re-establishes itself with a sufficient flow rate to blow any lingering deflagration toward the exit, the cycle repeats. The feed system may halt the combustion and avoid flashback by injecting fuel and oxidizer in separate streams. The difficulty addressed by this dissertation is in achieving a premixed system that will both blow off the deflagration left after the passage of the detonation and prevent flashback into the feed plenum.

6.2. Historical Research

Flame stability has been researched and understood for many years. Grumer et al. (30) performed a landmark study for the U.S. Bureau of Mines in 1956 which compiled a large body of data for burner flame stability. They compiled results from other research and ran new experiments for premixed combustion flame stability for a number of important industrial fuels and plotted the flashback, blowoff, and yellow-tip limits against equivalence ratio and the critical velocity gradients, g_c , as seen in Figure 31. In the two-dimensional coordinate reference frame; the fluid flows in the direction of the x axis through a tube or channel with velocity u . If the flow velocity varies along the y axis (generally measured as some distance y from the sidewall), the velocity gradient, g , is defined as

$$g = \frac{du}{dy} \quad (33)$$

where du is the differential change in fluid velocity, and dy is the distance from the side wall. Grumer et al. (30) directly applied the textbook formulae given by Lewis and Von

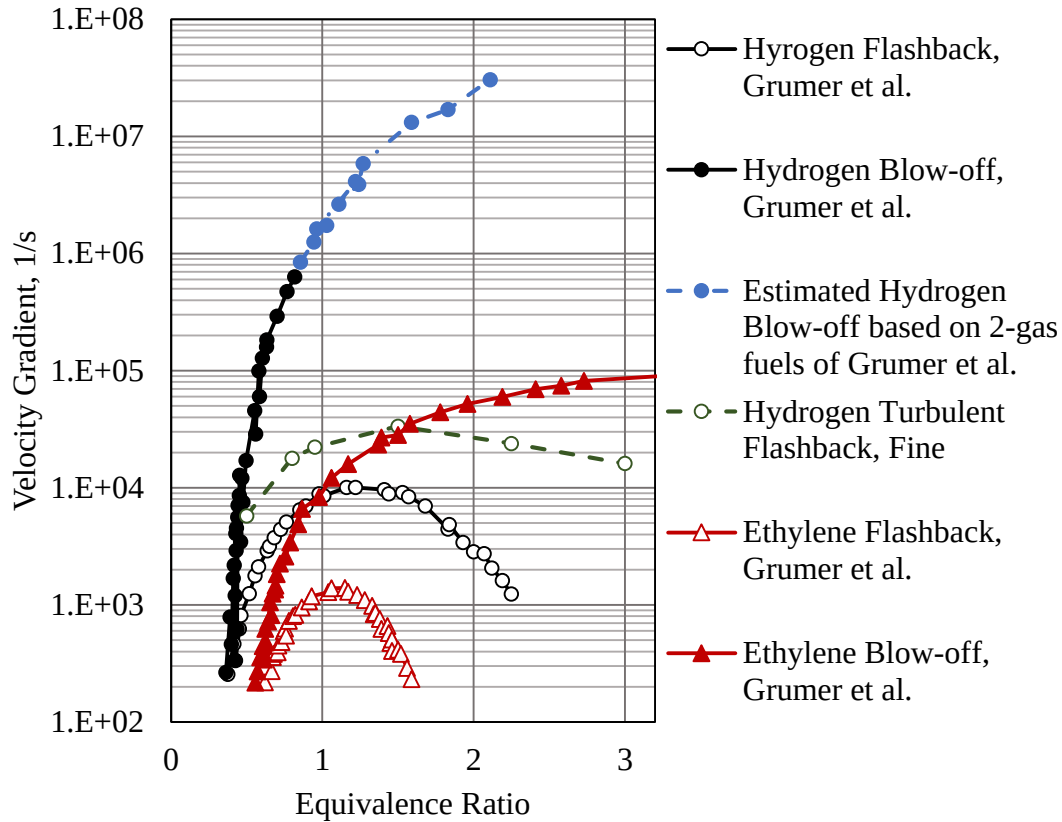


Figure 31. Critical boundary layer velocity gradients for hydrogen-air and ethylene-air fuel mixtures, standard temperature and pressure, data from Grumer et al. (30) and Fine (122,183)

Elbe (118) as described below to characterize the critical velocity gradients where flashback and blowoff occur for laminar premixed flames. In so doing, they accurately described the flow conditions required for stable flame. For normal burner technologies, when the velocity gradient of a flow lies above that of flashback (g_f) and below that of blow-off (g_b), the flame is said to be stable. However, for an RDE it is necessary that the flow be constrained so that the velocity gradients in any premixed feed system always be above the flashback line, and the flow in the detonation channel should maintain a velocity gradient above that for blowoff. Obviously, a premixed RDE will unstart if the flashback criteria is violated. Less obvious is that the detonation will cease to operate if

the blow-off gradient is not maintained because of the need for the detonation to constantly be supplied with a finite region of premixed reactants as it cycles around the detonation annulus. If the premixed flow in the detonation channel is not in a blow-off condition, deflagration will constantly consume the reactants and prevent detonation.

The critical velocity gradient g_c of the velocity profile for laminar flow in a circular tube may be derived (30) from the assumed parabolic velocity profile of Poiseuille flow, and is given as

$$g_{c} = \frac{4\dot{V}}{\pi r^3} \quad (34)$$

where $\dot{V}$ is the volumetric flow rate, and r is the radius of the circular tube. This velocity gradient is the ratio of the change in the axial flow velocity in a channel with respect to the change in distance from the channel wall. Fluid dynamicists may be more familiar with the terminology $\partial u / \partial y$, but, in order to be consistent with the combustion literature the term g_c will be used throughout this document. For turbulent flow, the appropriate formula is the Blasius relation which was cited by Grumer et al. (30) as:

$$g_c = \frac{0.316}{Re^{\frac{1}{4}}} \dot{V} \frac{Re}{16\pi r^3} \quad (35)$$

from this form, Grumer et al. further reduced the equation to:

$$g_c = c_f \dot{V} \frac{Re}{16\pi r^3} \quad (36)$$

where c_f is the coefficient of friction (also called the Fanning friction factor) defined by the geometry of the channel and the level of turbulence. Within this framework, for laminar Poiseuille flow $c_f = 64/Re$, while $c_f = 0.316/Re^{\frac{1}{4}}$ for turbulent flow in a

circular pipe. Other variations for c_f were collected for sharp edged ports (i.e. drilled holes in pipe: $c_f = 41.4/Re^{0.89}$), square tubes ($c_f = 156.4/Re^{1.22}$), triangular tubes ($c_f = 90.6/Re^{1.25}$), and rectangular tubes ($c_f = 125.8/Re^{1.24}$). These formulae for the friction coefficient were built for incompressible flows, whereas the premixed RDE feed system was a narrow channel with compressible friction flow.

There is significant bodies of data for incompressible turbulent flow in ducts that provide a far better approximation of friction coefficient. The Darcy-Weisbach friction factor (f) for turbulent flow may be computed using Colebrook-White equation (123, p. 432):

$$\frac{1}{\sqrt{f}} = -2 \log_{10} \left(\frac{\epsilon}{3.7D_h} + \frac{2.51}{Re\sqrt{f}} \right) \quad (37)$$

where ϵ is a surface roughness measurement taken from tables or measured directly, D_h is the hydraulic diameter for non-circular ducts calculated as:

$$D_h = 2b \quad (38)$$

for rectangular channels whose width a is much greater than height b , and Re is the Reynold's number, Re , for the flow given as:

$$Re = \frac{4\dot{m}}{\pi\mu D_h} \quad (39)$$

The Darcy-Weisbach friction factor (f) is related to the Fanning friction factor (c_f) as:

$$c_f = 4f \quad (40)$$

Blasius' definition of the pipe friction factor is given as:

$$c_f = \frac{2\tau_w}{\rho u_{av}^2} \quad (41)$$

where ρ is the fluid density, u_{av} is the average velocity in the duct, and τ_w is the wall shear stress. This can be solved for wall shear stress:

$$\tau_w = \frac{\rho u_{av}^2}{2c_f} \quad (42)$$

The wall shear stress can then be used to obtain the velocity gradient of the flow at the wall with the relation:

$$g_c = \frac{\partial u}{\partial y} = \frac{\tau_w}{\mu} \quad (43)$$

This relation should hold for turbulent flow in a narrow channel, but was developed under the assumption that the flow is incompressible.

6.3. Application Beyond Laminar Flames

The question arises as to whether stability limits developed with laminar flow apply to the flow in the narrow channels of an RDE. Notably, Grumer et al. (30, p. 92) stated that while blowoff limits collected in their study were good for laminar or turbulent conditions, flashback limits were generated strictly with laminar flames. Flashback of turbulent flames was noted at higher velocity gradients than the reported flashback limits, and the results were repeated by Eichler and Sattlemayer (124) for boundary layer flows.

When turbulence was induced in flashback studies, Fine (122) found the critical velocity gradient for flashback in hydrogen-air mixtures was a factor of 2 to 3 greater than laminar near stoichiometric conditions. A subset of his results are included in Figure 31, and showed flashback in the lean or rich mixture regions where flashback was

previously not observed. As the equivalence ratio moved away from unity in either direction, turbulence allowed flashback where a laminar flame did not. The larger gradient needed to avoid flashback was critical to planning an RDE, because it indicated that while it is desirable to operate a detonation channel in blowoff, the design must also account for the fact that flashback into the plenum is possible in a turbulent flow when the velocity gradient was above the reported flashback limits of Grumer et al. (30) The turbulent flashback limit also indicated that attempting to inject lean and rich streams might be just as problematic as attempting to inject stoichiometric mixtures. This would be particularly true for mixtures such as hydrogen-air, where laminar and turbulent flame speeds peaked at an equivalence ratio of 2, or ethylene-air mixtures, where flame speeds peaked at equivalence ratios of 1.2.

The relation for critical blowoff gradient when a premixed flame is venting into an unconfined space was given by Lewis and Von Elbe (118) as:

$$g_c = \frac{S_u}{d_{QB}} \quad (44)$$

where S_u is the flame speed relative to the unburned reactants (the laminar flame speed), and d_{QB} is the “quenching distance at blowoff, that is the width of the boundary layer wherein a noncombustible fuel-air mixture exists (30, p.105).” This quenching distance is different than the quenching distance discussed in Section 5; instead it is a distance that is mostly determined by diffusion of unvitiated air into the boundary layer. The diffusion (or alternatively entrainment) produces a mixture that is so lean at the edge of the premixed jet that the flame cannot propagate into it and is blown off by the higher

velocity stream of flammable reactants. When injecting into the detonation channel filled with hot detonation products, this quenching distance will not be achievable.

Flashback occurs when the flame speed exceeds the counter-flow of reactants and can occur in the middle of the reactant flow or within the viscous boundary layer near the side wall. Flashback may be arrested by forcing the reactant flow to be faster than the flame speed at all points in the freestream flow while forcing the boundary layer to be smaller than one-half the quenching distance. With this understanding, the flashback gradient, g_f , has been related to the quenching distance (118) through the relation:

$$g_F = \frac{S_u}{d_{QF}} \quad (45)$$

where d_{QF} is essentially a property of a given fuel-air mixture and is the thermal quenching distance discussed in Section 5 of this chapter. It is the maximum distance that successfully quenches the reaction just when the reaction reaches the same plane as the channel exit when channel flow is suddenly stopped. The term S_u is the velocity of the unburned gases flowing in the tube or channel. To use the flame stability curves shown in Figure 31, the experimental data must be adjusted back to the reference conditions in which the chart data were collected. The charts were constructed using laminar flame so that $S_u = S_L$ and the quenching distance was calculated for flows at approximately 1 atm pressure and 300 K initial temperature. To adjust the velocity gradient for conditions in a premixed RDE feed system, the relation of Equation 46 was used:

$$g_{f_{adj}} = g_{f_{ex}} \left(\frac{S_{L_{ref}}}{S_{obs}} \right) \left(\frac{d_{Q_{obs}}}{d_{Q_{ref}}} \right) \quad (46)$$

where g_{fex} is the time-averaged velocity gradient under the experimental conditions at flashback calculated with Equation 36, S_{obs} is the speed of the combustion wave relative to the side wall, S_{Lref} is the flame speed used for building the charts, d_{Qobs} is the theoretical quenching distance for the experimental conditions, and d_{Qref} is the theoretical quenching distance at the reference conditions for which the reference critical velocity gradients were measured. A derivation of Equation 46 may be found in Appendix IV.

The adjustments implied by Equation 46 may be quite large. Flashback driven into a premixed RDE feed system is shown in Chapter III to move at approximately the speed of sound relative to the gas flows. The observed speed of sound is calculated by subtracting the bulk velocity of the flowing gas from pressure wave speed:

$$S_{obs} = a - \bar{u}_{pl} \quad (47)$$

where S_{obs} is the observed wave speed used in the velocity gradient adjustment, a is the speed of sound in the flowing gas, and $\bar{u}_{pl}$ is the bulk velocity of the flowing mixture. The speed of sound is approximately three orders of magnitude greater than laminar flame speed (118). The quenching distance varies with the logarithm of the pressure (118,125) and results in another correction of approximately one or two orders of magnitude. Thus, the experimental combustion speed has a larger influence on the velocity gradient adjustment than quenching distance. Correlating the adjustment to temperature and pressure in the RDE system results in Equation 48:

$$g_{fadj} \propto \log(P) T^{-\frac{n}{2}} \quad (48)$$

where n is an experimentally determined coefficient of variation of the laminar flame speed with the temperature variation (approximately 1.5 for stoichiometric hydrogen air (126)). The proportionality of Equation 48 predicts that the flashback into the system will be far more sensitive to temperature than to pressure. Increasing temperature will result in a reduced adjusted gradient that indicates an increased probability of a flashback

The experimental setup for each of these studies generally allowed the reactants to vent into an open room, which is different from a theoretical RDE system which vents the premixed reactants into a narrow channel. More recently, Eichler (127) showed that venting into an open room gives a non-conservative prediction of flashback. When the exit is confined, as in a premixed burner, flashback occurs at significantly higher velocity gradients than the established stability diagrams report.

The material of the enclosure was also found to have an effect, with higher thermal conductivity of the burner reducing the velocity gradient required to prevent flashback. Duan et al. (128) used three materials to construct a low-swirl (turbulent) burner: brass, steel, and quartz glass. They also varied the steady state temperature of the three materials through active cooling, which changed the thermal conductivity at the flame-burner interface. This showed a direct connection between the thermal properties of the burner material and propensity for flashback. Additionally, the burner was operated in three configurations where the flame saw increased confinement. Figure 32 summarized the results of both studies and indicated that increasing thermal conductivity of the feed system and decreasing confinement should improve the safety and reliability of a premixed RDE. Their article also identified that placing a shroud around the port exit

to confine the flame promoted flashback in a manner that could not be overcome by material conductivity.

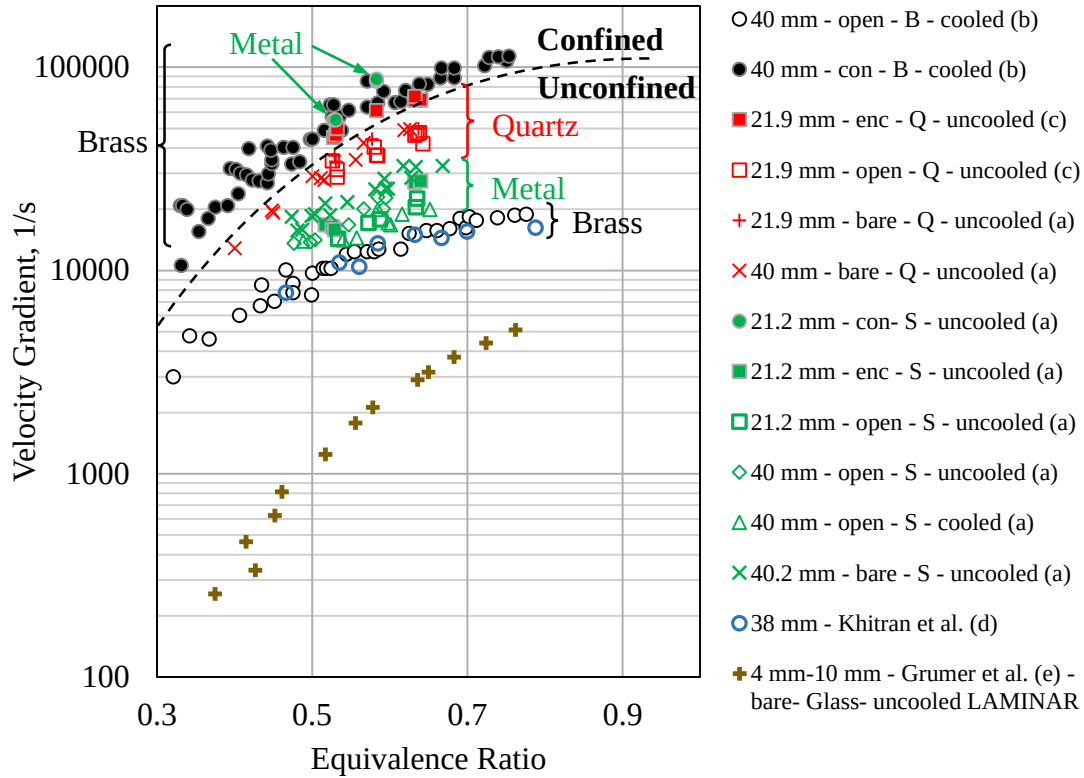


Figure 32. Flashback for a hydrogen-air low-swirl burner in confined and unconfined configurations of differing material types adapted from Duan et al. (128) and used by permission from ASME, data from a:(128), b:(184), c:(185), d:(186), and e:(30)

Flashback in turbulent flames occurs differently than in laminar flames. Flashback was shown to be less likely to occur (129) in the turbulent methane-hydrogen-air flames of a low-swirl injector when the bulk velocity and reactant temperature were increased. It was shown to be more likely when the feed pressure and flame temperature were increased. Turbulent flame speed was shown to have a linear relationship to the root mean squared velocity fluctuation of the turbulence, independent of pressure and temperature. For a premixed RDE, this indicates that increasing feed pressure or

turbulence will increase the propensity for flashback, and that increasing fluid velocity or moving to an equivalence ratio with a lower flame temperature will decrease it.

Turbulence also increases the propensity for flashback. Lin et al. (130) described the critical velocity gradient for a turbulent flame in terms of the cold flow gas properties:

$$g_c = \frac{S_T}{Le \delta_{L0}} \quad (49)$$

where S_T is the turbulent flame speed, δ_{L0} is the unstretched laminar flame thickness, and Le is the Lewis number defined as $Le = \mathcal{D}/\alpha$, where $\mathcal{D}$ is the diffusion constant for the mixture and α is the thermal diffusivity of the mixture. It has been shown that increasing turbulence changes the critical velocity gradient of the flame (108). Lin et al. (130) then defined the flashback velocity gradient with the Blasius correlation for circular pipe flow (123, p. 426):

$$g_f = 0.0396 u_0^{\frac{7}{4}} \nu^{\frac{-3}{4}} d^{\frac{-1}{4}} \quad (50)$$

and showed experimentally that when $g_c < g_f$ the feed system is in a flashback safe condition.

Friction flow in a narrow channel is compressible flow and has been discussed by many textbooks, such as Anderson (33). In a narrow channel the friction between the flowing fluid and the side wall increases the entropy within the fluid and unlocks an energy exchange between the potential energy of pressure and the kinetic energy of fluid velocity. The exchange accelerates subsonic flow and decelerates supersonic flow. When a pressure or expansion wave is pushed into the flow field, Vasu et al. (131) showed analytically that it acts in a non-linear fashion. If the friction flow is subsonic, it acts as a

diverging field where compressible waves are dissipated and expansion waves are amplified. In supersonic flow, the expansion waves are dissipated and compression waves are strengthened until they become shock waves. This is important for the detonation feed system since the detonation drives a pressure wave into the feed system. The work of Vasu (131) suggests that a supersonic flow in the feed system should be avoided and that friction flow dissipates the pressure wave.

A correction to the velocity gradient that accounts for the flame speed and quenching distance in the RDE feed system is described in Chapter III. The adjustment procedure allows the flame stability curves of Grumer et al. (30) to be used to estimate safe operating regions for the premixed RDE.

7. Conclusions

Detonation combustion research is moving rapidly forward to create an air breathing propulsion system that is more efficient than current technology. Computational and experimental RDE research efforts agree qualitatively on the fundamental structure of the RDE structure but disagree quantitatively with detonation wave speed and specific thrust predictions. The research community is working to understand the fundamental physics that have created these discrepancies by writing CFD codes that model separate stream injection, complex chemistry, and three dimensional geometries. Experimental efforts to build a premixed RDE have failed as a result of mixture delivery systems that did not account for the dynamic detonation cycle and its impact on theoretical quenching. Theoretical quenching and burner stability diagrams have been applied to traditional premixed laminar flame, and extensions have been made

to describe safe handling of turbulent flame. With further corrections discussed in Chapter III, the traditional burner stability diagrams were adjusted for the RDE conditions and informed the design and successful operation of a premixed RDE discussed in Chapters IV and V.

III. Arresting Flashback

1. Overview

Achieving a premixed detonation engine requires careful design of a feed system which delivers a well-mixed fluid while also preventing flashback. As seen in the literature review, flashback for a traditional burner has been studied and well characterized, but not for a detonation cycle engine. The goal of building a premixed RDE, then, must start with the first two objectives: “Discover the flow conditions that halt flashback into a premixed feed system exposed to a transient detonation,” and, “Characterize the correlations between flashback in a premixed flow exposed to a transient detonation front and traditional burner stability parameters, such as: quenching distance and critical boundary layer velocity gradient as a function of the temperature, pressure, equivalence ratio, mass flow rate, and fuel.”

An initial attempt to create a premixed RDE feed system using 0.43 mm holes in a steel bar failed to prevent flashback. A complete description is found in (26) and included as Appendix I. Hydrogen fuel and air were fed separately into a mixing chamber constructed by sandwiching a bank of feed nozzles between two polycarbonate sheets and sealing the opening edges. Grooves in the sidewall of the mixing chamber promoted mixing of the hydrogen and air before they passed through a series of feed nozzles.

The attempt to analogue an RDE with the linear combustor failed when combustion anchored at the exit of the premixture feed system and then was pushed into

the feed system with a subsequent pressure pulse. The failure destroyed the test section and highlighted the risk involved with operating premixed detonation engines.

The visualization of the flashback that accompanied the firing of the predetonators into the channel provided some key insights through careful observation. First, the flow rate of the reactants must be sufficient to blow any flame reaction away from the injector face or deflagration will consume the fuel before it can enter the detonation channel. Second, detonation appeared to rapidly de-couple when the mass flow rate through the detonation channel was small. Small holes appeared to limit the transmission of detonation and shock waves, but, in a transient cycle, they allowed a second blast to push flames ignited with the initial detonation attempt back into the mixture plenum. Finally, attempting to quench with flame quenching methods will require feed holes that are sized for the austere pressure and temperature fluctuations within a detonation engine.

After considering various feed geometries from the standpoint of manufacturability, a long narrow feed channel was selected as an optimal configuration to arrest flashback. Experimentation with this injection method showed probabilistic quenching of detonation initiated deflagrations in the feed orifice. Partial results were presented at the AIAA Dayton-Cincinnati Aerospace Sciences Symposium in March 2015, while complete results were presented in San Diego in 2016 (27). The remainder of this chapter is an amplification of that paper, leaving out the background which is more fully described in this document within Chapter II and adding additional thoughts, insights, and conclusions.

2. Premixed Injector Methodology

Flame quenching and blowoff gradient were identified as key principles for a successful premixed detonation engine design based on the previous study results (26). The observations that flashback could occur directly with a transient detonation, as well as when an anchored flame was pushed through the feed holes, spurred the construction of a premixed injector test assembly featuring long narrow feed slots. This effort took on two parts: an exploratory study injecting premixture into a pulsed detonation engine (PDE) host and a proof of concept study that injected premixture into an RDE host.

2.1. Premixed Detonation Engine Injector Apparatus

The first step to demonstrating the ability of a long narrow slot to arrest flashback was the design of an injector assembly that could be inserted into the side of a pulsed detonation tube. The slot was formed by sandwiching a U-shaped shim between steel plates. As shown in Figure 33, many variables affected the ability of the slot to arrest

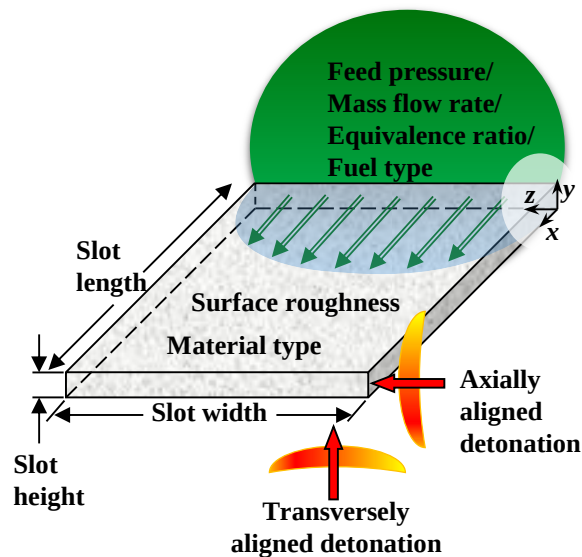


Figure 33. Diagram of the premixed injector feed slot segment control variables

flashback. Experimental variables from Figure 33 included slot height, slot length, fuel type, equivalence ratio, and mass flow rate. Other variables were controlled to minimize their influence on the results.

Two test sections were constructed to accept the injectors. The first used a pulsed detonation engine (PDE), while the second test section used a 15 cm modular research RDE modified by cutting an access slot in the outerbody. During each test, premixed fuel and oxidizer were pressure fed through the injector slot while a detonation traversed the slot exit. A pressure transducer, an ion probe, and a thermocouple, continuously sampled the flow for flashback indications.

2.1.1. Injector Segment Test Section

The test sections were conceived to mimic small segments of a premixed RDE feed system. Each injector assembly was designed for rapid reconfiguration and initially had no optical access. Two mild steel plates sized 7.62 cm x 12.7 cm x 1.91 cm were separated by shim stock layered in 0.127 mm increments. The brass shim stock was cut in a U-shape, as seen in Figure 34, to create a slot of variable height h , length of 7.9 cm, and width of 3.8 cm. The detonable mixture was pressure fed through the slot into the

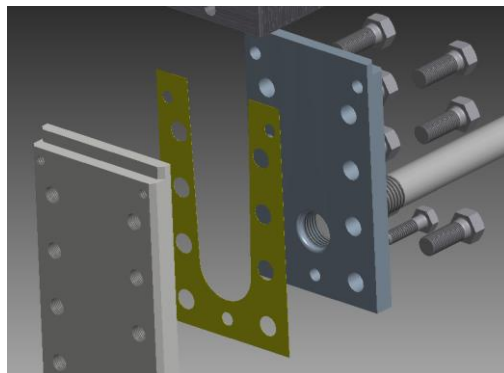


Figure 34. Drafting model of the premixed injector

functioning detonation engine. The slot width approximated an 8% segment of a single feed slot for a 15 cm diameter RDE. To keep a low profile in the detonation channel, the ends of the plates intended for the PDE were milled flat while the RDE plates maintained the curvature of the detonation channel. Surface roughness for the milled plates (132, p. 708) used in the PDE test section was estimated at $3.1\text{ }\mu\text{m}$. Plates used in the RDE test section were manufactured with tighter tolerances and maintained an estimated average surface roughness of $0.4\text{ }\mu\text{m}$.

Slot length was varied by inserting 0.48 mm D-shaped shims, as seen in Figure 35 a), between the two steel plates along with the U-shaped shims. These D-shims featured a central cut-out region that effectively increased the slot height near the mixture inlet when combined with the U shim. Only the portion of the length of the D-shim that crossed the open portion of the U-shim was recorded as slot length, as illustrated in Figure 35 b). The approximation of length using a D-shim was justified due to the demonstrated ability of the fluid to maintain flashback at the larger slot-heights. The underlying assumption was that any combustion front reaching the larger gap height

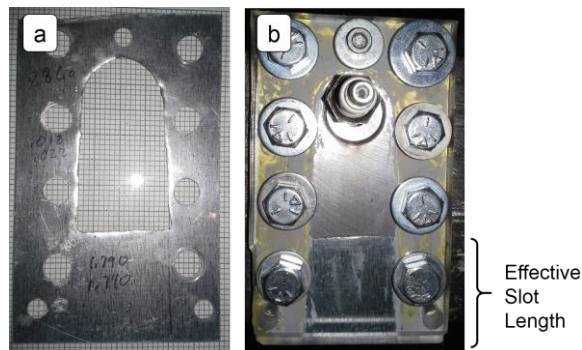


Figure 35. a) D-shaped shim that changes the effective slot length b) test section assembled with a plastic plate and with U and D-shaped shims

could successfully propagate the remainder of the distance into the mixing system and trigger a flashback response in the sensors.

2.1.2. Interface with Detonation

Once assembled, the test section was inserted either into an adapter welded onto a 5.08 cm diameter steel detonation tube host or into the side of a 15 cm RDE host outerbody. The set-up articles are shown in

Figure 36 with feed systems connected. The fuel and oxidizer for the premixed test section were combined at a tee union, and the mixture then flowed through an approximately 60 cm section of 6.35 mm steel tubing before entering the injector slot. The injector was initially oriented in a horizontal configuration, as shown in Figure 37, so that the detonation would pass along the major axis of the rectangular slot opening, in analogue of a continuous circumferential feed slot injector in an RDE. A minor variation in the RDE test section was made to allow a second configuration to be investigated. The injection slot was oriented parallel to the RDE axis, enabling an investigation to

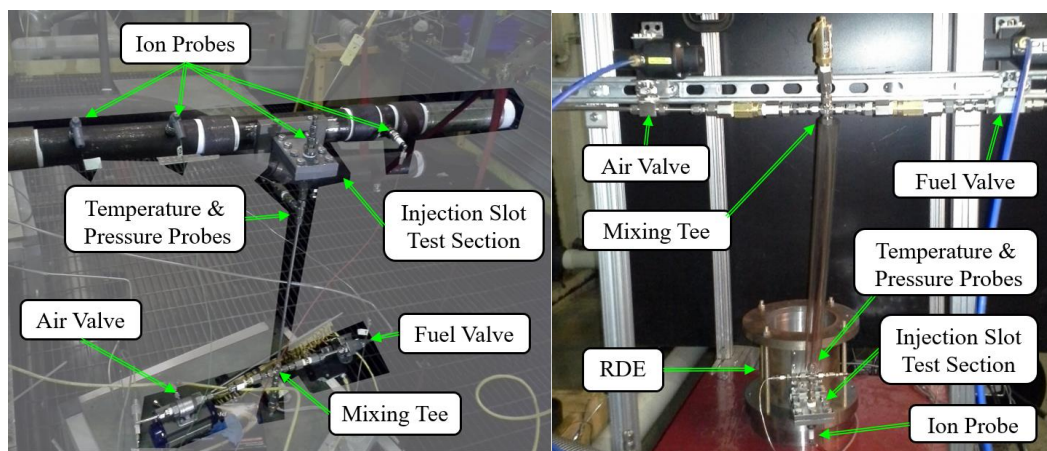


Figure 36. Assembled injector test apparatus inserted into a PDE host (left) and an AFRL 15 cm RDE host (right)

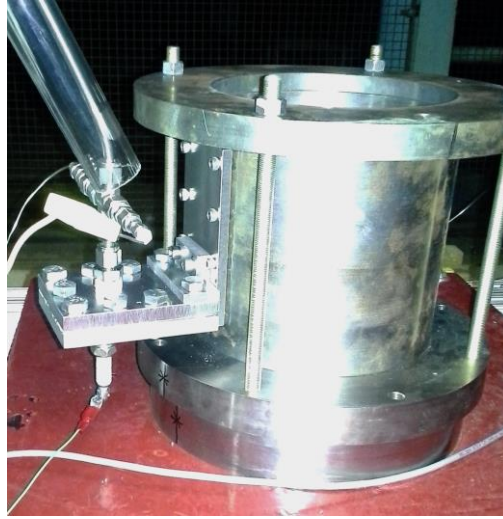


Figure 37. Close-up of the premixed injector connected in the horizontal configuration to the RDE host

understand if the RDE detonation flashback was affected by the orientation of the feed slot. Ion probes monitored the host detonation engine for detonation wave speeds and the test injector for signs of flashback.

2.1.3. Instrumentation

For the PDE test section, temperature and pressure were monitored at a tee immediately before the mixture entered the feed slot. The mixture entered the feed slot through a port in one plate. The opposing plate had a flashback sensor mounted in a similar port located coaxially to the mixture inlet port. Initially, only an exposed bead K-type thermocouple was used as a flashback sensor, but it was replaced with an ion probe. The response time of the thermocouple during flashback was hundredths of a second and could not be separated from potential noise during a test event.

Subsequent tests with the RDE injector assembly included an ion probe at the mixture entry point into the test section and an exposed bead K-type thermocouple and

pressure transducer located 6 cm upstream. All measurements from the RDE test section were time-synchronized and recorded for post-processing.

2.1.4. Uncertainty

Uncertainty in the measurements was tracked for all key measurements. The slot height was measured with a feeler gauge after the slot injectors were assembled, providing an uncertainty of 0.025 mm. Pressure and temperature measurements of the air, fuel, and mixture provided a statistical variation that was summed in quadrature with the instrument bias to obtain the total uncertainty plotted in error bars for mass flow rate and equivalence ratios. A complete derivation of the error formulae for mass flow rate, equivalence ratios, velocity gradients, and velocity measurements from video are included in Appendix II. The complex equations and fluid property models used to estimate the velocity gradient, theoretical quenching distance, and flame speed measurements did not permit analytic formulae to compute the uncertainty. Instead, a perturbation approach using the 2σ distribution of temperature and pressure variance was used. In this method, the experimental deviation from the mean of each signal was independently added to the mean value and the desired property was calculated. The variation of the property using the perturbed measurement was then summed in quadrature to generate the uncertainty of precision in the measurement. The models for fluid properties was assumed to be exact and not included in the error bars since they affect all the measurements identically, create a calculation bias, and this study was focused on identifying general trends. Thermocouples provided the noisiest data collected and uncertainties tended to range from one to five percent. Generally the uncertainty of

pressure sensors was less than two percent, mass flow rates for fuel and oxidizer were between three and five percent, total mass flow rates were five to seven percent, and equivalence ratios were six to eight percent.

2.2. Test Methodology

Results for each test condition were captured using multiple detonation events. Typically, 30 detonations would occur within a three second window for the PDE test section. The RDE host was operated continuously for 0.5 to 1.0 seconds, allowing several approximately 1000 cycles. A binomial distribution may be used (133, pp. 65-70) by assessing the passage of the host detonation, either with a success (no flashback), or a failure (flashback). For zero flashback events in a sample of 30 detonation events and a confidence level of 95%, the binomial theorem states that the injector configuration will arrest flashback at on at least 90% of all detonations. When zero flashback events occurred within the 1000 samples from the RDE host, the prediction improved to a minimum 99% reliability that flashback will be arrested with a 99.9% confidence level. The sensors were monitored for any indication that a combustion front had reached the feed system. For test conditions that were on the border between preventing and allowing flashback, flashback was found to occur inconsistently. Even if all the control variables were held constant within a given test, one detonation event might have led to flashback while another did not, highlighting the stochastic nature of detonation and identifying the need to push for high confidence and repeatability when using the binomial distribution (118, pp. 65-70). Ion probe data indicated that separate tests at approximately the same flow conditions showed flashback occurring with slightly different frequencies.

Therefore, if ion probe or thermocouple data showed indications of flashback occurred on any single detonation event within the test period for either the PDE or the RDE, then the test condition was designated as “Flashback”. When test conditions had no flashback indicators associated with any detonation event, the conditions were designated “No Flashback.” If multiple sensors were available and showed conflicting indications, such as a pressure rise without ion probe or thermocouple indications, then the conditions were designated “Inconclusive.” When flashback indications occurred while the mass flow rates in the injector were changing due to sequenced opening and closing of valves, the conditions were also designated “Inconclusive.”

For both the PDE and the RDE injectors, slot height was incrementally varied using U-shims until a boundary between flashback and non-flashback events could be established, and then slot length was incrementally shortened until a second flashback boundary could be found. It will be shown in sections 3.1.2 and 3.2.2 that variations in mass flow rates resulted in multiple flashback or no-flashback results at the same combination of slot height and length, so data were post-processed to generate estimates of velocity gradients.

3. Results

Overall injector configurations were found which prevented flashback from reaching the mixing region. Long narrow feed slots provided the best protection against flashback. If the separation between plates was too great, flashback occurred for several passing detonation events within a test condition. As the slot height became narrower, the prevalence of flashback decreased, but higher feed pressures were required to maintain

similar mass flow rates. Reduction in slot length was possible with a reduction in slot heights. Shorter slot lengths also reduced the required feed pressure for equivalent mass flows. When trading off slot height vs slot length, reducing slot height to allow reduced slot length always increased the overall feed pressure.

3.1. Premixed Injector in a PDE Host

The exploratory study using a premixed injector in a PDE host provided a quick method to evaluate if a long narrow slot would successfully arrest flashback into a premixed plenum. The rapid reconfiguration of the slot height, width, and length allowed for multiple test conditions to be tested in a short time period. The primary parameters of interest for this test were slot height and slot length. A visualization effort allowed the author to identify that the flashback was moving at the speed of sound through the slot. Height and length trade-space indicated that construction and operation of a premixed RDE was possible and provided a relationship for sizing the slot for hydrogen-air. Post processing identified that the flow conditions could be adjusted for the detonation cycle that would allow use of current burner stability diagrams.

3.1.1. The Speed of Flashback

A piece of polycarbonate replaced one of the steel plates on the PDE test section to visualize the flashback propagation. A color camera operating at 5,000 frames per second was positioned to optically record the flashback phenomenon. No similar modification was made for the RDE system. Figure 38 and Figure 39 show representative examples of quenching and flashback. In Figure 38, the combustion entered into the feed slot at Frame c, but was quenched by Frame f, thus resulting in a “no-flashback” event.

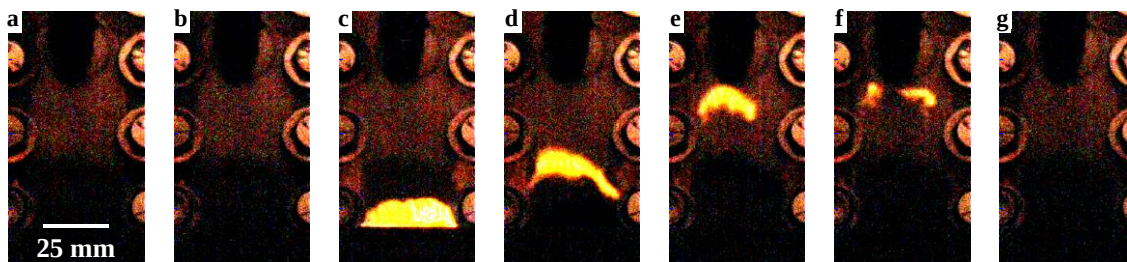


Figure 38. Flame quenching in a narrow premixed feed channel

However, Figure 39 indicates a sequence where the combustion propagated the length of the channel unquenched, entered the premixed supply in Frame g, and was considered a “flashback” event.

The sequence shown in Figure 39 was for an ethylene-air premixture at an equivalence ratio of 1.14, flowing at 0.0075 kg/s through a 3.8 cm x 7.9 cm x .035 cm slot. The sequence was collected at 5,000 fps with an integration time of 1/20,000 sec. The images were collected from a top view of the injector test section, with the premixture flowing from the inlet pipe at the top of the image into the detonation tube connected at the bottom of each image. The last 1.27 cm at the bottom of each frame was hidden by the mounting receptacle on the PDE tube. Flame speed measurements were

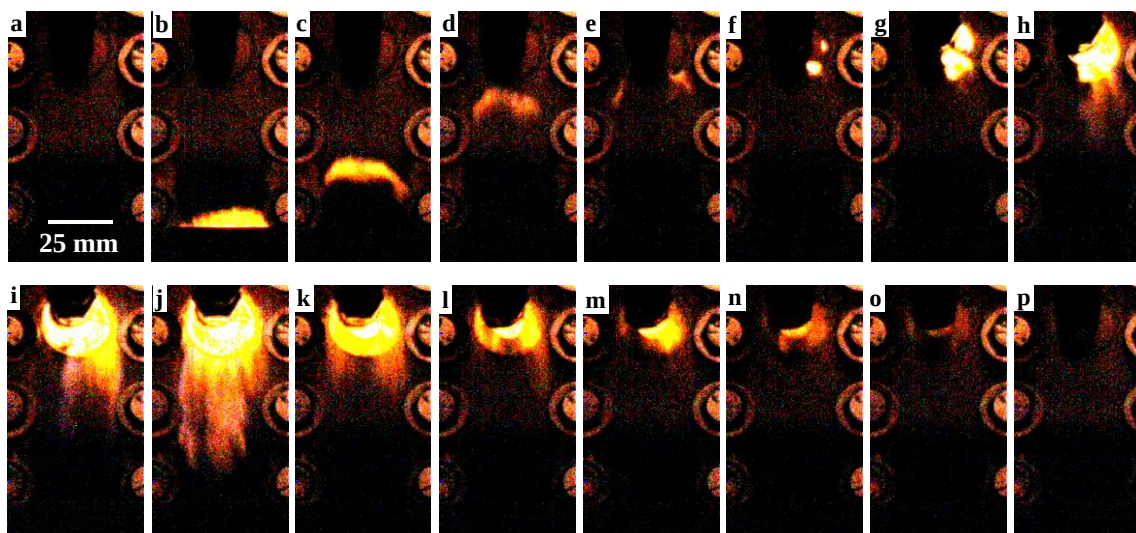


Figure 39. Flashback occurring in a narrow premixed feed channel

calculated from the video showing the combustion event moving into the feed system. In Frames b through e, the combustion event was moving at 130 m/s as calculated using the flame front movement between the frames. Cool reactant flows prior to the detonation event were calculated to be moving through the slot at 190 m/s based on upstream stagnation pressures, temperatures, and mass flow rates. Combining these two velocities the flame speed was calculated at 320 m/s relative to the reactant flow, or approximately the speed of sound in the cool reactants. This is a much higher flame speed than would normally be computed for ethylene air and required adjustments made in flame stability formulae as described in Section 3.2.3 of this chapter.

Ion probe data and pressure measurements, shown in Figure 40, were collected during the flashback event of Figure 39. The approximate time location of each photo is indicated in the plot. The combined figures showed that ion probe data was directly correlated to combustion. Combustion was clearly seen in the region of the ion probe when the corresponding probe data, shown in Figure 40, indicated ions in the gases. Mixture flow stagnation was probable when the static pressure at the injector exit rose

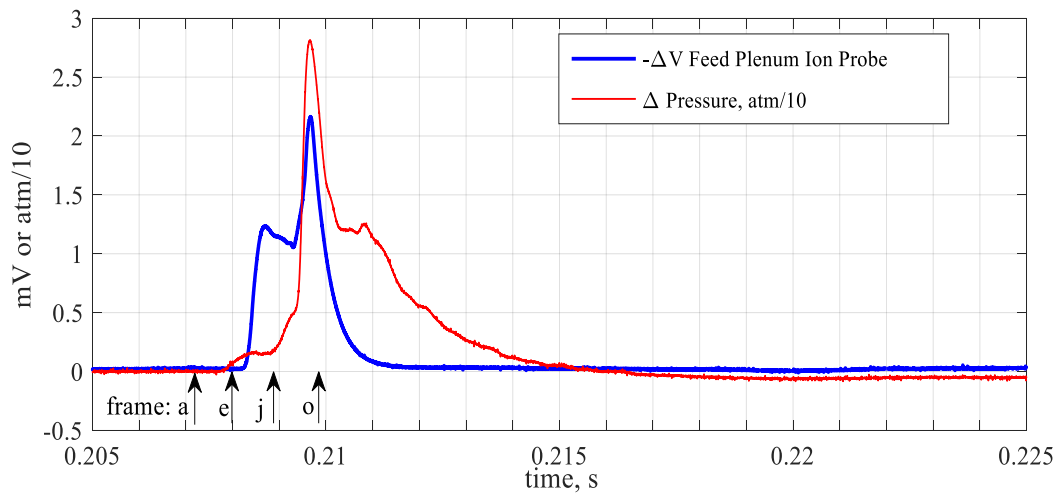


Figure 40. Pressure and ion probe data from a flashback into ethylene-air premixture

above the stagnation pressure of the injector flow. The ion probe data and pressure trace in Figure 40 indicated that a pressure rise was communicated to the mixing plenum at approximately the same time as combustion front and about two milliseconds after the detonation wave passed the test section. The chronologic sequence of indications in the ion probe and pressure data indicated that the combustion was associated with phenomenon moving at or near the speed of sound (approximately 340 m/s) relative to the cool reactants. Based on the chronologic sensor traces and video imagery evidence, adjustments to the velocity gradient using Equation 46 should use the observed flame speed, S_{obs} , calculated with Equation 47 so that the bulk flow velocity, $\bar{u}_{pl}$, is subtracted from the speed of sound in the cool reactants, a , to estimate the observed flame speed through the premixed detonation feed system in the laboratory frame of reference.

3.1.2. The Relation between Slot Height, Slot Length, and Quenching

Feed slot height was the principal parameter that was varied during the PDE hosted experiments. Feed slot length was the secondary variable parameter. A subset of

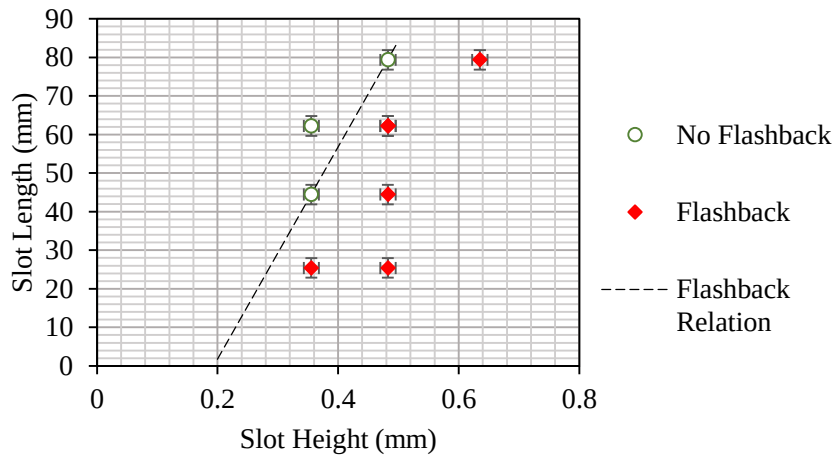


Figure 41. Flashback indication for premixed ethylene-air in slot of varying heights and lengths showing that a narrower channel allows for a quicker termination of flashback

the results in Figure 41 indicated that a shorter slot length could be used when the slot height was reduced. All the data plotted were ethylene-air mixtures flowing at approximately 0.006 kg/s, an equivalence ratio of approximately 1.1, and flowed through a 2.6 cm wide gap. A linear fit of the no-flashback slot dimensions of 0.35 mm by 45 mm and 0.48 mm by 80 mm produces a relation between the necessary feed slot dimensions:

$$l = 275h - 53.3 \quad (51)$$

where l is the slot length in mm, h is the slot height in mm, and the flow conditions are as described above into a pulsed detonation tube. Variation in mixture mass flow rates, equivalence ratios, or detonation profiles at the exit of the feed system, will likely change the relationship between the required slot length and slot height needed to halt detonation.

Figure 42 illustrated the relationship between slot length, height, and feed pressure. The mass flow rate for this data set was held relatively constant at 0.006 kg/s with an equivalence ratio of $\phi \sim 1.08$. The feed pressure followed the trends of friction flow, and feed pressure increased when slot height decreased from 0.48 mm to 0.36 mm

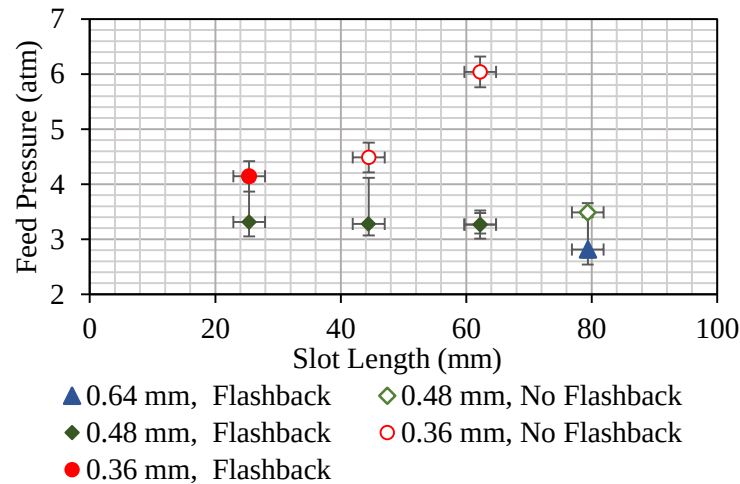


Figure 42. Mixture pressure, slot length, slot height, and flashback indication for ethylene-air showing that narrower slots require higher feed pressure and arrest flashback more quickly

or when slot length increased. However, flashback was still arrested in the 0.48 mm channel when the slot was just over 76 mm long. The ability to arrest flashback in a wider slot with lower feed pressure indicated that the increased back-pressure in the system was not the sole contributor to the quicker flashback arrest in a narrower slot.

3.1.3. Adjusted Velocity Gradient Comparison with Published Blowoff and Flashback Limits

The boundary layer velocity gradients were calculated assuming steady state flow conditions at the entrance of the feed slot and were compared in Figure 43 to the published stability limits (27). Two issues with this comparison are 1) the current experimental flashback conditions were at much higher pressure and velocity than the

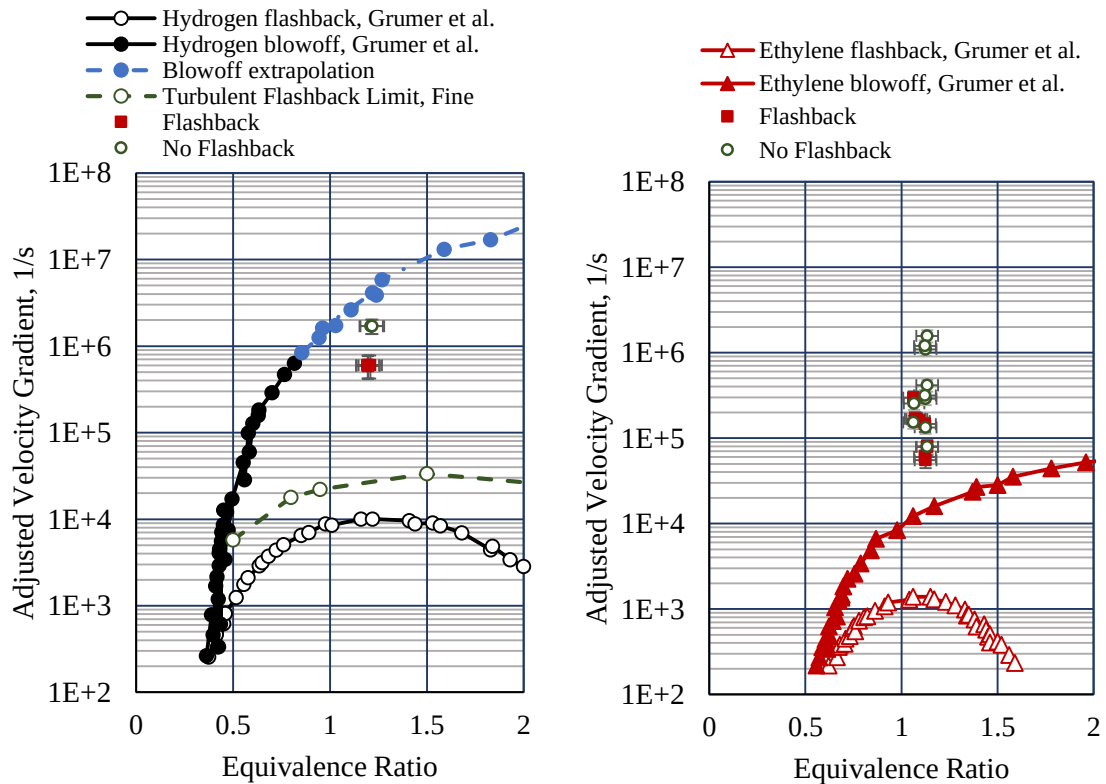


Figure 43. Adjusted gradient comparison with published premixed flame stability limits from Grumer et al. (30)

published data, and 2) the current experimental velocity gradients were estimated from the time averaged flow conditions established by flow metering several meters upstream of the mixing tee and injector instead of the transient pressure spike conditions generated by the detonation wave as it moved past the feed slot. Each problem was addressed separately.

The data from Grumer et al. (27, p. 1) represent premixtures at room temperature flowing through tubes into a room at approximately 1 atm pressure with flame speeds measured on the order of cm/s. The unadjusted velocity gradients in the detonation injector test sections were collected from flows that were 3 atm to 12 atm, and flashback was seen to occur at hundreds of meters per second as described in Section 4.1.1. Experimental velocity gradient data plotted in Figure 43 were adjusted with Equation 46. This adjusted the velocity gradient down by 3 to 4 orders of magnitude. The reference quenching distance and laminar flame speed used in the adjustment were calculated at 1 atm and 300 K. Still, many of the flashback data points lie above the reference flashback limits, a trend most notable in the ethylene-air data. One possible explanation for the discrepancies is that the adjusted velocity did not account for time-varying changes in the flow as the pressure wave penetrates into the feed slot. Another possible explanation for the large ethylene discrepancy is that during stagnation of the feed system during the PDE blowdown, the PDE may have been forcing partially-reacted hydrogen-air mixture into the premixed feed.

Using the feed slot entrance pressure and temperature provided the most conservative estimate for the flashback conditions during the PDE operation. Fanno flow dominated the premixed feed so the pressure was highest and the velocity lowest at the

entrance of the feed slot. Conversely, a pressure wave arriving with a flashback event slowed the mixture so that the calculated velocity was higher and the measured pressure lower than the actual flashback conditions, and the calculated velocity gradient was higher than the actual gradient during the transient flashback. In both cases, using the plenum feed conditions resulted in the most conservative empirically-based estimate of where flashback would occur in the premixed RDE. No measurement of the transient pressure spike was attempted since this effort was originally intended as an exploratory study to establish viability of this premixed feed approach.

3.2. Premixed Injector Hosted by an RDE

The exploratory study with the PDE hosted injector showed a detonation flashback could be arrested in a long narrow slot, and the success led to the construction of an injector that could be inserted into an RDE host for a characterization of flashback arrest. The slot height and length were again varied to build a relationship describing slot combinations that arrested flashback. The results highlighted the risk of using hydrogen-air mixtures which in turn influenced the decision to use ethylene as the fuel for the premixed RDE. The velocity gradients of the mixture fed into the RDE host were calculated using the adjustments of Chapter II Section 6.3 and found to agree qualitatively with current flame stability diagrams. A new equation was developed from an assumed RDE cycle that related detonation channel refresh requirements to the slot length required to quench flashback. The adjusted burner stability, length-to-height flashback relationship, and feed-to-quench length relationship provided the characterizations needed to design a successful premixed RDE.

3.2.1. The Relationship between Feed Slot Height and Length in an RDE

Flashback in the RDE hosted injector when slot height and length were varied produced a different model than the PDE host. As shown in Figure 44 (a), no linear fit could be formed from the data as presented for hydrogen-air injection since flashback occurred for the same geometry as a no-flashback event for the slot geometry of 0.013 cm height by 1.3 cm length, and flashback was seen at every slot height greater than 0.013 cm. No satisfactory separation of the flow conditions could be found to separate the flashback events of the 0.013 cm by 1.3 cm geometry from the non-flashback events. For the data point collected in the 0.013 cm by 1.3 cm slot, the flashback occurred as three discrete events during the 0.6 seconds of RDE operation that sent an estimated 1000 detonations past the injector. When the binomial theorem is used (133, pp. 65-70), this ratio of 3 flashback events out of 1000 detonation cycles represents a low but unacceptable probability of flashback.

A model for ethylene-air flashback, slot height, and slot length was constructed, as shown in Figure 44. The relation is:

$$l = 45.082h + 1.4574 \quad (52)$$

(given here in millimeters rather than centimeters) where l is the slot length in millimeters, and h is the slot height in mm. This model assumed that the inconclusive test events were not flashback, and this assumption represented an inherent risk when using Equation 52 to design a premixed RDE since the length-to-height model line passed through a point that could not definitively be ruled a no-flashback event. Further, the inconclusive points at the slot length of 9.7 mm existed in a region where the slot

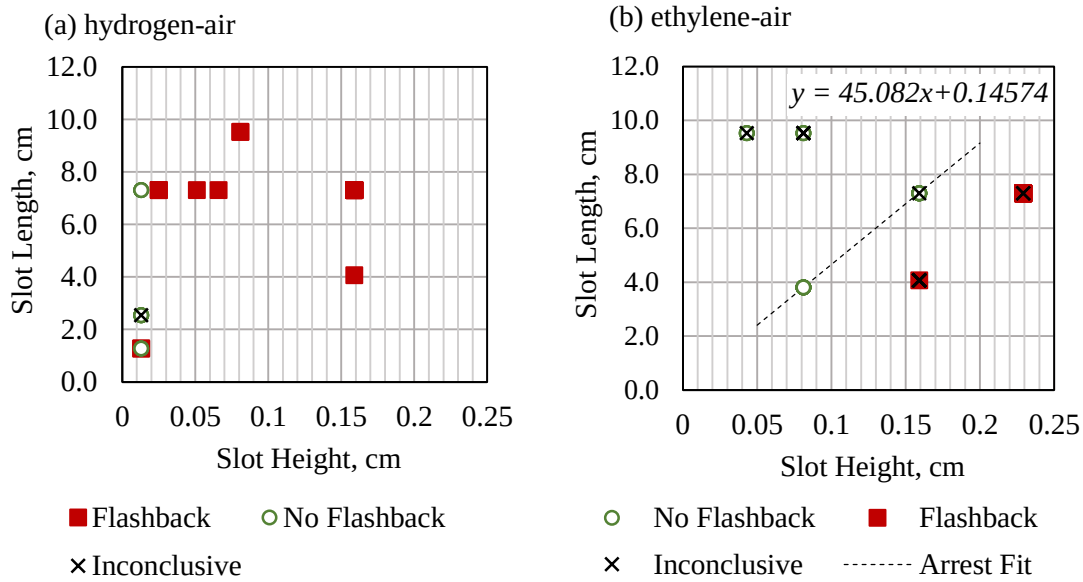


Figure 44. Relationship between slot height and length for arresting flashback in an RDE-hosted premixed injector

geometry was anticipated to arrest flashback based on the data points at 0.7 cm height and 3.95 cm length. If those points were actual flashback events, it would have indicated that the possibility of flashback for the long narrow feed slots always existed at an unacceptable level of probability. A decision was made to assume the risk of flashback and mitigate the presumed flashback effects with the design described in Chapter IV that could survive a flashback event.

Feed pressures varied with mass flow rate and slot height as shown in Figure 45. Unlike the PDE injector data set shown in Figure 42 of Section 3.1.2 of this chapter, mass flow rates were allowed to vary for this data set. The long narrow slots as wide as 1.5 mm were so successful at arresting flashback that minimal modification of slot length was performed. The resulting data set does not allow the grouping sets of data by slot height and slot length as was done in Figure 42. Consequently, the pressure reduction with

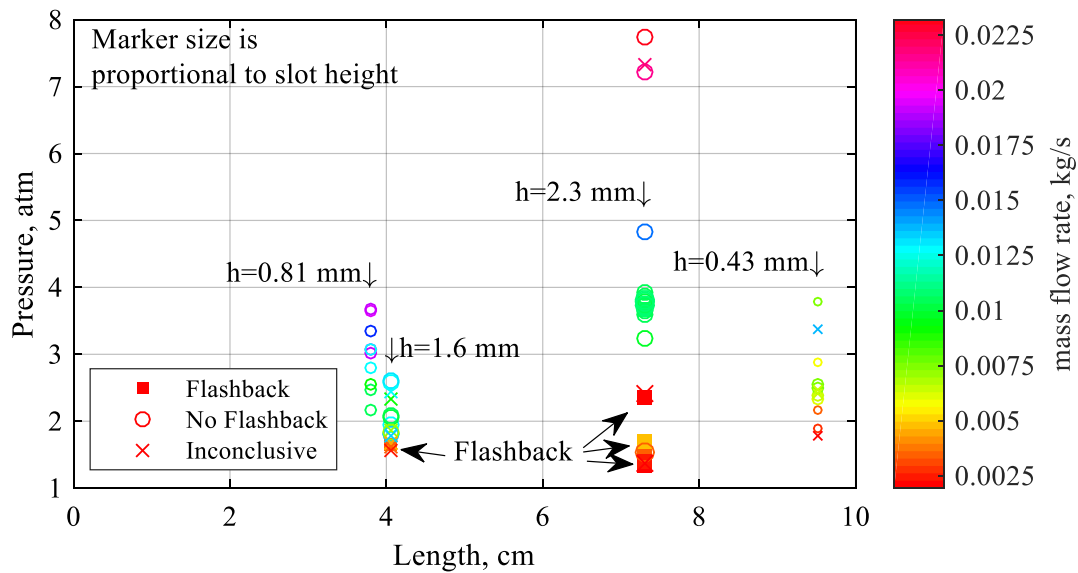


Figure 45. Variation of ethylene-air injector feed pressure with slot length, mass flow rate, and slot height

shorter slot length is not as apparent. Pressure was seen to rise with both decreased slot height and increased slot length. This matched trends described by the compressible friction flow equations (33), and the trends seen in the PDE injector rig were assumed to still be present. Generally the plot of Figure 45 indicated that flashback occurred at the largest slot heights when mass flow rates were very low, and that it was possible to arrest flashback with moderate feed pressures.

3.2.2. Adjusted Velocity Gradient Comparison with Published Flashback and Blowoff Limits

The boundary layer velocity gradients at the entrance of the feed slot were compared to the published stability limits (30) for flashback in Figure 46. In the same manner as the PDE hosted results presented in Section 3.1.3, the RDE hosted results face two issues; 1) the current experimental flashback conditions were at much higher

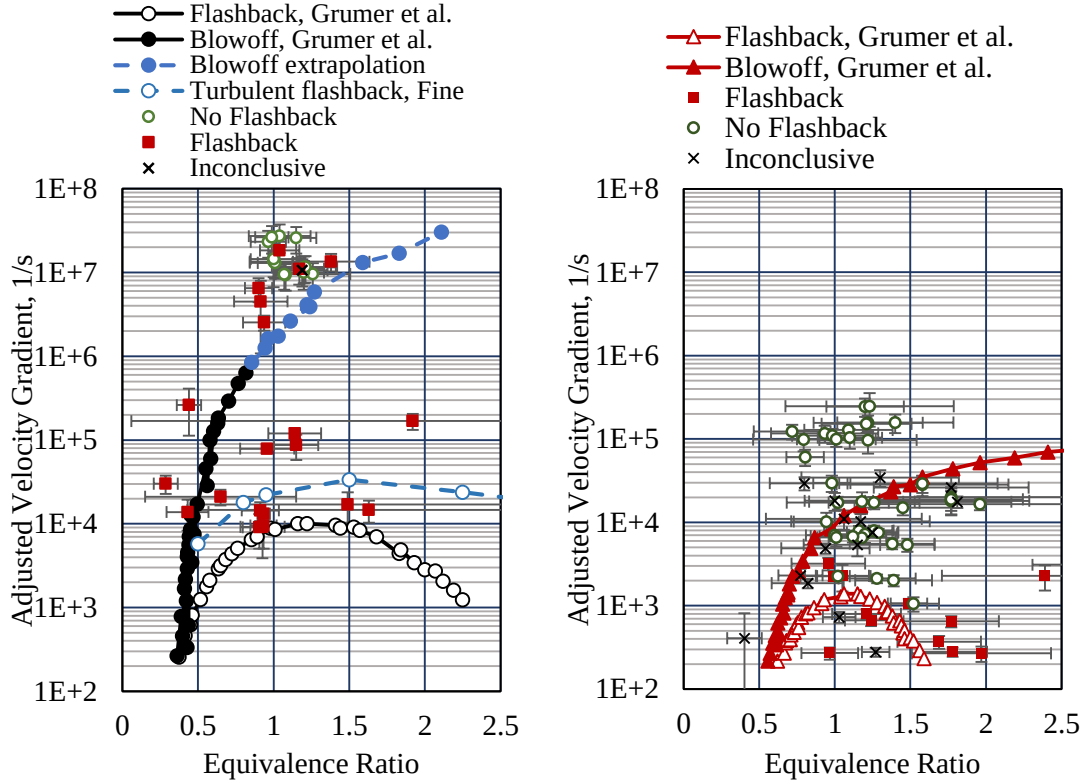


Figure 46. Injector adjusted velocity gradients for hydrogen-air (left) and ethylene-air (right) premixture flowing into an RDE host and compared with historical data

pressure and velocity than the published data, and 2) the current experimental velocity gradients were estimated from the time averaged flow conditions instead of the transient pressure spike conditions generated by the detonation wave as it moved past the feed slot. Each problem was addressed by adjusting the velocity gradient as discussed in Section 3.1.3 of this chapter and Section 6.3 of Chapter 2.

Each experimental velocity gradient datum plotted in Figure 46 was adjusted using Equation 46. This reduced the unadjusted velocity gradient by 3 to 4 orders of magnitude and was more successful in describing flashback from the RDE host than from the PDE hosted results in Section 3.1.3. Still, many of the flashback data points continued to lie above the reference flashback limits. As with the PDE hosted results, using the steady state feed conditions to calculate the adjusted velocity gradients of Figure 46 did

not account for time-varying changes in the flow as the pressure wave penetrated into the feed slot. Using the feed slot entrance pressure and temperature provided the most conservative estimate for the flashback conditions during RDE operation, as described in Section 3.1.3 of this chapter. No measurement of the transient pressure spike was attempted since this effort was originally intended as an exploratory study to establish viability of this premixed feed approach. Large pressure spikes from the RDE detonation were observed in the feed systems when flashback occurred. When the host RDE was operating, the 1 kHz pressure measurements appeared to be constant, while a high-speed pressure sensor collected feed pressure fluctuations occurring at approximately twice the frequency of those in the RDE. The pressure waves from the rotating detonation flowing into the slot momentarily slowed the out-flowing reactants, and the additional pressure rise undoubtedly reduced the quenching distance within the physical span of the pressure wave. Using the premixed feed flow conditions to calculate the velocity gradient imperfectly captured the time-variance of the flashback conditions but allowed characterization of the design space with respect to variables that were important to implementation: mass flow rates, equivalence ratios and feed pressures. Additionally, in an RDE, the constant flow of pressure waves into the feed system causes the feed system pressure to increase, so using the steady-state conditions from an RDE host captured the detonation channel influence on the velocity gradient better than the PDE host.

Orientation of the slot injector was changed from horizontal to vertical. The ethylene-air flashback results shown in Figure 46 were sorted by injector orientation in Figure 47 and show very little overlap between the two slot orientations. The vertical orientation operated with higher adjusted velocity gradients than the horizontal

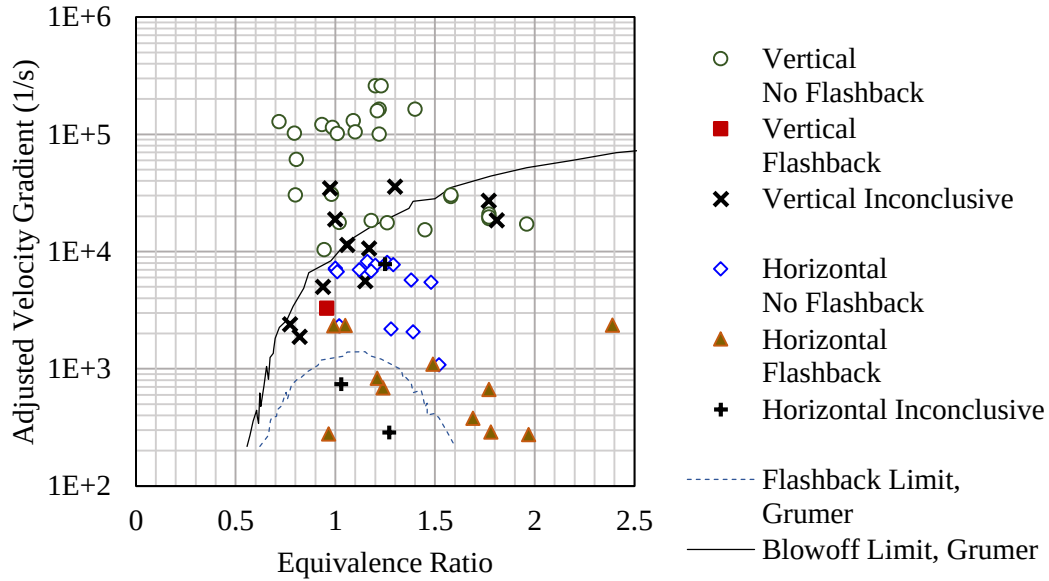


Figure 47. Distribution of the flashback and no-flashback results separated by injector orientation in the RDE Host

orientation. The confirmed flashback data points for the vertical orientation were at the lower range of the vertical orientation's velocity gradient and bordered the upper range of the horizontal orientation's flashback. The many inconclusive data were a result of a flashback indication on one or more sensors during startup or shutdown while mass flow rates were changing, and the reported velocity gradient is a conservative estimate based on the steady state run conditions. Flashback indications at startup and shutdown were more prevalent with a vertical orientation than with the horizontal orientation and were probably due to a varying pressure profile at the exit as described in the RDE detonation channel data of Rankin et al. (23). Few conclusions may be drawn from the data regarding the influence of slot orientation on arresting flashback since they had so little overlap. Other conclusions in this chapter were made assuming that the feed slot orientation was not a significant factor.

A noticeable difference between the velocity gradients where the PDE hosted injector and the RDE hosted injector arrested flashback may be seen by comparing Figure 43 and Figure 46. The difference in the velocity gradient relative to the flashback limits may be due to the differences in the detonation cycles. The RDE detonation cycle (21) involves a large pressure spike associated with the detonation wave, as shown in an idealized plot in Figure 48. The pressure spike is followed by a continuous expansion which is halted when the detonation front returns. A pressure time history of several cycles looks like a saw edge. The gases in a PDE, on the other hand, are restricted in the tube until the detonation wave has traversed the entire length; then the expansion wave initiates at the back of the tube and moves forward. The result is that the premixed injector inserted into the PDE host sees a much longer period of high pressure than the injector inserted into an RDE host. This allows a longer period in which the pressure can create a flow reversal and push mass into the feed slot.

3.2.3. Comparison of Theoretical Quench Distance and Slot Height

To determine the influence of thermal quenching on the probability of flashback, theoretical quenching distances were compared to the premixed feed slot heights in

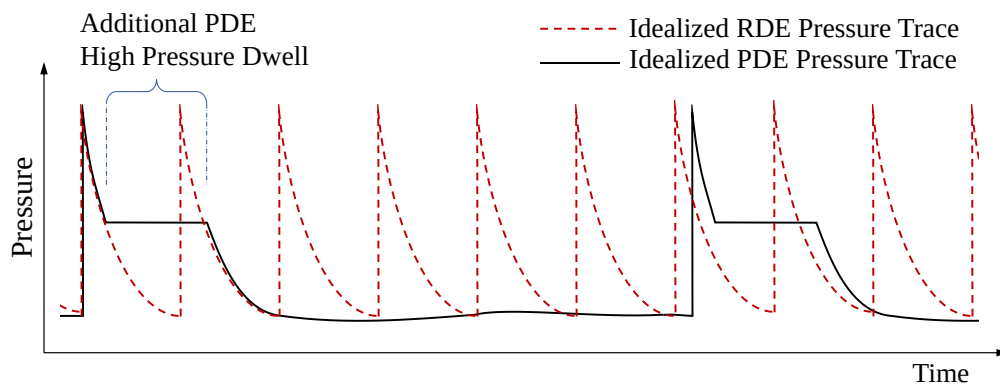


Figure 48. Idealized pressure trace of a PDE and an RDE highlighting the additional dwell at high pressure of a PDE

Figure 49. This plot includes data from the ethylene-air and the hydrogen-air mixtures injected into the RDE host. The black diagonal line separates the plot into two sections and represents where the experimental slot height exactly matches the theoretical quenching distance for the flow conditions at the entrance of the feed slot. Mixtures for data points plotted above the black line flowed through a slot whose height was greater than the theoretical quenching distance. In this upper region, the flow must have been moving fast enough to push back the combustion front everywhere except within half the quenching distance from the wall of the slot. Below the black line, the theoretical quenching distance was larger than the slot and no flashback should ever be observed. Quenching distances calculated using the mixture feed flow conditions were conservative for both the flashback and no-flashback data points for the same reasons described in the velocity gradient description above.

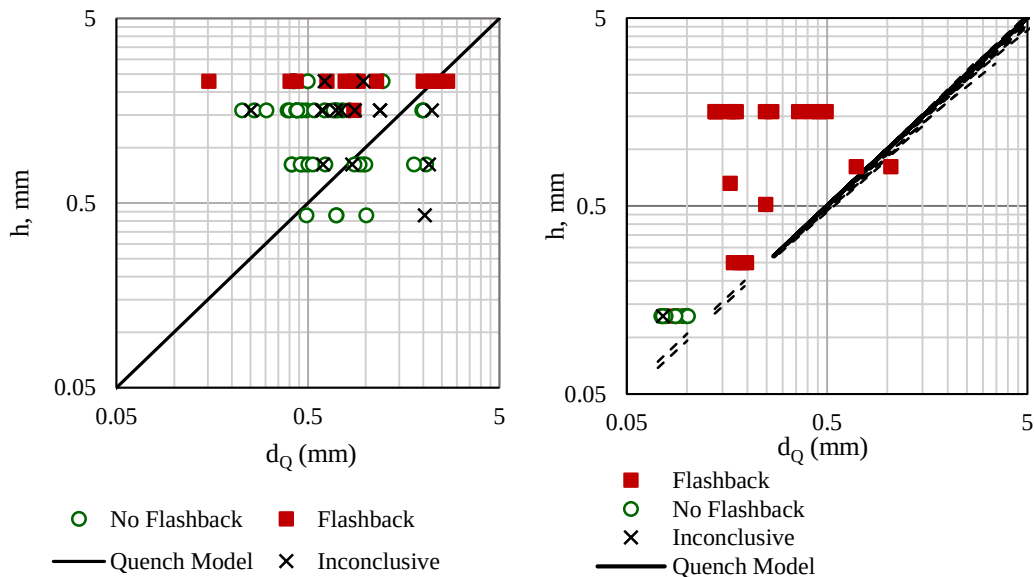


Figure 49. Comparison of slot height, h , to the theoretical quenching distance, d_Q , calculated with the average feed pressure for ethylene-air (left) and hydrogen-air (right) in the RDE hosted injector

All of the experimental slot heights, except one, were larger than the theoretical quenching distances for hydrogen-air test conditions and appear above the theory-experiment matching line. The presence of no-flashback data above the theory-experiment matching line indicated that quenching theory does not fully describe how to arrest flashback. Further, the single test point where the theoretical quenching distance was larger than the experimental failed to halt flashback, and showed that flashback would only be halted for hydrogen-air mixtures if flow conditions created an extremely high velocity gradient. Counterintuitively, this would require increasing the feed pressure to levels that drive the theoretical quenching limits smaller than can reliably be manufactured using feed holes. A multiple slot geometry would allow the feed system to achieve increased mass flow at the minimum required velocity gradient without requiring additional feed pressurization. Slot injectors would also be easier to manufacture than multiple small holes.

As shown in Figure 49 for the ethylene-air mixtures, flashback was arrested in multiple feed conditions where the feed slots were larger than the predicted quenching distance, and some flashback data was collected in slots smaller than the theoretical quenching distance. This demonstrated that quenching theory was part of, but not the complete solution to flashback avoidance in ethylene-air mixtures.

If a design relies solely on the theoretical quenching distance to determine the feed system spacing, it must account for the quenching distance encountered in the detonation wave. Specifically, the feed system must have a sidewall spacing for the mixture flow that results in a data point below the theory-experiment matching line of Figure 49. With respect to the discussion in Section 3.1.2, it would be designing a system

with a slot length of 0. The resulting feed geometry holes for a hydrogen-air mixture would be so small that it could not be constructed. Figure 39 and Figure 40 showed that arresting flashback occurred over some finite distance, and that the distance varied with the channel height and feed pressure. These variations indicated that the narrow feed channel is changing the flashback wave in a manner that has yet to be determined rather than simply quenching the combustion reaction.

3.2.4. Cycle Timeline Considerations

The ability to vary the height of the feed slot creates a trade space that affects feed pressure, quenching times, and refill height. For equivalent flow rates, a longer gap requires a higher feed pressure. Successful quenching in a shorter slot length indicates a faster quench. The trade between feed slot height and length is constrained by the competing needs of operating the machinery at low pressures where quenching occurs quickly and the need to flow sufficient quantities of uncombusted reactants before the detonation wave arrives to sustain the detonation cycle. If the total RDE cycle were divided into small segments, shown in Figure 50, it could be seen that the flashback must have been arrested in a fraction of the total cycle's time.

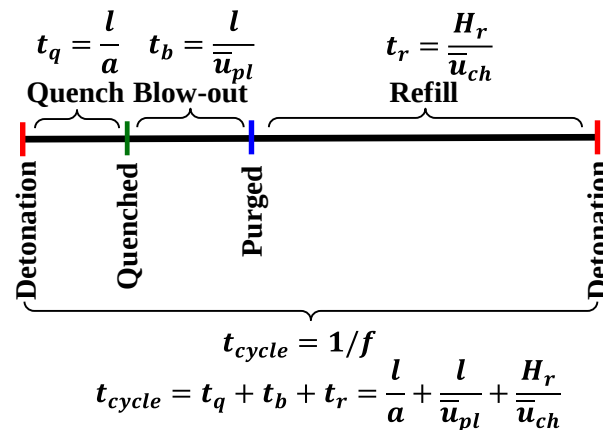


Figure 50. Diagram of the detonation cycle timeline

For a 15 cm RDE operating with a detonation cycle frequency of 3800 Hz, there are only 263 μs per cycle. If a liberal estimate of the fill time is $\frac{3}{4}$ of the cycle time, then only 66 μs are available for the quenching and combustion product blow-out. Consider the flashback event recorded in Figure 39: the flow was estimated to be moving at 190 m/s during the 5 frames it took the flame to travel from the detonation tube to the ion probe, and 1000 μs elapsed. That would be equivalent to starving the RDE of reactants during 3.8 detonation cycles thereby terminating the detonation wave. Recall that Figure 49 showed a reaction moving at approximately 130 m/s relative to the feed slot. Having assumed that the flashback should be quenched after approximately 60 μs to adequately support detonation would restrict the penetration distance into the slot of no more than 7.8 mm (0.30"). Blowing out the burned gases at 190 m/s would then take an additional 41 μs , using more than $\frac{1}{2}$ the cycle time. This example illustrates the relationship between the quenching problem and the RDE feed cycle. The total RDE cycle time can be expressed as:

$$t_{cycle} = \frac{1}{f} \quad (53)$$

where t_{cycle} is the time to complete one cycle, and f is the cycle frequency. The detonation wave speed is described as:

$$D = \frac{\pi f \bar{d}_{RDE}}{n} \quad (54)$$

where D is the detonation wave speed, f is the frequency of the detonation, $\bar{d}_{RDE}$ is the mean diameter of the detonation annulus, and n is the number of detonation waves.

The cycle time can also be broken into various times as discussed previously, and shown in Figure 50:

$$t_{cycle} = t_q + t_b + t_r + t_{ind} + t_c \quad (55)$$

where t_q is the time required to quench a flashback and may be a statistical average for a large sample size of cycles, t_b is the time required to push the burned gases back out of the feed channel, t_r is the time that fresh mixture is flowing into the detonation channel, t_{ind} is the induction time for the detonation, and t_c is the combustion time for the detonation. In this analysis, t_{ind} and t_c are assumed to be approximately zero so that a relationship for the fraction of time spent refilling τ_r , takes on the form:

$$\tau_r = \frac{t_r}{t_{cycle}} = \frac{t_r}{t_q + t_b + t_r} \quad (56)$$

The quenching and purge times are related to the geometry, mixture properties, and feed pressure. The example above calculated quenching time as:

$$t_q = \frac{l}{a} \quad (57)$$

where a is the speed of sound that was shown to be the approximate reaction velocity relative to the cold flow and l is the length required to quench the flashback (assumed to be the slot length). The purge time is calculated based on the cold flow velocity as

$$t_b = \frac{l}{\bar{u}_{pl}} \quad (58)$$

where $\bar{u}_{pl}$ is the bulk velocity of the unburned reactants and l is the length required to quench the flashback. The engineering design problem is to find what quenching length allows for re-fill without interruption in the RDE cycle.

It is anticipated that to sustain a premixed RDE, $\tau_r \geq 0.7$, but future experimentation may provide a better understanding. Substituting Equations 57 and 58 back into Equation 56 generates the relation:

$$\tau_r = \frac{t_r}{\frac{l}{\bar{u}_{pl}} + \frac{l}{a} + t_r} \quad (59)$$

Solving for minimum slot length to quench flashback gives:

$$l = \frac{t_r \left(\frac{1}{\tau_r} - \tau_r \right)}{\left(\frac{1}{\bar{u}_{pl}} + \frac{1}{a} \right)} \quad (60)$$

Substituting in the relations for refresh time, $t_r = \tau_r t_{cycle}$, and Mach number of the reactant flow in the plenum, $M_{pl} = \frac{\bar{u}_{pl}}{a}$, into Equation 60 yields:

$$l = \frac{t_{cycle}(1 - \tau_r^2)M_{pl}a}{(1 + M_{pl})} = \frac{(1 - \tau_r^2)M_{pl}a}{f(1 + M_{pl})} \quad (61)$$

where l is the feed slot length based on quenching, t_{cycle} is the cycle time of the rotating detonation, τ_r is the ratio of refill time to cycle time, M_{pl} is the Mach number based on the bulk velocity of the mixture in the plenum, a is the speed of sound in the mixture which approximates the speed of the combustion that must be quenched, and f is the frequency of the RDE detonation cycle. Equation 61 would be used in conjunction with Equation 52, which was described in Section 3.2.1 as the RDE host analog of Equation

51 in section 3.1.2 for the PDE host. Equations 51 and 52 allow the designer to determine the slot length and slot height combinations that will successfully support RDE operation. The next desired step was to obtain a relationship that facilitates prediction of slot height and length combinations for multiple operating conditions. This was similar to the problem faced by combustion research in the 1940s and 1950s that was solved when Lewis and Von Elbe (134) resolved flame stability differences with critical velocity gradient measurements and led to the flame stability diagrams of Grumer et al. (30).

4. Conclusions & Recommendations

This chapter fulfilled the requirements of Objective 1: “Discover the flow conditions that halt flashback into a premixed feed system exposed to a transient detonation.” The principles of traditional premixed burner stability and a method to adjust the curves to the detonation feed system using Equation 46 were identified to successfully describe the flow conditions that arrest flashback in a detonation engine feed system. Also, Equation 61 was derived to relate the detonation cycle requirements to the maximum quenching length that will support rotating detonation operation.

Objective 2, “Characterize the correlations between flashback in a premixed flow exposed to a transient detonation front and traditional burner stability parameters, such as: quenching distance and critical boundary layer velocity gradient as functions of the temperature, pressure, equivalence ratio, mass flow rate, and fuel,” was also fulfilled. The probability of flashback was measured and characterized in a slot injector with a statistical repeatability of 99% using a 99.9% confidence level. Equations 51 and 52 characterized the slot length-to-height requirements for the slot feed systems as shown in

the flashback measurements of Figure 41 and Figure 44 respectively. Equations 51 and 52 were demonstrated to correlate flashback to the published burner stability diagrams when Equation 46 was used to adjust the velocity gradient based on the feed conditions.

Deviations from the burner stability diagrams are attributed to conservative estimates based on feed conditions rather than measurements of a detonation generated pressure pulse that penetrates into the feed slot. The ability of the velocity gradient adjustment to predict whether a mixture will flashback or not was demonstrated with Figure 43 and Figure 46. The ability to use the traditional flame stability diagrams with the adjustment of Equation 46 informs the slot height design choice with a relationship between mass flow, pressure, and slot height in a manner unavailable from the arresting length-to-feed time relation of Equation 61 or the slot height-to-length relationships of Equations 51 and 52. Estimates for the detonation cycle pressure transients at the feed slot exit may come from non-premixed experimental data or from CFD results. The a priori knowledge of how the feed slot size, quantity, surface roughness, and entrance and exit geometry will influence feed pressures should be taken from standard textbooks on thermodynamics (39), incompressible (123,135) and compressible flow (33).

Feed systems for premixed detonation should employ quenching distances and feed slot lengths based on desired plenum feed conditions, the anticipated detonation cycle overpressure conditions, and the detonation cycle timing. Adjusting the theoretical quenching distances and boundary layer velocity gradients for detonation conditions was shown to successfully describe the conditions that arrest flashback, opening the opportunity for the design and operation of a premixed RDE.

Fuel selection for a premixed RDE should take into account the risk tolerance of the application. Hydrogen will require higher feed pressures than hydrocarbons due to the need to achieve higher velocity gradients. Also, a properly designed hydrogen feed system must arrest flashback quickly enough that the RDE cycle will continue without interruption. With these observations, ethylene-air mixtures were selected as the preferred fuel-oxidizer combination for a premixed RDE (28).

IV. Construction and Operation of a Premixed RDE

Based on the result of the premixed feed system study described in Chapter 3, a premixed RDE was successfully constructed, operated, and reported (28) at the 2016 AIAA SciTech Conference. The contents of that report have been copied here and amplified with additional data when possible. The construction and operation of the premixed RDE meets Objective 3 listed in Chapter 1: “Explore the ability of traditional burner stability design principles to effectively arrest flashback in a premixed rotating detonation engine.” Traditional stability design principles were found to adequately describe design criteria for a premixed RDE when adjusted for the detonation operating conditions, and no flashback has been seen in the current data set. Objective 4, “Experimentally characterize the operation of a premixed rotating detonation engine,” was met with the construction of an operating map that showed a more limited operating range when compared with non-premixed RDEs. Differences in wave speed were also found to disagree with wave speeds reported in CFD studies.

1. Background

A difference between the wave speed measured in current non-premixed RDEs and the theoretical Chapman-Jouguet detonation velocity was noted in experimental (19,81,103) studies. It was hypothesized that the velocity deficit was a result of poor fuel-oxidizer mixing within the mixing channel (1,19,101). It was further hypothesized that the operating maps of non-premixed RDE were constrained and defined by the geometries that promoted or inhibited rapid fuel-oxidizer mixing. Development and

successful operation of the premixed RDE allows the research community to test fundamental hypotheses regarding the fuel-air mixing effects in the operation of current RDE.

It is proposed that the fuel and air feed variations in the reviewed experiments (2,19,23,80,81,83) promote or inhibit mixing timescales, and that poor mixing inhibits the RDE operation. Premixing fuel and oxidizer removes the diffusive and turbulent mixing mechanism time delays from detonation experiments and represents the best possible mixing available. This ideally mixed system would establish a benchmark for basic research regarding the mixing effects in an RDE. The premixed RDE could also be used to test if the differences between CFD and non-premixed experimental wave speeds and specific thrust measurements are due to inaccurate assumptions regarding combustion chemistry and the influence of three-dimensional flow structures on detonation. To that end, implementation of the long narrow slot feed system geometries suggested by the preliminary design study, discussed in Chapter 3, and reported in (27), successfully overcame flashback hazards and allowed the first-ever successful operation of an air-breathing premixed RDE.

2. Methodology

An adjustable premixed RDE, shown in Figure 51 was constructed with a new premixed feed system that interfaced with the existing outerbody and centerbody hardware from the modular 15 cm radial outflow RDE described in Chapter II, Section 4.3.2.4. This new feed system, described in the following subsections, premixed fuel and oxidizer well upstream so that there was no mixing delay. Unlike non-premixed RDE, the

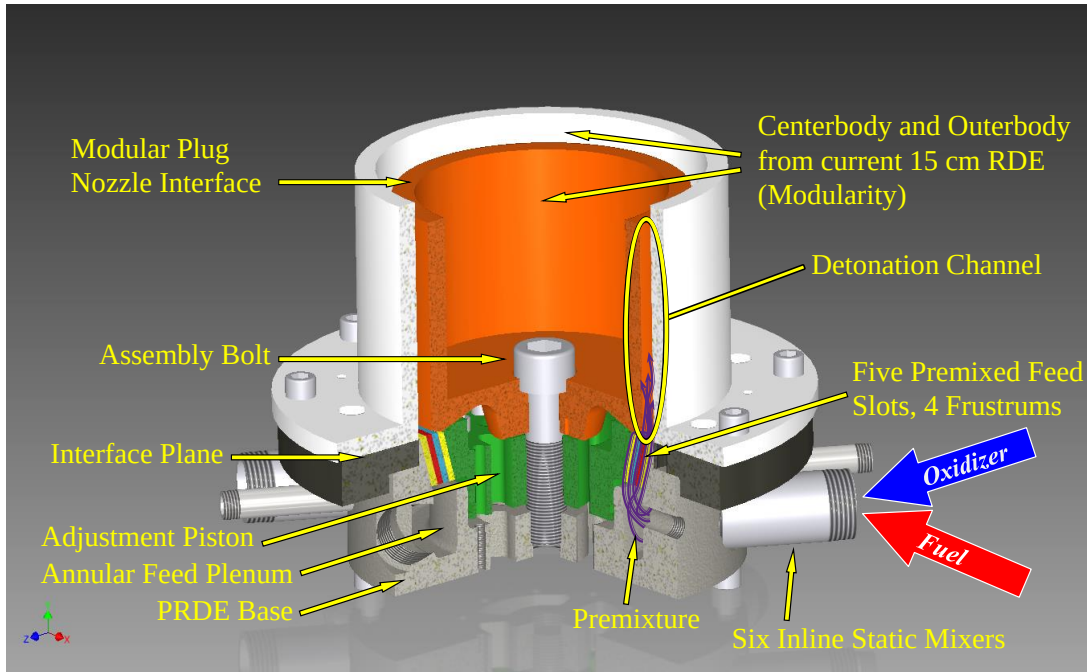


Figure 51. CAD model of an easily adjustable premixed RDE

premixed RDE provided an ideal fuel-oxidizer mixture that was ready to react immediately upon introduction into the detonation channel. It was assumed that if the detonation channel geometry affected premixed RDE operation in the same manner as the non-premixed RDE, then the geometry was more critical than mixing. Conversely, if the operation maps for analogous geometries changed for the premixed RDE compared with non-premixed RDE, then mixing effects were more critical.

2.1. Test Apparatus

The new premixed RDE design was constrained by safety concerns, reusability of existing hardware, and similarity with the intention of reducing experimental variability between premixed and non-premixed RDE.

2.1.1. Baseline RDE Design Parameters

The premixed RDE was designed with a dual focus of maintaining similarity with the non-premixed RDE and allowing flexibility with fuel selection. Although ethylene was ultimately selected, the design was driven primarily by the constraints of operating with a hydrogen-air mixture. The design envelope described in Table 4 is based off of the DERF's 15 cm modular non-premixed hardware, described in Chapter II Section 4.3.2.4, operating with a total mass flow through the system between 0.15 kg/s and 1.5 kg/s. Wave speed frequencies in the non-premixed RDE were observed between 700-1400 m/s for ethylene-air (82) and between 900 and 1800 m/s for hydrogen-air (23).

Table 4. Design parameters for premixed RDE

Parameter	Value	Units
Nominal detonation channel diameter	15	cm
Nominal detonation channel length	15	cm
Nominal detonation channel width	1-2.3	cm
Number of feed slots	1-5	
Slot length	25	mm
Slot height	0.5	mm
Radial spacing of slots	3.1	mm
Plenum feed pressure operational limit	≤ 6.8	atm
Theoretical quenching distance	≥ 0.25	mm
Minimum mass flow rate	0.15	kg/s
Maximum mass flow rate	1.5	kg/s
Fuel type	Ethylene or Hydrogen	
Equivalence ratio range	0.6-1.6	

2.1.2. Mixing Assembly

Premixing was accomplished by feeding fuel and oxidizer into the RDE base through six inline static mixers housed in 2.5 cm pipe. The coefficient of variance for the mixtures was estimated to be well below 0.5%. The oxidizer stream was metered far upstream with a single sonic nozzle, split into six feed lines, and combined with fuel at six separate mixing tees. Fuel was metered using precision flow orifices at each mixing

tee. The mixers were inserted into the premixed RDE base at 6 radial locations and equally spaced at 60° intervals. Each mixer fed tangentially into a common annular plenum, a design intended to circumferentially distribute the dynamic pressure more evenly than a direct radial inflow. The annular plenum opened upward to the feed plenum comprised of long narrow slots. The design of the feed slots will be described next.

2.1.3. Detailed Design of a Premixed RDE Feed System

Designing the feed system was a multi-step iterative process. First, the maximum arresting length that supported the desired detonation cycle was calculated using Equation 61. Second, the slot height that would guarantee flashback was arrested was calculated using the arresting length from the previous step and Equation 52. Finally, the slot geometry was evaluated against flashback gradients using the adjustment described by Equation 46. This methodology requires multiple assumptions guided by experience from non-premixed RDE and, as such, allows for future improvement through implementation of improved modeling of flow conditions that are currently assumed.

The maximum desirable quench distance, based on a refill to detonation cycle ratio of 0.75 was calculated at 19 mm using Equation 61. The solution point was illustrated in Figure 52 with lines that showed how independent variation of each assumption influenced the solution. This length was calculated using the assumptions that the maximum frequency would be 1800 m/s, the refill-to-cycle time ratio should be approximately 0.75, the Mach number in the feed plenum would be approximately 0.3, and the speed of sound in the mixture would be approximately 340 m/s. The quenching length of 19 mm represents the maximum length that the flashback should be allowed to

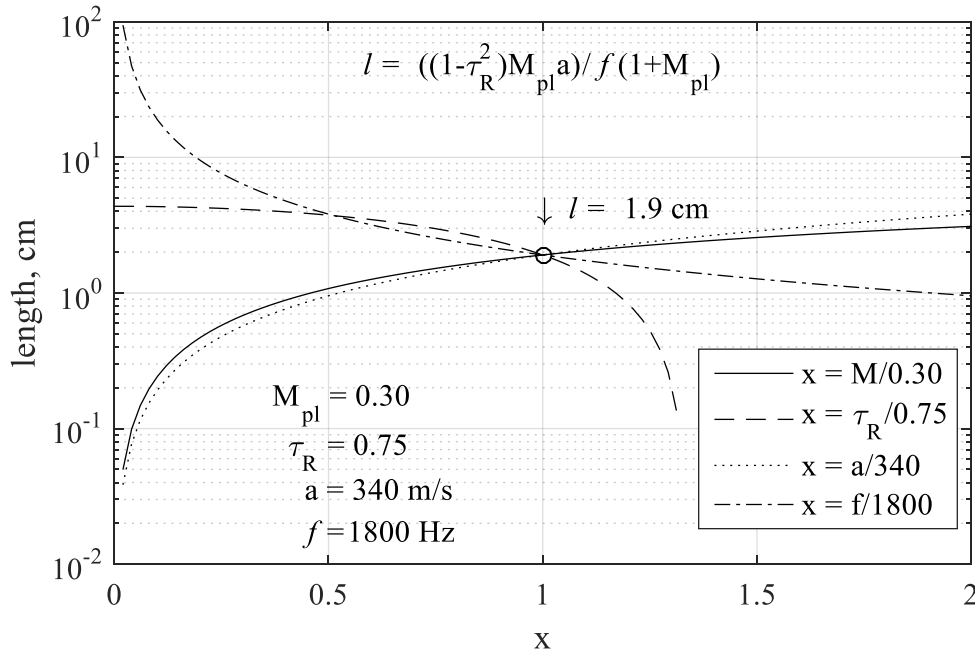


Figure 52. Length calculation using Equation 61 with the inputs shown in the lower left, lines representing the independent variation of single variables indicate the influence of that variable on the quenching length needed to support the assumed cycle

propagate if the RDE cycle is to be maintained with the assumptions listed above. Figure 52 plotted the design point using normalized variables. The independent variation lines should be used to identify if the design is conservative based on variation with that parameter. When the variations indicate that the flashback should be arrested in a shorter distance, the solution point will not support the new assumed cycle. However if the variation indicates that quenching can occur over a longer distance, the design point will arrest flashback within the required distance, and the design will be considered conservative. For example, if the cycle requires more than the assumed refresh, has a higher frequency, the mixture flow velocity decreases, or the mixture has a slower speed of sound then the slot length would need to be shorter to support the cycle and detonation may not be sustained. Similarly, a feed system designed to quench with 19 mm for the assumptions listed above will successfully quench when the Mach number in the plenum

increases, the mixture speed of sound is faster, the frequency decreases, or ratio of refresh to cycle time decreases. With the predicted maximum arresting length, the design process next calls for calculation of a channel height that would guarantee the flashback was quenched in this distance.

The relationship described in Chapter III, Equation 52, was solved for slot height, h , and evaluated at $l = 19 \text{ mm}$. The predicted slot height was 0.39 mm. Equation 52 represented a less conservative estimate than Equation 51 (which predicts a slot height of 0.26 mm) and was used since the pressure profile for the RDE host was more representative of the system being designed. An extrapolation of the height-to-length arresting model occurs when calculating slot height from either Equation 51 or 52, incurring risk due to uncertainty in a model built essentially upon two data points and an assumption of linearity. A conservative approach would be to use the narrower slot height as an initial starting point, but a slot 19 mm x 0.26 mm would drive feed pressures very high. Additionally, small errors in spacing affect mass flow through a narrower slot, increasing the risk of uneven flow into the channel.

To accommodate a possible mass flow rate of 1.2 kg/s and lower feed pressures, the number of feed slots for the premixed RDE design was increased from one to five. This increased the injector area to slot height ratio and lowered feed pressures. Additionally, since Equation 52 was tied to a hydrogen-air RDE operating at $\phi \approx 1.0$ between 0.45 kg/s and 0.8 kg/s, there was an inherent assumption that the detonation profile would be the same. A better understanding of the slot geometry was sought with the adjusted velocity gradient calculations.

Slot height evaluation involved calculation of the predicted adjusted velocity gradient with assumed values for mass flow rate, feed pressure, and equivalence ratio. This portion of the analysis was coded as the *DesignVelGradCalc* script found in Appendix V Section 2 because of the need to accurately model the flame speed, quenching distance, mixture viscosity, and velocity gradient calculations. Both the slot height and the mass flow rate were coded as a range of variables, resulting in Figure 53. After following the minimum desired flow rate of 0.2 kg/s line to the intersection of the blowoff gradient for the ethylene mixture, the minimum required slot height was read from the horizontal axis. The algorithm predicts that the initial design point of 0.39 mm slot height is conservative and that safe operation may be obtained with a slot height as large as 0.7 mm based on the conservative assumption that it requires 6.8 atm to feed 0.2 kg/s of an ethylene-air mixture at $\phi = 1.05$ through a 5-slot injector whose nominal diameters are 15 cm. This analysis makes the simple assumption that the feed pressure is 6.8 atm regardless of the feed slot total cross-sectional area. In practice, the feed pressure is a function of the feed slot design, and feed pressure is determined by the mass flow rate

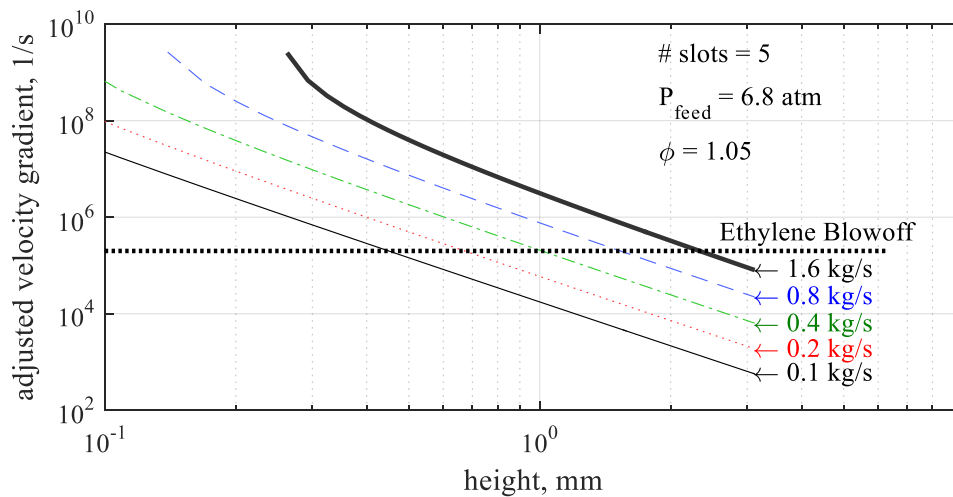


Figure 53. Adjusted velocity gradient predictions as a function of slot height

equations described in Appendix II Section 1 and the friction flow equations described in a compressible fluid text such as Anderson (33). Based on the testing described in Chapter II, the feed pressure was estimated to be less than 6.8 atm for the flow rate. The slot height of 0.39 mm generated as the initial design point from the first two steps of the design process is shown in Figure 53 to support a blow-off velocity gradient when adjusted for detonation conditions at all desired mass flow rates (0.1 kg/s to 1.2 kg/s).

The premixed RDE design included the ability to adjust the slot height through the use of shims as an engineering measure that mitigated the risk of selecting a slot height too large to arrest flashback or too narrow to achieve desired mass flow rate. Initially, a slot height of 0.25 mm was employed but quickly adjusted to 0.51 mm and eventually to 0.8 mm, where detonation operation was noted without flashback. An exploration of the trade space between slot height, feed pressure, and mass flow rate was not attempted. Instead, efforts focused on achieving detonation at higher mass flow rates.

Operational procedures limited plenum pressures to 6.8 atm so that during a flashback event the system and sensors would survive at their design point of 68 atm. No detailed analysis was performed for this RDE to evaluate if the feed system would allow adequate mass flow within the range of allowable pressures. Instead, rough estimates from the injection test work of Chapter III were used in the design phase. Before operating with fuel, air was forced through the system to obtain a calibration for the pressure loss through the feed system and establish safety limits for mass flow.

2.1.4. Premixed Feed / Flashback Arrestor Design

The premixed fuel and oxidizer flowed from the annular plenum described in Section 2.1.2 into the feed slots formed by stacking four truncated conical rings (hereafter referred to as ‘frustra’) sandwiched between the base and the slot adjustment piston. Figure 54 shows the assembled premixed RDE with the centerbody and outerbody removed, providing a top-view of the interface plane. The top of the frustra are visible as rings expanding concentrically outside the red gland seal (O-ring). The frustra created con-annular feed slots which expanded the flow laterally. A red gland seal sits atop the adjustment piston, secured by nine assembly bolts to the base. As described in Section 2.1.3 of this chapter, experimental parameterization indicated that the initial feed slot height of 0.39 mm could be increased to 0.51 mm and provide sufficient flashback arresting capability for these experiments. Spacing between the frustra was maintained through shimming with flat 1.0 mm x 0.5 mm stainless steel wire. Shims were spaced at 18° intervals, as shown in Figure 54 and Figure 55. Careful shim alignment achieved a

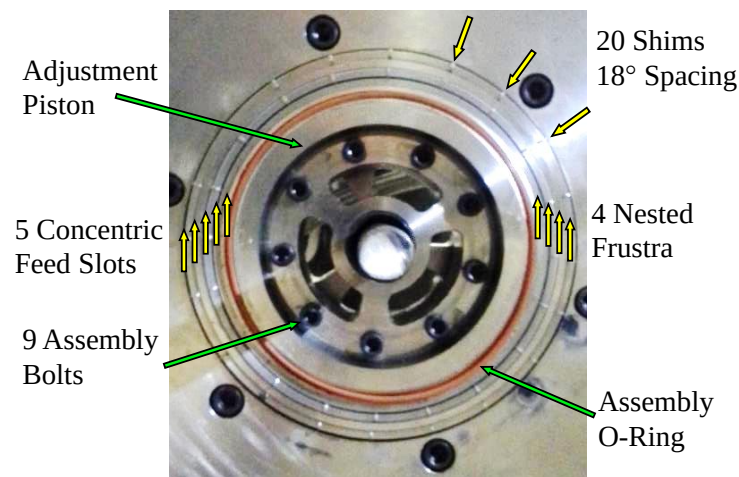


Figure 54. Interface plane of the premixed RDE showing shim spacing in the feed slots

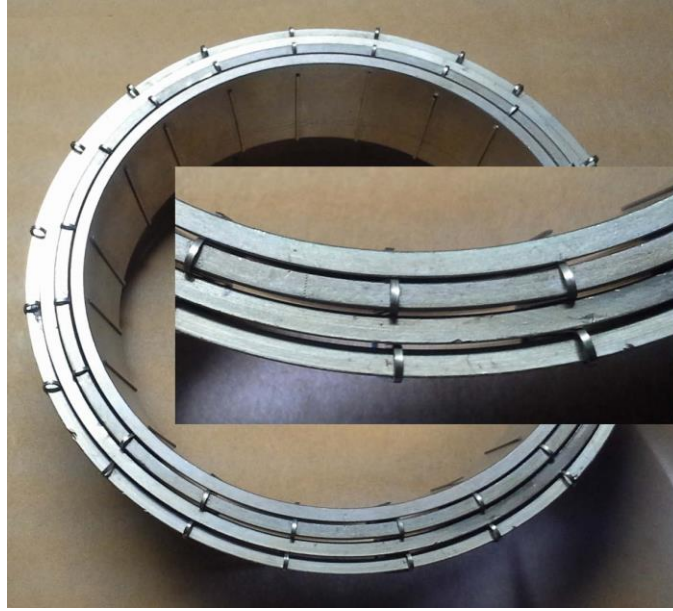


Figure 55. Photograph of assembled frustra stack with inset showing segmented con-annular slot

circumferentially uniform flow field into the detonation channel, a prerequisite for achieving continuous rotating detonation.

The premixed RDE was designed to support mass flow rates that were similar to those run in non-premixed RDE. Achieving mass flow rates of 1.5 kg/s with a maximum feed pressure of 6.8 atm drove the design to use at least five feed slots. Initial slot height and quantity was determined based on the desired mass flow rate and the slot height/feed pressure requirements seen in the companion study (27). As slot height increased, the nested frustrum stack expanded axially. The adjustment piston was designed to maintain a pressure seal during piston extension, thereby avoiding the need to manufacture new frustra. Each slot was approximately 45 cm in circumference and divided into 20 segments with the shims as shown in Figure 55. Flowing radially outward, the 20 feed slots expanded the gases 4.7° laterally as shown in Figure 56 and calculated according to Equation 62:

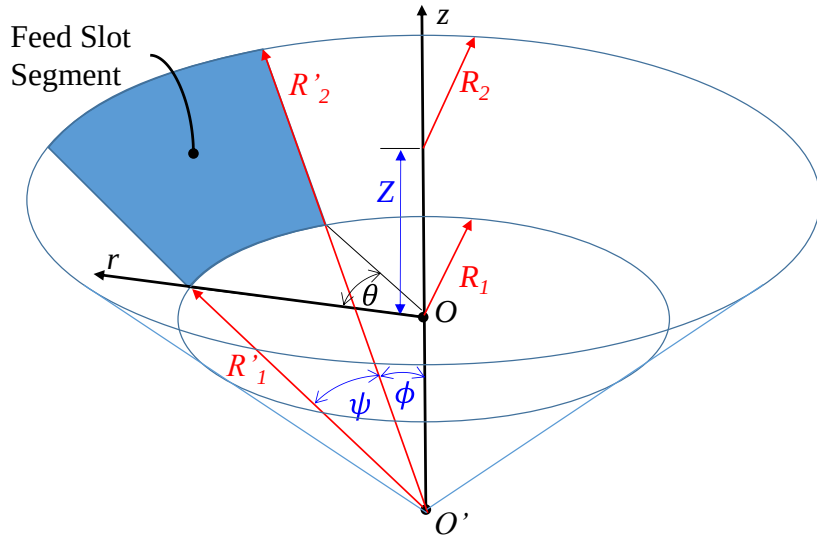


Figure 56. Diagram of a feed slot segment between frustra

$$\psi = \theta \sin(\phi) \quad (62)$$

where ψ is the expansion angle, θ is the segment angle of 18° , and ϕ is the frustrum's half-cone angle of 15° . In practice, the narrow con-annular slot is an expanding diffuser and the expansion angle needs to be limited to prevent flow separation which creates stagnant and recirculating flow within the feed slot. Based on a desired expansion angle of less than five degree, the segment angle was calculated from Equation 62. Given the segment angle the number of slots, n , is calculated as:

$$n = \frac{360}{\theta} \quad (63)$$

where n is the number of feed slots, and θ is the expansion angle from Equation 62.

2.1.5. Detonation Channel

The detonation channel was formed by re-using external parts from other DERF 15 cm RDE. The outerbody was a cylindrical steel shell and served as the outer wall of

the detonation channel. A smaller cylinder, the centerbody, nested inside the outerbody. Multiple plug nozzle attachments were connected to the centerbody to create a choke point at the detonation channel exit and pressurize the flow within the detonation channel. Channel width was set at 2.3 cm by reusing an outerbody and centerbody from the modular non-premixed RDE. The reuse of parts reduced the number of independent variables when comparing the premixed RDE and the non-premixed RDE test results.

2.1.6. Ignition of the Premixed RDE

Detonation within the channel was initiated with a hydrogen-oxygen predetonator (not shown). The predetonator was mounted tangential to the detonation channel on the outer body and fired a single detonation directly into the flowing RDE reactants. For startup, only one detonation from the predetonator was required. However, direct coupling of the detonation was not observed. Instead, the discharge only initiated deflagration in the ethylene-air premixture, and rotating detonation was observed only after a deflagration to detonation transition (DDT) occurred.

Upon DDT, the detonation traveled circumferentially around the annular channel, and its progress was monitored with the use of ion probes, pressure transducers, and thermocouples, as described in Section 2.3 of this chapter.

2.2. Fuel Selection

Ethylene fuel was selected for this study after balancing the desire to compare available results with the need to minimize the flashback risk. Hydrogen is the easiest available fuel to detonate, and many experimental (2,23,103) and CFD studies (8,21,75,94) have been performed with premixed hydrogen-air mixtures. Ease of

detonation comes with a significant drawback: a high propensity for flashback. Ethylene detonation was demonstrated in an RDE (105) with minimal design changes from hydrogen fuels while flashback was significantly less likely to occur. Since ethylene-air combustion achieved blow-off velocity gradients at lower mass flow rates than hydrogen (30) and had larger quenching distances for similar pressures, lower risk of flashback was assumed to operate the same hardware with an ethylene-air mixture.

2.3. Instrumentation

Temperature, pressure, and ionization timing (via ion probe) were collected in both the RDE feed system and at the RDE detonation channel. In Figure 57, the schematic highlights the interconnectivity between the instrumentation, control loops and the safety panel. Gas feed pressures and temperatures were collected at 1 kHz for all tests to provide global mass flow rate and equivalence ratios. Pressure and temperature measurements were post-processed to calculate mass flow rates and global equivalence

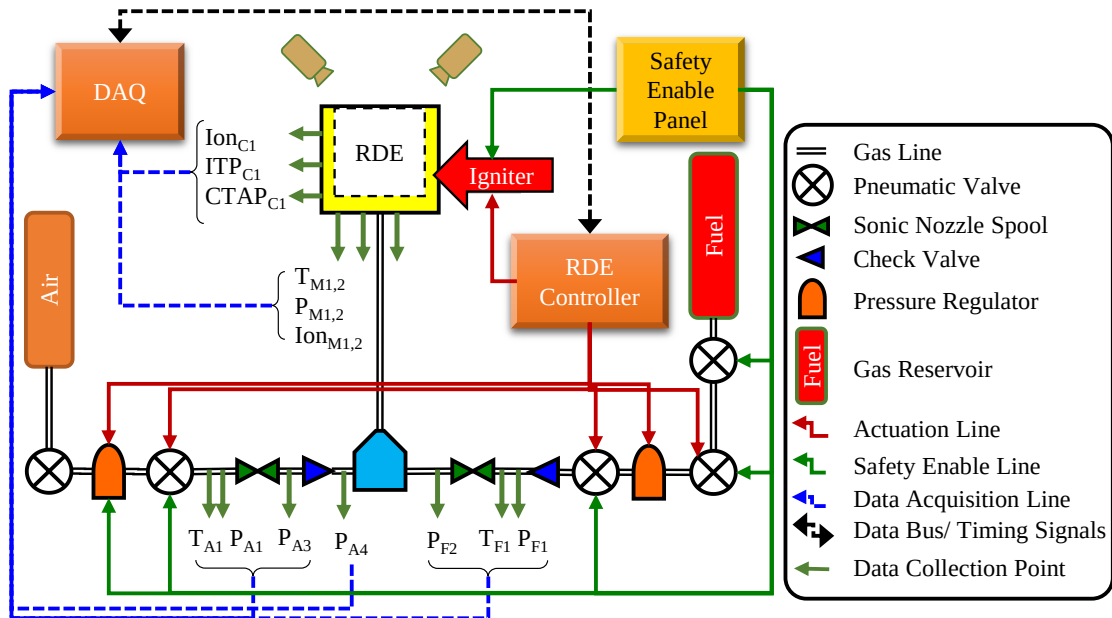


Figure 57. Premixed RDE sensing and control diagram

ratios, and the standard deviation of each measurements was added in quadrature with uncertainties for assumed quantities and calibration uncertainties to calculate total uncertainty.

For a one second duration after the predetonator was triggered, a 1 MHz data stream collected high speed pressure measurements from the detonation channel and feed plenum. The high speed signals showed the passage of the detonation in the detonation channel and captured the spectral response of the premixed RDE operating pressures. All recorded signals were post processed to build operating maps and verify operation modes.

Streaming temperature measurements from a K-type exposed bead thermocouple and ion probe voltages were monitored for signs of flashback in the feed plenum. Operating software was programmed to close the fuel valve if the set threshold values of 400 K for the thermocouples or 9.5 V for the ion probes were surpassed.

Two different pressure measurements common to the DERF were used: the infinite tube pressure (ITP) and the capillary tube attenuated pressure (CTAP). Fotia (136) described form and function for both measurements, and only a summary is given here. The CTAP sensor was located at 3.8 cm above the interface plane, measured the time averaged pressure in the detonation channel, and was collected on the 1 kHz data acquisition system. The CTAP provided accurate time averaged pressures in the detonation channel, but the capillary tube attenuates transients, thereby losing any insight into the structure of the passing detonation. The ITP sensor was approximately 180° circumferentially from the ITP and was 2.5 cm from the interface plane. The ITP reacted to detonation channel pressure transients, and its signal was collected at 1 MHz, but it

was not able to provide calibrated pressure values. The ITP also provided the pressure wave shape that allowed a determination of whether the test event was a rotating detonation or an acoustic mode. Both the ITP and the CTAP measurements supported comparisons to other RDE experiments and computational studies.

A periodogram of each high speed signal was generated. When the characteristic loud tone was heard, (usually louder than 100 dB and around C₇, or about 3 octaves above middle C at approximately 2000 Hz) and a combustion was seen to stay primarily within the detonation channel, RDE operation was assumed. Further verification of the specific mode was performed by looking at the high speed ITP signal and its spectrum. For detonation operation, the ITP signal had a sharp, almost instantaneous rise followed by an exponential decay. The ITP signal periodogram assisted in wave speed calculation. The maximum frequency from the ITP in the 500 Hz to 5000 Hz range was identified as the predominant frequency and was verified by overlaying a sinusoidal plot on the raw ITP signal. The predominant frequency was then used to calculate the wave speed as:

$$D = \pi f d_{RDE} / n \quad (64)$$

where D is the detonation wave speed, f is the predominant frequency, d_{RDE} is the mean diameter of the detonation channel, and n is the number of detonation waves.

The predominant frequency was very repeatable throughout any given test event and provided a consistent measure of wave speed in the laboratory frame of reference. Uncertainty for the wave speed error included the uncertainty of the mean diameter with the uncertainty of the frequency, but since the uncertainty in the mean diameter was three orders of magnitude smaller than the measurement, it was ignored and the uncertainty of the frequency predominated. The one-sided uncertainty for frequency measurements,

based on repeated measurement using the periodogram, was estimated to be 40 Hz or about 2%. The large channel width to diameter ratio created uncertainty regarding detonation wave speed; a detonation traveling on the outer perimeter of the detonation channel will be underestimated by 14% with this measurement, while a detonation traveling on the inner radius of the channel will be over predicted by 14%. This uncertainty applied to all data points identically, was not plotted in the charts, and was part of the total uncertainty in the measurement. The number of detonation waves, n , represented a very large uncertainty. Most of the ITP data was collected using only a single collection point, and the wave speed was assumed to be one unless the wave speed was greater than V_{CJ} , as calculated using the global equivalence ratio, or was out-of-family for the RDE configuration.

High and low speed video footage collected during test events allowed validation of premixed RDE wave speed calculations, operating modes, and sources of error in measurements. Monochrome high-speed imagery collected chemiluminescence from the side or from the exit at frame rates as high as 50,000 fps. The side looking videos required the use of a quartz outerbody created for the DERF chemiluminescence studies (82). The positions of chemiluminescent structures were tracked frame-to-frame as they moved within the field of view of the camera. A coordinate transformation between the Cartesian frame of reference and cylindrical coordinates provided circumferential and axial velocity measurements. Uncertainties related to pixel spacing, radial variation in the field of view, and the detonation front relative to the cycle were not rigorously tracked. Instead, five independent features were tracked using the same method, and their span provides the relative uncertainty in the measurement.

3. Results

Testing initially involved iterations of channel width, back pressurization using annular nozzles, and premixture injection geometries until a configuration and flow rate conditions allowed a rotating detonation, referred to hereafter as an operating point. An initial operating point was eventually found at a mass flow rate of 0.34 kg/s and an equivalence ratio of approximately 1.0 in a detonation channel of 2.3 cm radial depth and with a bluff centerbody installed. The test apparatus functioned reliably and repeatably in that configuration with an ethylene and air mixture. With a single point of operation, mass flow rates were varied between 0.15 and 1.0 kg/s using equivalence ratios between 0.6 and 1.6. The boundaries between the operating modes of detonation, acoustic pulsing, and deflagration defined the premixed RDE operating map and are discussed in Section 3.1.1. The performance of the RDE to arrest flashback is shown in Section 3.1.2 in terms of the burner stability adjustments. The operating maps and wave speeds of the premixed RDE and comparable non-premixed RDE are shown and discussed in Section 3.1.3.

3.1. Premixed RDE Operating Modes

No flashback indications appeared in any of the collected temperature or ion probe signals. Similar to Naples' et al. (103), one of three modes of operation were noted for each run with successful ignition: 1) detonation, 2) acoustic pulsing and 3) deflagration. The detonation mode was characterized by a loud audible tone, a combustion region within the detonation channel, and a distinctive pressure signal that exhibited a sharp rise in the pressure followed by a long expansion period as seen in Figure 58 (a). The periodogram shown in Figure 58 (b) shows the typical spectrum for a

triangular wave, with multiple higher harmonics of decreasing amplitude. Acoustic pulsing also exhibited a loud audible tone, but combustion tended to extend outside of the detonation channel, and the pressure signal had a notably more gradual rise as seen in Figure 58 (c). The amplitude of the pressure signal for an acoustic mode varied between 0.015 mV and 0.25mV, with the larger amplitude corresponding to sharper rises in the pressure signal. The periodogram of the acoustic mode is shown in Figure 58 (d) and exhibits a signal with relatively few higher harmonic overtones. Deflagration was an operation mode where ignition of the mixture occurred, but the premixed RDE never transitioned to either a pulsing acoustic or a rotating detonation mode. The deflagration mode occurred either within the channel or anchored at the bluff exit region depending on the mass flow rate and the flame speed, but no effort was made to track the anchor location since detonation was the mode of interest.

The ITP spectral signals of Figure 58 (b) and (d) provided the best estimate of the time averaged wave frequency. The periodogram was generated for the time period of interest, and the highest peak in the 500-5000 Hz range was found to match the time averaged wave frequency. The predominant frequency (usually the lowest frequency

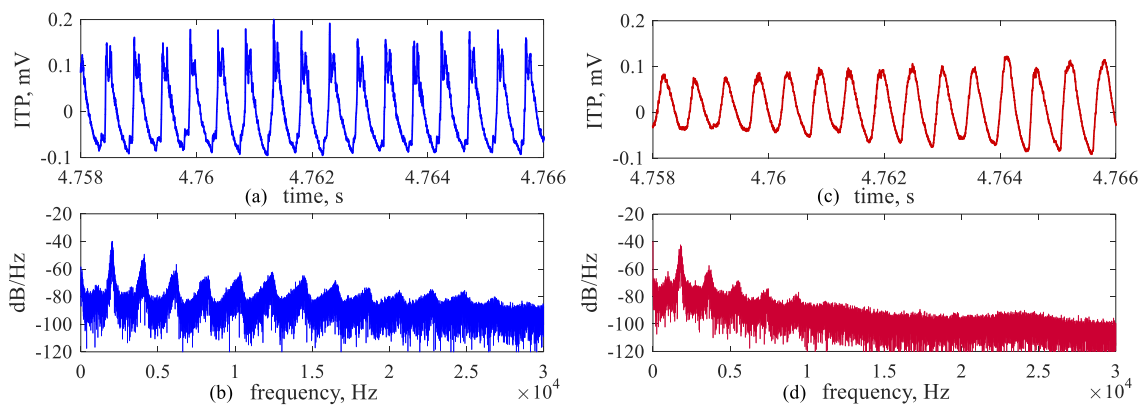


Figure 58. premixed RDE operation with ethylene-air showing detonation mode (a) waveform and (b) spectrum, and acoustic mode (c) waveform and (d) spectrum

peak) was used with Equation 62 to calculate the time averaged wave speed in the laboratory frame of reference. Generally the acoustic mode wave speed was slightly lower than the detonation wave speed. Attempts to measure the wave speed in the gaseous frame of reference (i.e. relative to the shock wave) were not made.

The tangential mounting of the predetonator had no effect on initiation or directional preference of the rotating detonation. Similar to Fotia et al. (105), the detonation never coupled into the ethylene-air premixture. Harmonic axial and circumferential pulsing preceded every observed deflagration to detonation transition. Detonation was seen to travel in both directions, occasionally changing direction during a single 0.7 s run. Multiple detonation wave operation was not noted.

3.2. Comparison to Burner Stability

The estimated quenching distance, velocity gradient, and adjusted velocity gradients were calculated as described in Sections 5 and 6 of Chapter II, and in (27), and indicated safe operation for these fuels and this mass flow rate, as shown in Figure 59. The large separation between the observed velocity gradient and the published flashback curve (30) indicates a future opportunity to explore the trade space between the feed slot height and the feed pressure. Slot heights and mass flow rates can both be increased while also moving the system away from flame anchoring, maintaining a low feed pressure, and retaining a blow-off adjusted velocity gradient.

3.3. Operating Map Comparison between a Premixed and Non-Premixed RDE

The operating maps for both the premixed and non-premixed RDE are shown in Figure 60. Contrary to initial assumptions, this premixed RDE operated within a narrower

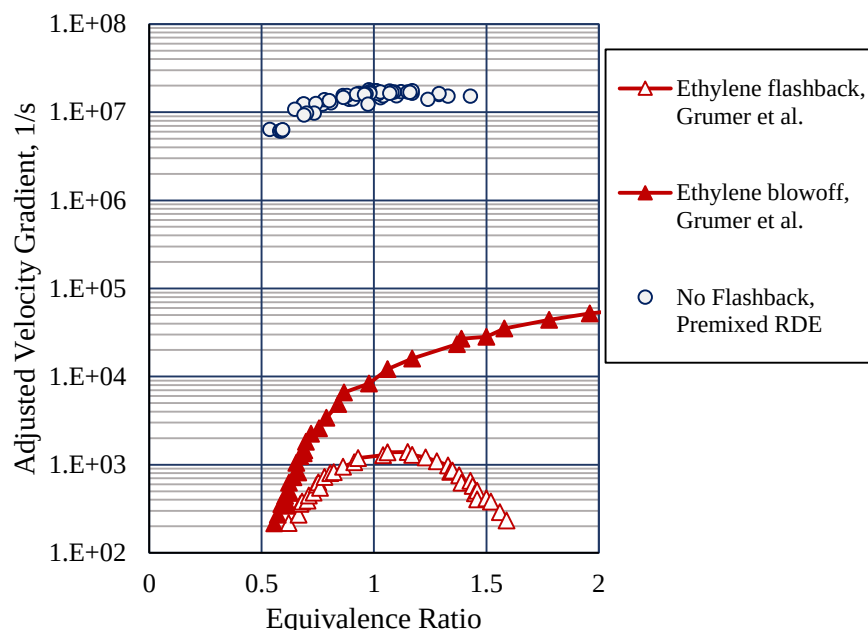


Figure 59. Velocity gradient observations for the premixed RDE compared with published (30) flashback and blowoff limits for detonation and acoustic operation modes

band of equivalence ratios and mass flow rates than the non-premixed RDE with similar channel geometries. The RDE hardware used to build the operation maps of Figure 60 (a) and Figure 60 (b) had similar geometries, and the different regions of detonation operation suggested that mixing delays influenced the RDE operation. The smaller operating range of the premixed RDE suggested that incomplete fuel-oxidizer mixing was not restricting RDE operation. Instead, incomplete fuel-oxidizer mixing may have helped to expand the range of operation. It was possible that the diffusive mixing provided a thin layer of highly detonable mixture across a wider range of global equivalence ratios. Further, as the fuel and oxidizer streams mixed in the detonation channel, a region would have always existed that was at the minimum ignition energy. The remainder of the detonation channel would have been filled with less ideally mixed (either rich or lean) reagents which existed with a higher initiation energy. The proposed strata of rich, ideal, and lean mixtures could be envisioned like nested bowls within the

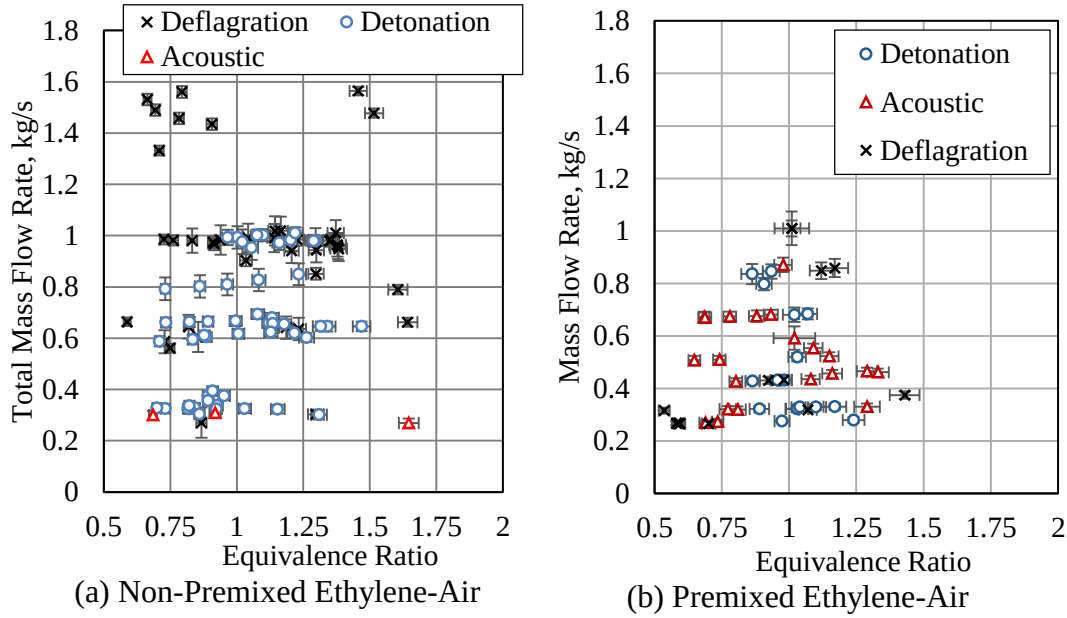


Figure 60. Operating maps for a) non-premixed and b) premixed RDE using ethylene and air

detonation channel, with radial gradients and circumferential uniformity. The variation of available and consumed energy within the mixture presented to the detonation wave would make the wave speed calculation multi-dimensional, and the V_{CJ} calculation could no longer assume the global equivalence ratio for the initial condition.

The current data set is unable to separate the influence of mixing from geometry upon the detonation wave speeds. Wave speeds shown in Figure 61 indicate that the premixed RDE operated with roughly the same wave speeds as the non-premixed RDE, and that both are significantly slower than V_{CJ} predictions. The non-premixed data of Figure 61 (a) was carefully collected so that the air injection sizing was within 20 percent of the premixed RDE mixture injection area of Figure 61 (b). Also, the detonation channel was identical so that the flow patterns would be similar. Differences exist only in the injection scheme and the fact that the premixed RDE has no mixing delay for the fuel and oxidizer.

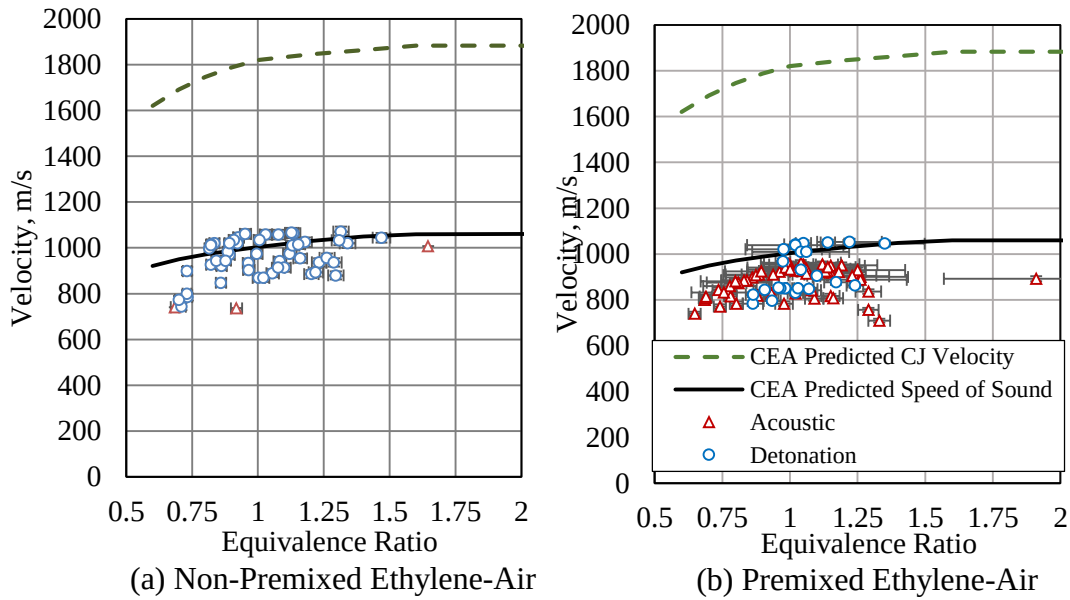


Figure 61. Wave speed calculations for (a) non-premixed and (b) premixed RDE operating with ethylene-air

Similar operating modes would appear at first glance to indicate that detonation channel geometry has a much larger influence on operating mode than mixing timescales. However, the premixed RDE delivered premixed fuel and oxidizer to the channel, and mixing between the reagents and the combustion products was occurring at the point of insertion. Unlike the non-premixed RDE where the flow field was stratified with varying levels of ignition energy, the premixed RDE was stratified with layers of highly detonable gases interleaved with undetonable products. The individual frames of the high speed video from the premixed RDE reinforce this proposal for non-premixed RDE, are shown in Figure 62, and are discussed next.

A high speed video camera collected the broad-band chemiluminescent flow within the premixed RDE at 25,000 frames per second. Video captured before the ignition event displayed no chemiluminescence from the flow. The 12 individual frames of Figure 62 show one complete lap of the detonation around an optically accessible

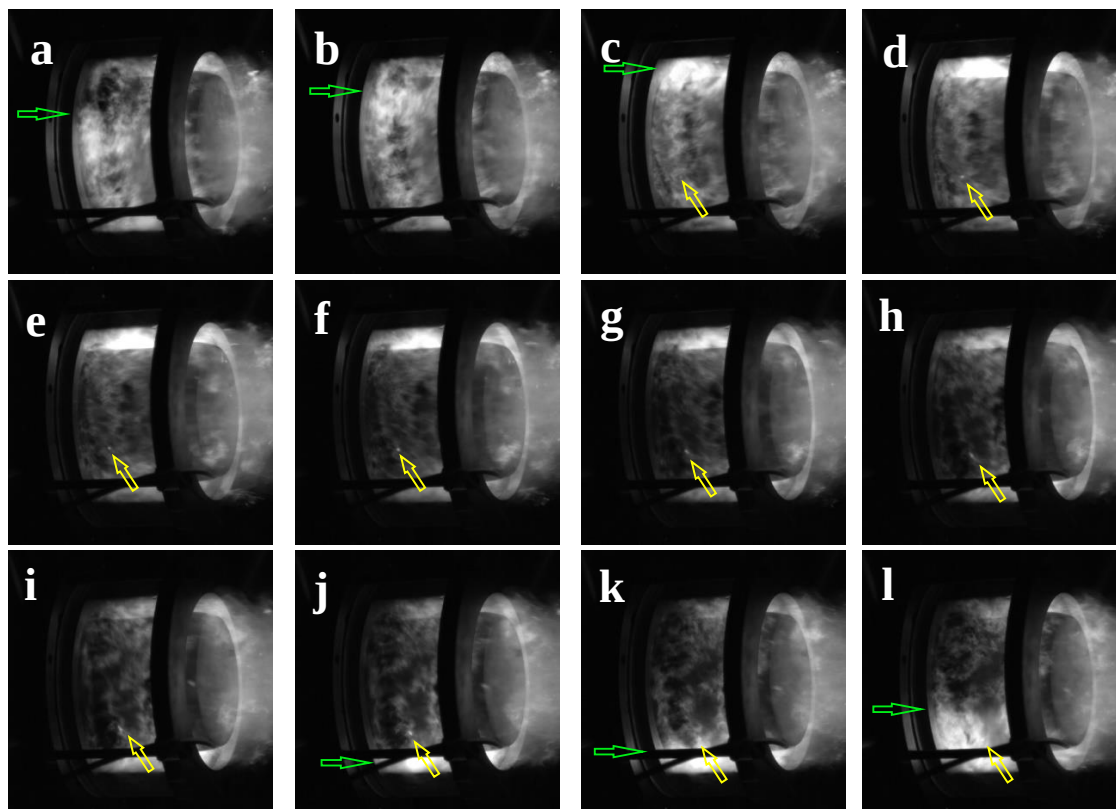


Figure 62. Time sequence of ethylene air detonation during 1 detonation cycle

premixed RDE, and the frames were recorded approximately 0.2 seconds after ignition when the detonation cycle was well established. The gamma correction was changed to 2.0 to improve contrast of the chemiluminescent structures within the detonation channel. The visible structures in the flow were assumed to be chemiluminescence emitted by deflagration continuously ignited by a deflagration zone anchored within the detonation channel at the plenum feed slots. The presence of deflagration within the flowing channel indicated that while the fuel and oxidizer were ideally mixed, the reactants, reacting ions, and combustion products were not.

The detonation front, highlighted with a green horizontal arrow, is centered in Frame a and progresses toward the top of the image in successive frames until it reaches

the apex of the detonation channel annulus in Frame c. Immediately after the detonation passed, a dark band issued from the feed plenum and persisted as it moved axially from the plenum on the left to the channel exit on the right. The detonation continued around the detonation channel and was still visible at the top of the annulus in Frames d through h, after which the detonation front traveled behind the centerbody. The front then re-emerged in Frame j at the bottom of the image. In Frame l, the detonation wave completed one lap, and the cycle repeated. Note that the dark band did not luminesce as the detonation front traversed it, indicating that it was quenched products.

The dark band is seen more easily when the individual frames of Figure 62 are cropped and collected into the collage image of Figure 63. The detonation wave fronts are identified with the “D” above an arrow in frames a, m, and y. A second pass of the detonation begins in Figure 63 Frame m and the dark band is highlighted with the yellow ellipses. The wide detonation annulus allowed for vorticity to swirl the flame structures, and the band may appear to be a series of dark dots in Frames a through h. The second dark band that enters the bottom of the image in Frame g is almost obscured by the swirling flames by the time it reaches the opaque steel band in Frame t. A third band

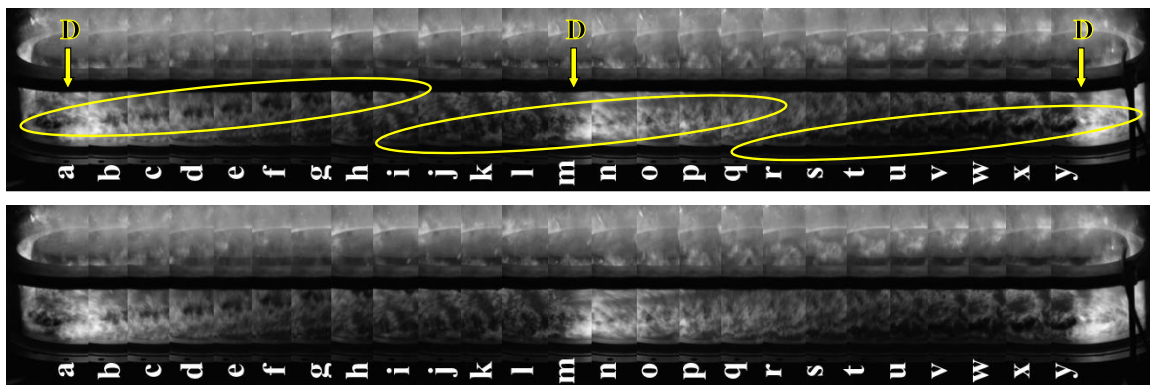


Figure 63. Collage of two complete laps of the detonation: with highlighting showing the dark band highlighted in yellow ellipses (top) and without highlighting (bottom)

enters at the bottom of the channel in frame t and persists through the remaining frames. Multi-spectral imagery of the detonation cycle and further discussion regarding the dark band are found in Chapter V.

3.4. Circumferential Velocities

The visible structures within the reacting flows allowed visual tracking of the flow fields within the detonation channel. A small firefly (heated particle), located in the lower portion of the individual frames in Figure 62 and highlighted with a canted yellow arrow, allowed the author to track the flow movement from frame to frame. The movement of the particle highlighted the circumferential variation in velocity. The particle also provided a qualitative assessment of temperature variation over time since its radiance changed as it moved. The flow field exhibited significant unsteady movement before exiting. For a separate series of images, flow field features were tracked manually through two complete cycles of the detonation. The pathlines and flow velocities were plotted as Figure 64. Since the location and timing of the track points was not uniform, the pathlines of Figure 64 a) do not represent an entire cycle's pathlines, and the figure should not be misconstrued as an analogous figure to Nordeen et al. (8) (copied in Section 4.2.3 of Chapter II as Figure 15). Both Figure 64 b) and c) were transformed from Cartesian coordinates in the laboratory frame of reference to cylindrical coordinates in the rotating detonation frame of reference. The rotating detonation frame of reference holds the detonation wave at 0 azimuth and allows the fluid particles to move circumferentially around the annulus and through the detonation wave. The preceding detonation wave would be projected at -2π radians and $+2\pi$ radians. Since the location

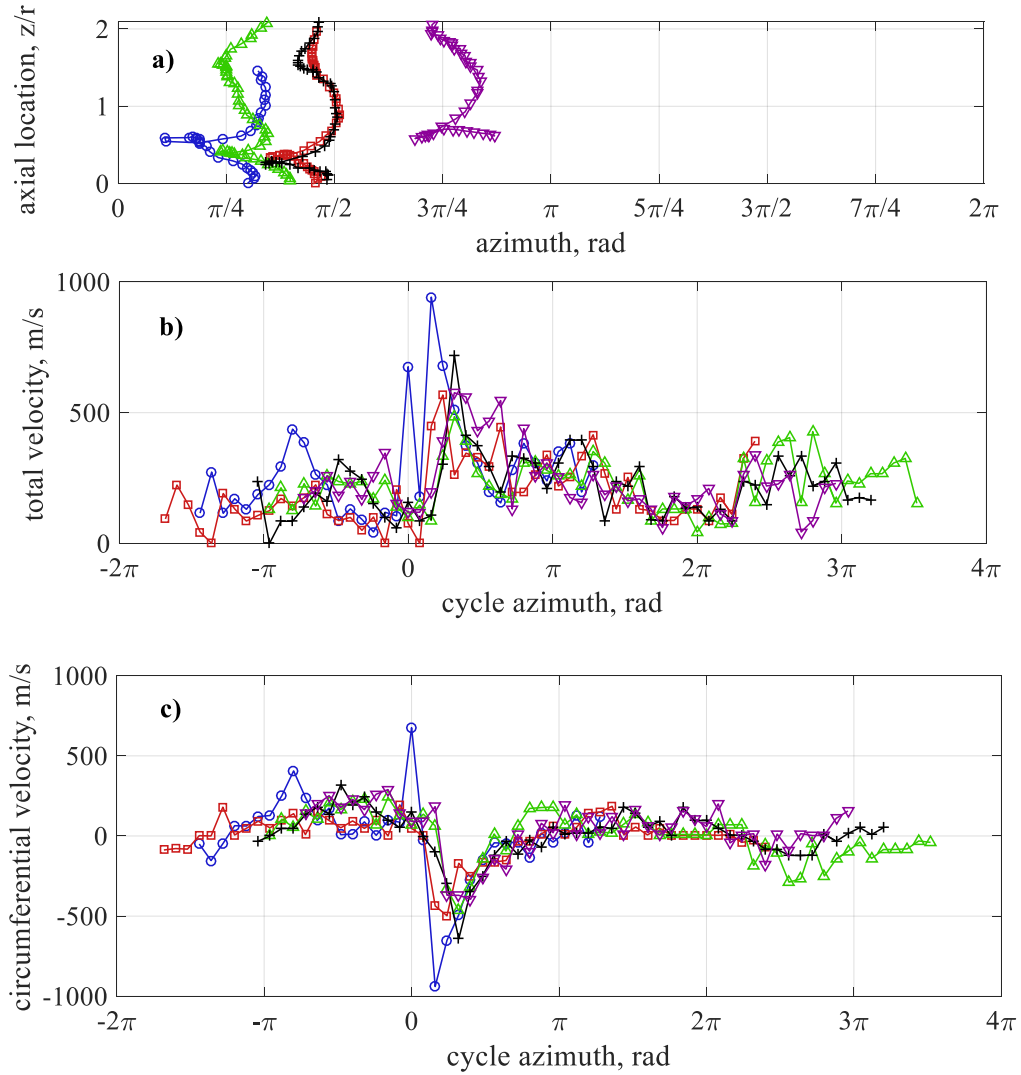


Figure 64. Pathlines and velocity profiles for manually tracked points

and timing of the track points was not uniform across the RDE cycle, the pathlines of Figure 64 a) should not be misconstrued as representative pathlines of an entire cycle. The circumferential swirl appears comparatively large when compared to any of the pathlines of Nordeen's study (8).

The point-to-point distance traveled, as tracked in Figure 64 a), was divided by the time between frames to get a total velocity magnitude, and the time was shifted so that a cycle time of zero corresponded to the frame where the detonation wave first met

the tracked feature. A cycle period of 2π corresponds to the time when the detonation wave arrived back at the same azimuth in the camera's field of view. The resulting velocity diagram is shown in Figure 64 b). The circumferential velocity component was separated and plotted in Figure 64 c), and the plot indicates that the fluid is moving at a net rate of approximately 50 to 100 m/s toward the detonation. It was then accelerated to a velocity of 600-1000 m/s in the opposite direction by the detonation wave. The counter-rotation of the fluid relative to the detonation wave accounted for between 6% and 25% of the difference between the V_{CJ} estimate and the laboratory measurements of wave speed and should not be ignored. However, the circumferential movement and velocity decreased as the combustion products move toward the exit so that this combustor can be called low-swirl overall when considering the exit flow at that plane.

A periodic region of combustion (shown as a light gray band in Figure 62 and Figure 63) entered the detonation channel from the plenum after the dark band noted above. This region of combustion is associated with a zone of fresh reactants being injected into the detonation channel. The amount of reactants injected generally follows the criteria given by Bykovskii [72] of $h_r \cong (12 \pm 5)\lambda$ where h_r is the height of the refreshed mixture, and λ is the detonation cell width. Estimating cell size incurs large uncertainties due to inherent inexactness and variation in the published detonation cell size data [49] and sensitivity to measurement error associated with test conditions, estimated flow temperatures, and local pressures. This elongated deflagration zone associated with refill matched the patterns reported by Schwer and Kailasanath (77) (shown in Chapter II, Section 4.2.3 as Figure 19) and supports their conclusion that finite injection simulations should include a low-pressure reaction model. One difference

between the modeled and experimental geometry was that the modeled geometry spaced the slots circumferentially like spokes on a wheel, whereas the experimental premixed RDE spaced feed slots radially like concentric rings.

The presence of detonation in a combustor flow is a key insight into the relatively slow wave speed and narrow band of equivalence ratios that allow this premixed RDE to operate. The feed slots provide lamina of fresh mixture and flame analogous to the layers of varying stoichiometric ratios found in a non-premixed RDE. Unlike the non-premixed RDE, the entire chemistry driving the detonation forward has changed from the common assumption of a supply of cool reactants, as highlighted in Figure 4 of Chapter II, Section 2.1. The final Chapman-Jouguet wave speed calculation should account for the hot combustion products and non-equilibrium chemistry.

Figure 65 displays Chapman-Jouguet detonation velocities computed with CEA (137) where a portion of the flow was initialized as fully combusted products. The products were assumed to be a mixture of CO_2 , H_2O , and N_2 from a stoichiometric initial mixture. The remaining un-burned portion was assumed to be an ethylene-air mixture at an equivalence ratio of 1.05. The V_{CJ} estimates are plotted as a function of initial temperature representing the temperature trends associated with combustion completion. Therefore, this chart represents a first estimate of V_{CJ} under partially burned conditions, and no attempt was made to match the actual species concentrations (which were not measured) in the experiment. The plot indicates both that the increased temperature and the introduction of inert products decreased the predicted wave speed consistent with the experiment. Conversely, the low wave speeds observed with the premixed RDE suggest the energy released in the experimental premixed RDE was limited due to the

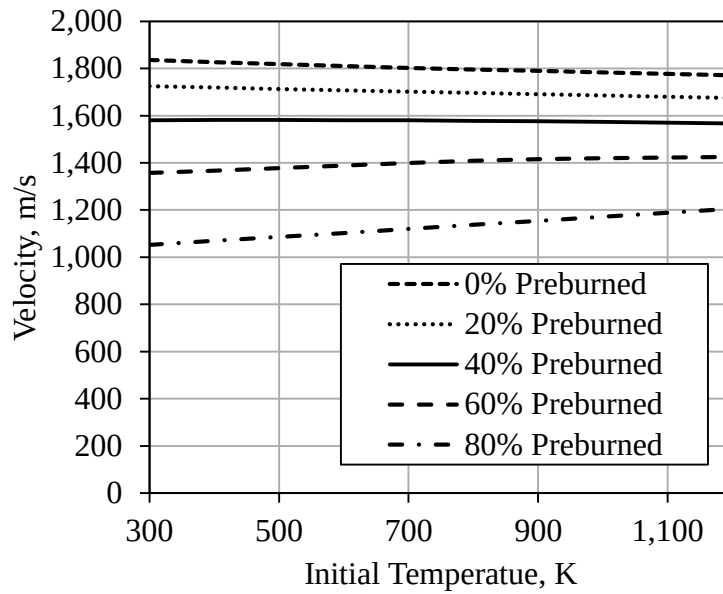


Figure 65. Chapman-Jouguet detonation velocity for ethylene-air, assuming a mixture of reactants and a percentage by mass of pre-combusted products

combination of a detonation event coupled with deflagration. In parallel to non-premixed RDE, it is proposed that the layers of ideally mixed reactant allow the detonation to progress, while the off-nominal mixture absorbs a significant portion of the energy and slows the detonation wave. The off-nominal regions change the initial conditions and assumptions that feed Chapman-Jouguet predictions. Clearly, 1400 m/s wave speed of a 60% inert mixture at 1000 K does not account for the entire deficit between the predicted 1800 m/s V_{CJ} and the 800 m/s to 1000 m/s observed wave speed, but it takes a significant step.

4. Conclusions

This is the first reported operation of a premixed rotating detonation in the modern era. The successful operation of a premixed RDE based on the design criteria established in Chapter II completes Objective 3: “Explore the ability of traditional burner

stability design principles to effectively arrest flashback in a premixed rotating detonation engine.” The current premixed RDE operated with an ethylene-air premixture without any indications of flashback into the feed plenum. The premixed RDE operated successfully with mass flow rates between 0.25 and 0.85 kg/s, and equivalence ratios between 0.9 and 1.2. The exploration allowed the creation of an operating map that was compared to non-premixed ethylene-air with similar detonation channel geometries, meeting the fourth objective: “Experimentally characterize the operation of a premixed rotating detonation engine.”

The ideally mixed fuel-oxidizer stream was subject to a non-ideally mixed reactant-product environment during operation, yet the premixed RDE continued to operate with a propagating detonation wave in the presence of anchored flames at the mixture injection slots. Flow visualization confirmed that detonation in this engine propagated through a region of combustion. Chapman-Jouguet predictions were found to be slower in mixtures containing reaction products. Although non-premixed RDE visualizations reviewed for this work show no evidence of flame-holding, they do have significant portions of the flow where the fuel-oxidizer mixture requires additional energy to achieve ignition and cannot support the detonation velocity calculated with the global mass equivalence ratio. Visualization also showed that RDE wave speeds measured at 1000 m/s in the laboratory frame of reference under-predicted the wave speed by 50-150 m/s when circumferential movement of the fluid due to expansion was present. Both of these corrections explain some of the difference between current RDE wave speeds and simple V_{CJ} predictions based on global equivalence ratios.

The premixed RDE operated with the same wave speeds and over narrower regions of equivalence ratios and mass flow rates than non-premixed RDE, suggesting that mixing does affect premixed RDE operation. One proposed explanation regarding the difference is that diffusive and turbulent mixing mechanisms in a non-premixed RDE provide a small volume of highly detonable mixture over a wider range of global mass flow rates. Similar wave speed measurements were obtained for identical detonation channels, but the presence of reactant-product mixing prevents the clear separation of the mixing delay influence on wave speed from channel geometry influence. Opportunities to explore more of the mixing effects are now within reach. Modifications to the feed geometry and flow conditions should minimize premixed burning and provide fresh reactants to sustain detonation at higher mass flows and with greater wave speeds.

V. Multi-Spectral Chemiluminescence

1. Introduction

The high speed chemiluminescence imagery of Figure 62 in Chapter IV showed a dark layer issuing from the feed plenum after the detonation wave had passed. By selecting only the middle portion of each image and setting them side by side, a panoramic complete cycle of the chemiluminescence can be constructed, as shown in Figure 66. The laboratory frame of reference has been changed to a detonation-wave frame of reference in Figure 66, so that the detonation wave is fixed in the middle of the image and the reactants flow in from the bottom and pass through the detonation from right to left following pathlines, as highlighted in Figure 67. Dark regions that follow the pathlines may be seen in both the broad-band chemiluminescence of Figure 62 and the ultra-violet bandpass filtered imagery of Figure 66 and Figure 67. This dark band is different from the band of deflagration in CFD models which occurs between the region of detonated products and the region of fresh reactants. The CFD predicted zone of deflagration would chemiluminesce. Also, the dark band does not appear to be the fresh

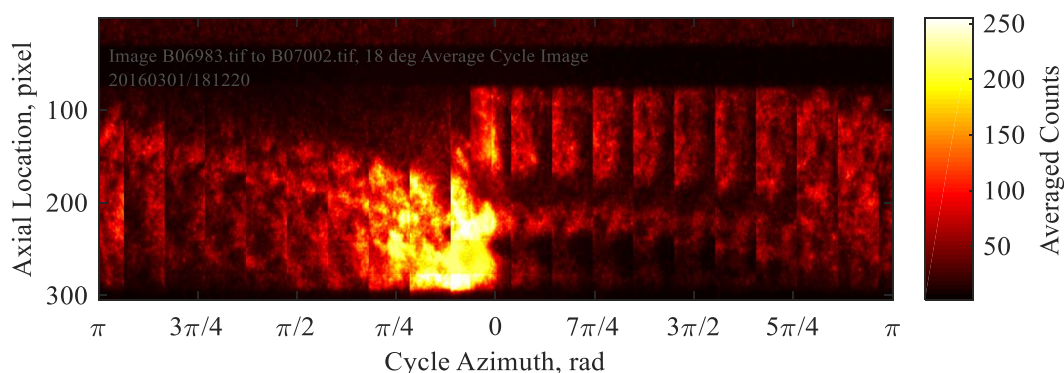


Figure 66. Chemiluminescence from a single cycle of an ethylene-air premixed detonation moving from left to right in the RDE and imaged through a 300 nm to 342 nm bandpass filter corresponding with OH emission

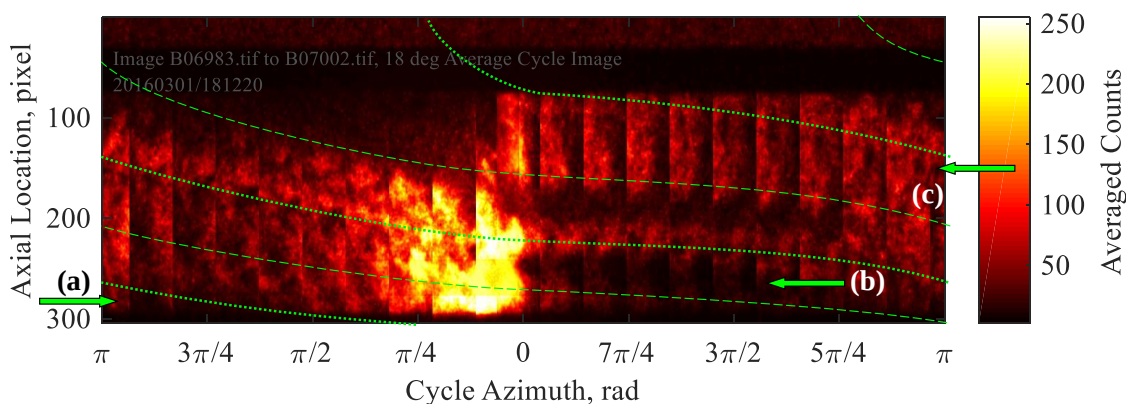


Figure 67. Pathlines for a detonation wave cycle: two approximate pathlines are drawn as dashed lines that flow from the bottom to the top, wrap around the cycle image right to left, and pass through the rotating wave 2 times before exit; the dark band of products is indicated with arrows at locations (a), (b), and (c)

reactants since the detonation wave emits chemiluminescence everywhere except within the dark region. This chapter discusses the impact of that dark band and adds additional information to Objective 4 by providing greater detail about the detonation cycle in a premixed RDE.

2. Background

Computational simulations (77,78) of RDEs have been helpful in describing the continuous detonation cycle. The literature from these studies has defined the terminology used to describe the RDE engine. They predicted that the portion of the flow subjected to the detonation driven shock wave would push the reactants to complete combustion. The portion of the flow still in the feed plenum that did not experience the shock would not combust and might have continued to deflagrate. The NRL simulations (21,22,77,78) showed that this deflagration region separates the cool reactants from the detonated products, and that a shear layer exists. The complex equations dealing with fluid flow, mixing, and chemical reactions required refined grids and long computational

times to converge to a solution, so simplifications were often made to speed the CFD process. One of the simplifications has been to ignore the fuel plenum altogether, or when it is modeled, to ignore heat transfer within the feed system. As described in Section 5 of Chapter 2, thermal quenching can halt deflagration passing through narrow channels. Since quenching is not modeled, the numeric solution from the CFD will never predict a quenching effect in the feed system.

Rankin et al. (23) and Cho et al. (82) performed experimental visualization studies of non-premixed RDEs using hydroxyl chemiluminescence that provided qualitative comparison with the CFD studies of Schwer et al. (77,78). The experimental studies allowed the authors to provide experimental comparison of wave speeds, refill heights, and thrust performance correlations. Qualitative comparison with CFD results showed that the cycle as described by Schwer et al. (77,78) was generally in agreement with the wave structure and detonation cycle dynamics. Cho et al. (82) even showed a correlation between an injection geometry that is thought to inhibit fuel-air mixing and detonation wave liftoff similar to the numeric predictions of Nordeen et al (22).

This study discovered the flow field of a premixed ethylene-air RDE using chemiluminescent imaging, and identified presence of delayed combustion and quenched products using multi-spectral band-pass filtering. Band-pass filtering allowed a non-intrusive indication of three chemical radicals within RDE cycle: hydroxyl (OH), ethenediylidene or bicarbon (C-C), and methylidyne (CH). These three radicals are closely tied to combustion within ethylene, served as markers for the combustion zones, and provided a qualitative measurement of the combustion rates. Location and rate of

combustion within the RDE flow field demonstrated that the dark band shown within the flow field in Figure 62 and Figure 63 was non-reactive.

3. Methodology

A spectrum of the premixed ethylene-air RDE described in Chapter IV was collected to inform the band-pass requirements for a multi-spectral system. The RDE was configured with a quartz outerbody and imaged through band-pass filters at 40,000 fps with a high-speed broadband camera connected to a high-speed image intensifier. Data was post-processed to collect the nearly flat central sector of the detonation channel and convert it to a panoramic detonation cycle still image like that shown in Figure 66. Each step of the process is described in greater detail in this section, as well as a description of the errors impacting the imagery.

3.1. Preliminary Spectrum

A spectrum shown in Figure 68 was collected from the premixed RDE operating at 0.99 kg/s total mass flow with ethylene-air and an equivalence ratio of 1.02. The spectrum was collected 8 cm from the injector face with an Ocean Optics USB 2000+ UV-Vis spectrometer. The spectrometer had a stated bandwidth of 199-886 nm, a grating with 600 lines blazed at 400 nm, an optical slit of 200 μm , and a resolution estimated at 7.9 nm. Similar instruments instrumented with a 5 μm slit have an estimated resolution of 1.0 nm, but an instrument with the smaller aperture was not available for this test. Possible band heads noted in the spectrum were compared to published combustion spectra described in the CRC Handbook of Spectroscopy (138) and with known spectra for carbon combustion in air provided by Captain William Bauer (AFIT/ENP), although

the low resolution of the spectrometer prevented peak matching. Three bands of interest were identified:

1. Hydroxyl, 300-330 nm, OH, transition: $A^2\Sigma^+ - X^2\Pi_i$, $\Delta v = 0$
2. Methylidyne, 430-440 nm, CH, transition: $A^2\Delta - X^2\Pi$, $\Delta v = 0$
3. Ethenediylidene, 535-575 nm, C-C, transition: $A^3\Pi_g - X^3\Pi_u$, $\Delta v = -1$

Optical bandpass filters were already available for the OH, CH, and C-C bands, and each was tested for transmission by dividing a filtered spectrum by an unfiltered spectrum. Additionally, each filter was tested using a different light source, without a collimator or fiber in the optical path. Different light sources were used to test the transmissivity of each filter. A 300 nm to 342 nm ultra-violet bandpass filter was used to capture OH. The OH filter was tested using sunlight where there was sufficient ultra-violet signal. The results showed that the ultra-violet filter had nearly full transmission

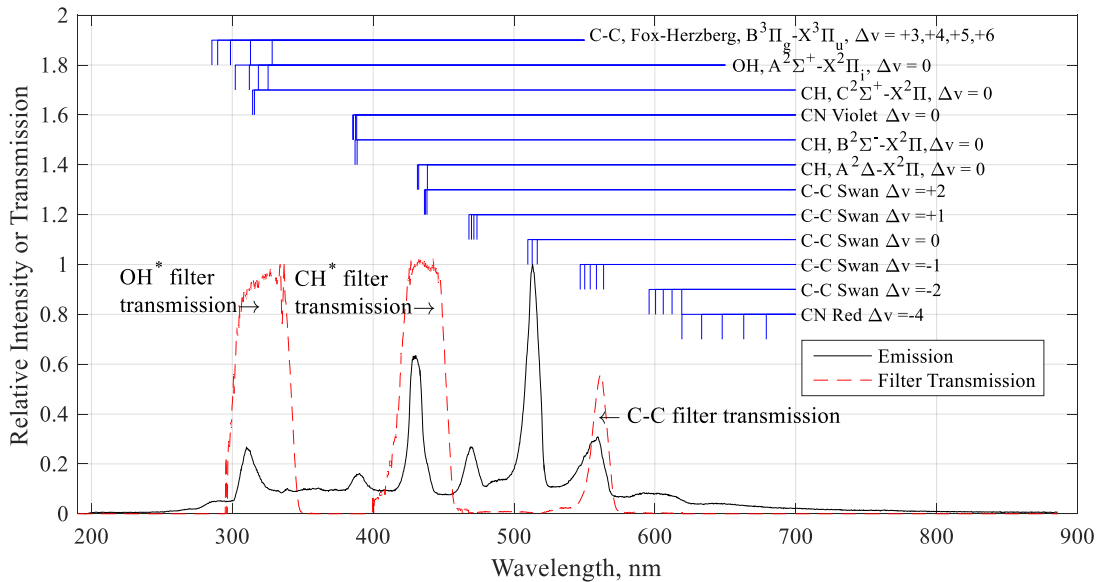


Figure 68. Spectrum of an ethylene-air RDE operating at 0.99 kg/s and $\phi = 1.02$ showing anticipated emission bands and available filter transmission curves

over the 300 nm to 330 nm emission range of OH. Based on other combustion emission spectra (138,139), the intensity of the CH and C-C in the 300 nm to 330 nm range was anticipated to be low enough that its contribution to the OH emission was ignored. A 400 nm to 480 nm bandpass filter was used to capture CH emission. The CH filter was tested using the diffuse reflection from overhead fluorescent lights which had a good signal in the 400 nm to 480 nm wavelengths. The results indicated that the blue CH filter would provide nearly full transmission for the 410 nm to 440 nm CH emission while also passing the low-intensity CN Violet $\Delta v + 1$ and C-C $\Delta v + 2$ emissions. Based on other combustion emission spectra (138,139), the intensity of the CN and C-C in the 410 nm to 440 nm was anticipated to be low enough that its contribution to the CH emission was ignored. Finally, a 554 nm to 568 nm green filter was used to capture C-C emission. Fluorescent lights had a significant drop off in intensity at approximately 570 nm so the C-C filter was tested using the diffuse reflection of a 25 W incandescent projector bulb. The results for the green C-C filter indicated it would block over 50 percent of the light emitted from the 535 nm to 575 nm C-C $\Delta v = -1$ band, requiring an image intensifier.

The resulting transmission curves, shown as a red dashed line in Figure 68, agreed to within ± 5 percent with the anticipated transmission and were intended only to provide a qualitative estimate of what the filtered image was actually passing to the sensor.

The bandpass filters allowed more than just the desired radical emissions through to the camera. An underlying baseline rises above the noise floor at about 250 nm, and extends to 780 nm. This baseline is a wide low-intensity curve that persists through the sampled spectrum and the electronic rovibronic transition emissions created intensity peaks in the spectrum of Figure 68 that appear to rest on the baseline. This low intensity

band will continue to emit and presents a noise floor to the video image. The floor is likely some sort of blackbody emission from a carbon compound. Broadband color images of the RDE in operation show blue emissions, indicating that there is likely very little contribution of the black-body baseline by soot. Relative levels of intensity may be found by integrating the total emission spectrum over the region of interest and subtracting the integral of the baseline. Using this method, the ratio of hydroxyl specific to baseline emissions is estimated to be 1 to 1. For both methylidyne and ethenediylidene, the ratio of radical to baseline emissions is roughly 2 to 1. Thus, using the filtered images is a fair, but not absolute, indicator of the presence and relative concentration of the various radicals.

3.2. Configuration of the RDE for Optical Access

The premixed RDE described in Chapter IV was configured with a quartz outerbody with a 2.3 cm channel, as shown in Figure 69. A Phantom v7.1 high speed camera was coupled with an IRO image intensifier and positioned approximately 2 m from the RDE. The camera was set so that the field of view captured 200 degrees of

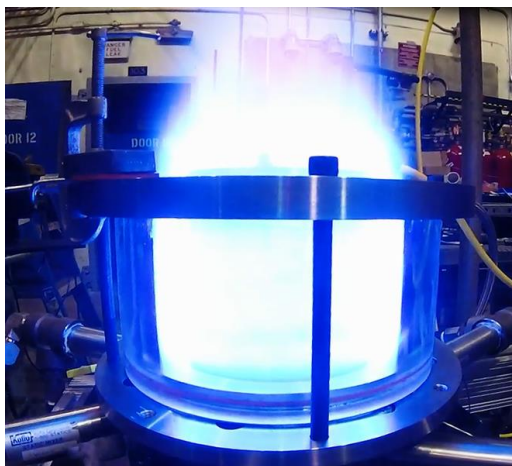


Figure 69. Premixed RDE configured with a quartz outerbody for optical access and operating at 0.33 kg/s and $\phi = 0.86$

azimuth and was level with the optically accessible portion of the detonation channel as shown in Figure 70. The opaque mounting plate for the quartz outerbody obscured approximately 0.6 cm at the bottom of the detonation channel where the premixed fuel and air were injected. A second opaque plate at the exit of the channel held the quartz outerbody in place with the assistance of 4 long bolts. The 60 degrees of RDE azimuth centered within the camera's field of view are highlighted with dashed lines and was used during post-processing to build the single-cycle image of Figure 66, Figure 67, and the subsequent time averaged cycle images shown in this chapter.

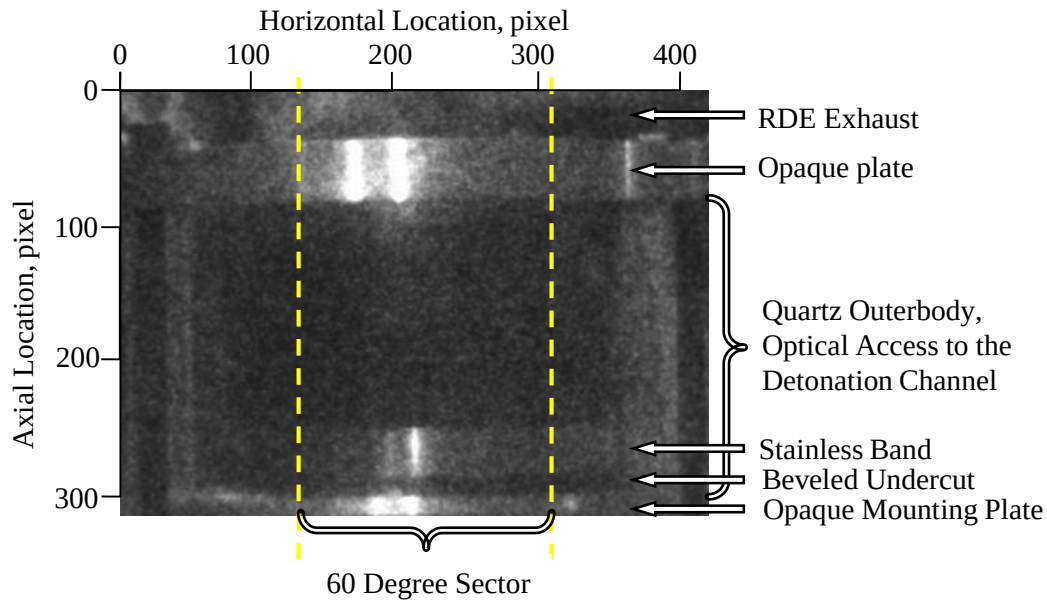


Figure 70. Field of view image for the multi-spectral video showing the premixed RDE configured with a quartz outerbody, opaque plates, and 60 degree sector used to time-average the detonation cycle

The lower portion of the centerbody was freshly machined stainless steel and reflected approximately 15% more light in a horizontal band between axial locations 243 and 278. The increased intensity was corrected by multiplying the band with a correction factor of 0.87. The multiplicative correction factor was found by iterating. Some artifacts

of the increased intensity and subsequent correction may still be seen in the images. No correction was attempted for the horizontal band in the image just below the increased reflectance where an undercut on the centerbody reduced the intensity by providing reflectance away from the camera.

3.3. Conversion of Video to Detonation Phase Angle-Averaged Stills

High speed video was post processed to create a two-dimensional static display of the RDE cycle. The first step was to track the rotating detonation for approximately 25 cycles through the field of view diagrammed in Figure 71. The detonation was seen in the field of view within the detonation channel which extended from x_1 to x_4 . The opaque centerbody obscured the detonation between the x_2 and x_3 datums for that portion of the cycle where the wave was passing behind it. The centerline datum, x_c , was calculated as the arithmetic mean of x_2 and x_3 , or, alternatively, x_1 and x_4 . The centerbody radius, r_i , was calculated with the relation:

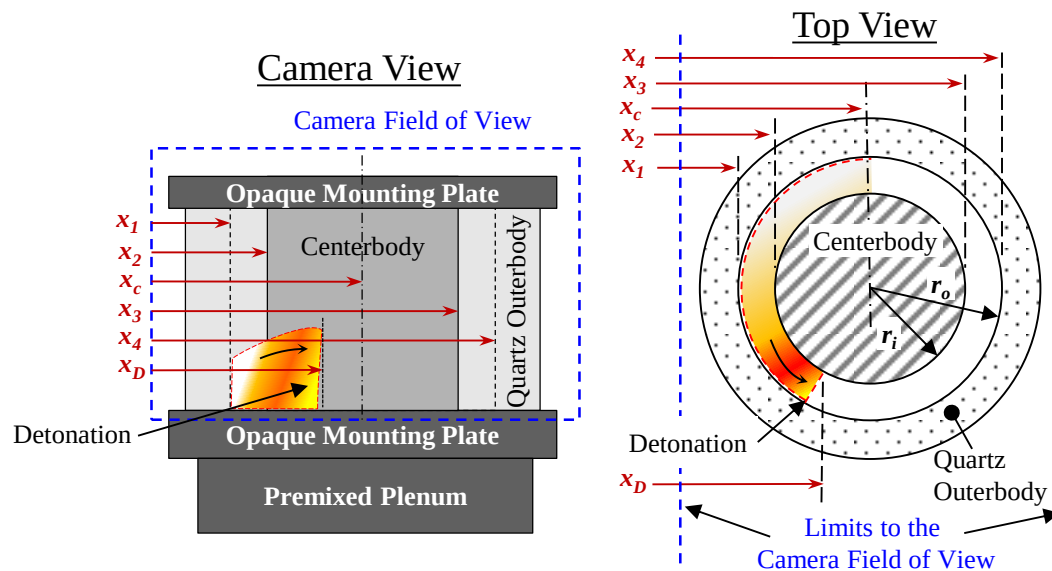


Figure 71. Diagram of the field of view and significant datum lines used to track the detonation wave front in high speed video imagery

$$r_i = \frac{x_3 - x_2}{2} \quad (65)$$

and the outer radius of the detonation channel, r_o , was calculated with the relation:

$$r_o = \frac{x_4 - x_1}{2} \quad (66)$$

In the diagram, the detonation wave travels from left to right in front of the centerbody, corresponding to a counter-clockwise movement if viewed from the exhaust end of the RDE. The detonation wave front was assumed to be normal to the channel walls, and the angle of the leading edge tracked at x_D was calculated using the outer wall radius, r_o , in the following regions: 1) between x_1 and x_2 as the wave was emerging from behind the centerbody, and 2) between x_c and x_4 as the detonation passed from left to right. The leading edge datum was measured on the inner radius, r_i , when the leading edge of the wave was between x_2 and x_c . The phase angle of the detonation was calculated using the location with the relation

$$\theta = \begin{cases} \cos^{-1}\left(\frac{x_D - x_c}{r_o}\right) & \text{if } \begin{cases} x_D > x_c \\ x_1 \leq x_D < x_2 \end{cases} \\ \cos^{-1}\left(\frac{x_D - x_c}{r_i}\right) & \text{if } x_2 \leq x_D \leq x_c \end{cases} \quad (67)$$

where θ is the phase angle of the detonation wave, x_D is the location of the leading edge of the detonation wave in the video, r_o is the outer radius of the detonation channel, r_i is the inner radius of the detonation channel, x_1 is the left most edge of the detonation channel's outer wall, x_2 is the left most edge of the detonation channel's inner wall, x_c is the axial centerline of the detonation channel, and x_D is the measurement from the left most edge of the image to the leading edge of the detonation wave.

A least squares fit of the accumulating detonation phase angle with respect to time was performed in Microsoft Excel and takes on the form:

$$\theta = \beta_1 F + \beta_0 \quad (68)$$

where θ is the phase angle, β_1 is the mean rate of detonation wave phase angle increase per frame, F is the frame number, and β_0 is an intercept that allows the phase angle from the first frame to exist between $-\pi$ and π . An example of the curve fit is shown in the top portion of Figure 72 with the horizontal axis identifying that time may be reported in frame numbers. The relation between time in seconds and frame number is:

$$t = \frac{F}{f} \quad (69)$$

where t is the time in seconds from the beginning of a frame, F is the frame number, and f is the frame rate of the video. The cumulative phase angle was tracked by using a conversion from Cartesian to cylindrical coordinates that provided a measurement in each frame on a circle that was approximately 325 pixels in diameter. Tracked over 400 frames, the cumulative start-to finish resolution of roughly 130,000 pixels permits wave front location within the data set to six significant digits of accuracy. Time was tracked within the video camera to 10 significant digits for each frame. The linear fit to the data represents a simple $\Delta s / \Delta t$ measurement, and accuracy may, therefore, be stated to six significant digits since the least significant digit is associated with the cumulative phase angle calculated as the start-to-finish number of azimuthal pixels, and the span of the cumulative angle covered approximately 400,000 pixels. The coefficient of determination, R^2 , for this fit was 0.999984, indicating that the linear regression has almost perfectly captured the mean rate detonation wave speed over the sampled period.

However, the coefficient of determination does not indicate the goodness of fit during any single cycle. The residual error between the model of Equation 68 and the measured phase angle is plotted in the lower portion of Figure 72 as a function of detonation cycle phase angle. Although the error carries a standard deviation of 11.7° , the standard deviation over the -30° to 30° interval is smaller, such that two standard deviations capture an uncertainty of $\pm 12.5^\circ$ using a 95% confidence interval or about $\pm 3.4\%$ of the cycle. Although the trend is distributed normally about the mean, the residual error displays a non-linear trend when plotted as a function of phase angle. The variation of the error when plotted against some third variable, such as phase angle, is termed heteroscedasticity from the Greek terms for “different” and “dispersion.”

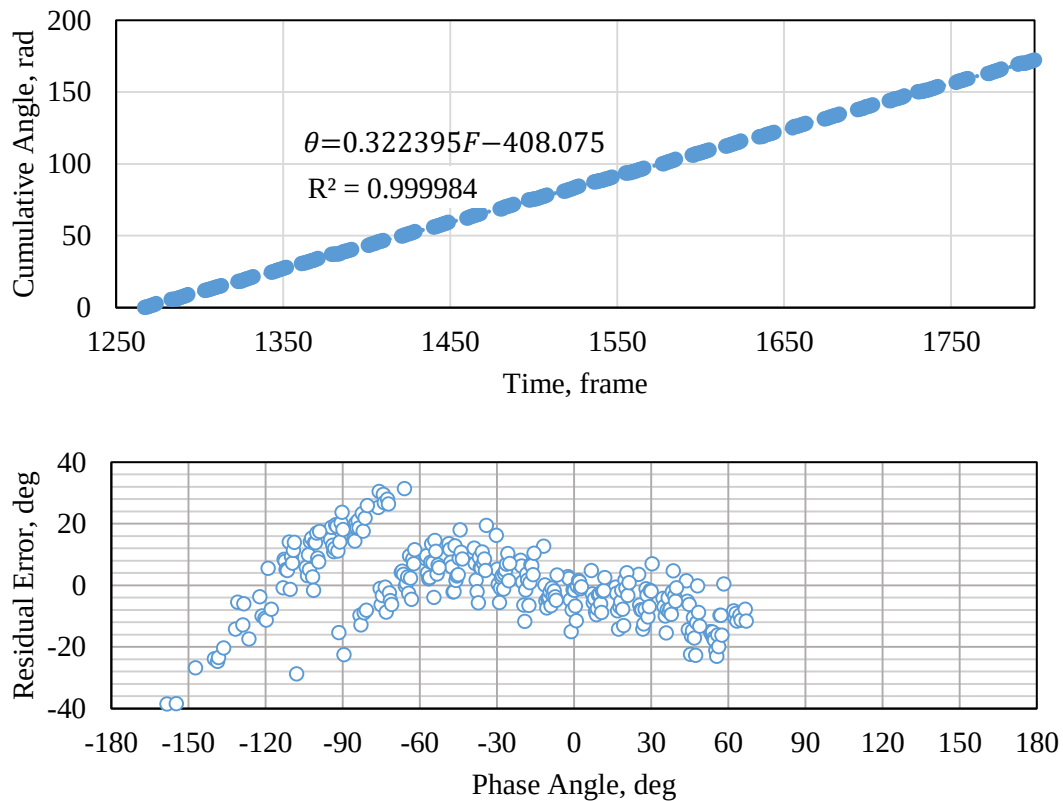


Figure 72. Linear fit to the cumulative phase angle (top) and residual error to the least squares regression (bottom) as a function of time

Heteroscedasticity means there is some variation in the data that was not accounted for in the linear regression model. The discontinuity in the residuals between -120° and -160° phase angle is due to tracking the detonation wave front as it emerges from behind the outerbody, where the outer radius is used in Equation 67 for the group of data points extending from -150° to -60° phase angle.

The data points extending from -90° to 0° used the inner radius for calculating the phase angle as the wave front appeared to move in front of the centerbody. The discontinuity indicates that the assumption of a planar wave front that is normal to the channel and extends from the inner radius to the outer radius is not valid; suggesting instead a curved wave front that leads in the middle of the channel and trails at the inner and outer radii of the detonation channel may either be due to an artifact of the detonation phase measurement technique or an accurate representation of a detonation wave that varies its wave speed periodically with the cycle. More information on wave speeds that vary cyclically may be found in Appendix VI. An ensemble average of the phase angle rate is captured by using a linear fit to the data spread across many cycles, and the linear fit avoids accumulating errors due to randomness of the phase angle rate within the cycle. Between 0° and $+90^\circ$, the formula again transitioned to the outer radius for wavefront location but did so without a discontinuity because of the shallow angle.

The coefficient of phase angle rate, β_1 , may be used to calculate the time-averaged detonation wave speed with the formula

$$D = \frac{\beta_1 f}{2\pi} \pi d_{RDE} \quad (70)$$

where D is the detonation wave speed, β_1 is the coefficient of phase angle rate from the linear regression of Equation 68 in radians per second, f is the video frame rate, and d_{RDE} is the mean diameter of the detonation annulus. The detonation wave speed calculated in this manner is analogous to the a wave speed calculated from the ITP or ion probe signals discussed in Chapter IV Section 2.3, and does not capture the relative circumferential velocity of the swirling flow.

The central portion of the video representing 60° of RDE azimuth could be captured from each frame and placed in a single layer of a sparse data cube sized to represent 360° of azimuth, as shown in Figure 73. Each 60° segment was assigned a phase angle azimuth using the β_1 coefficient from the linear regression of Equation 68.

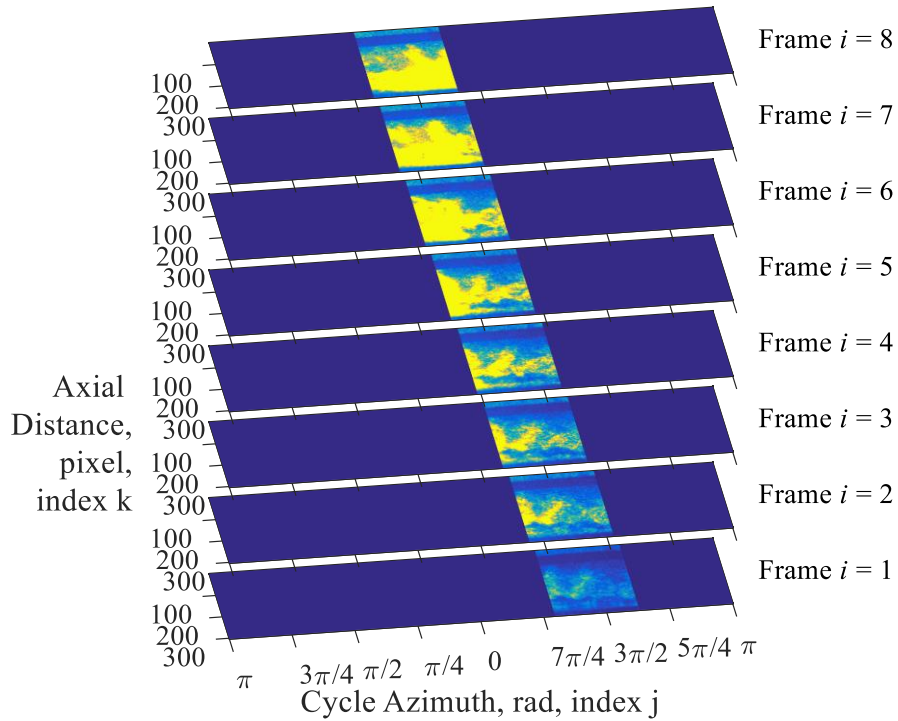


Figure 73. Data cube collecting 60 degrees of azimuth from 8 frames of video imagery and storing it in the appropriate cycle azimuth for time averaging

The assignment of each column of pixels within the 60 degree sector was done without a rigorous transformation and resampling, so that:

$$C_{i,\theta_j,k} = V_{i,x_j,k} \quad (71)$$

where C is the sparse data matrix depicted in Figure 73, i is the index location associated with the time or frame, θ_j is the discrete phase angle index in Matrix C that will be assigned data from the image frame Matrix V , x_j is the column index in the video frame V to be assigned, and k is the row in both the C and V matrices. The columns assignment from the x_j image Matrix V employed the small angle assumption:

$$\theta_j = \text{mod}[x_j + \beta_1 i, 2\pi] \quad (72)$$

where θ_j is the discrete phase angle index of the sparse data Matrix S that will be assigned data from the column index x_j image of the video frame Matrix V , β_1 is the coefficient of phase angle rate from Equation 68, i is the frame increment of the image Matrix V , and “mod” is the modulus function that returns the remainder of the phase angle after division in the range $[0, 2\pi]$. A truer transformation would be

$$\begin{cases} x_j = r_m \sin(\theta + \beta_1 F_i) \\ \theta_j = \text{nint}\left(\text{mod}\left[\text{asin}\left(\frac{x_j}{r_m}\right) + \beta_1 i, 2\pi\right]\right) \end{cases} \quad (73)$$

where x_j is the index in the image Frame F , r_m is the mean radius of the detonation channel, θ is the azimuth angle of the column, θ_j is the angle index, and “nint” is a rounding function that assigns the nearest integer. Using the relations of Equation 73 induces loss of data due to dropped or averaged columns while removing very little error as will be discussed in Section 3.5 of this chapter. The approach used for this analysis was to employ Equation 72 with the inherent assumption that the angular span of each

column in image Frame F was an unchanging constant, and that each column of the 60 degree sector from the video image can be placed in the sparse Matrix C without re-sampling, removing columns, or averaging columns.

Averaging the cube across the time (or frame) domain provided a time-averaged panoramic image of the entire cycle. Care was taken to remove the portions of the cube that contained no data from the average. The azimuth of the detonation wave within the annulus defined the phase angle of the cycle, and uncertainty of phase angle indicated by the residual errors from the model of Equation 68 translated into uncertainty regarding the total amount of lateral averaging that may be occurring with the time averaging. Assuming no variation of the phase angle rate within the detonation cycle, the phase angle within the detonation cycle may be converted to a cycle time with the relation

$$t = \frac{\theta}{\beta_1} \quad (74)$$

where t is the time within the detonation cycle, θ is the phase angle, and β_1 is the coefficient of phase angle rate from Equation 68.

3.4. False-Color Recombination of Multi-Spectral Data

The time averaged images from each cycle were combined in a red-green-blue (RGB) format to create a false-color image. This process involved normalizing each of the three filtered images with the maximum intensity contained in each and ensuring that

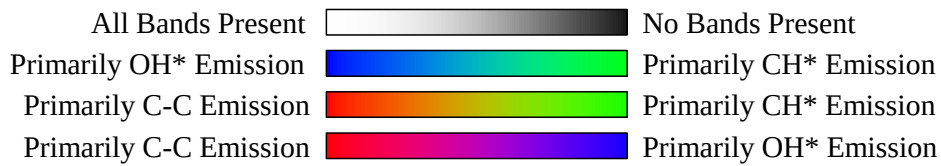


Figure 74. Color distributions for the false-color recombined multi-spectral imagery

their phase angle was matched as closely as possible by aligning the steep gradient at the front of the shock. When combined, the four color scales shown in Figure 74 represented the relative distribution of the different emitters within the flow field, and the separate layers combined to qualitatively indicate where combustion occurred. When the three emitters were present in equal parts the image will display a shade of gray: white when all three are present at their peak intensity, black when all three are absent. The OH emission was arbitrarily assigned to the blue vector, CH to the green vector, and C-C to the red vector. When both OH and CH are emitting from similar locations in the cycle, the imagery will appear blue-green. When C-C and CH are emitting from similar locations, that sector will be in the yellow-orange spectrum, and when C-C and OH are emitting from similar location, that sector will appear a shade of purple.

3.5. Error and Uncertainty of Phase Angle and Intensity

Error and uncertainty manifest themselves as lateral averaging of the phase angle in the imagery. Uncertainty regarding cycle location due to small variations in cycle time was directly measured as the residual error from the phase angle model, as shown in Figure 72. If the residual errors are an artifact of how the detonation azimuth was measured, the linear fit over 25 cycles will wash out most of the variability. On the other hand, real variations of the detonation wave speed within the selected averaging time will be manifest as a lateral averaging of the intensity along the phase angle.

The detonation wave front was assumed to be normal to the direction of propagation. When tracking the wave front, the tracking method is vulnerable to error caused by the azimuthal ambiguity of an oblique wave front in an annular channel. The

annular channel has a width to outer radius ratio of 1:3.7, allowing the detonation wave front to vary across the width of the channel. The variation includes pushing a portion of the detonation wave further along the inner radius or outer radius while the mean of the detonation front lags behind. The lead-lag may then reverse and may erroneously skew the wave front tracking ahead or behind the median, causing the residual errors in the linear fit described in Section 3.3 and causing additional phase averaging in the time-averaged imagery. Within the video imagery field of view, the measurement and quantification of this wavefront variability was not measured. This uncertainty is estimated at approximately one percent of the wave speed.

Wave position was calculated from the horizontal location of the detonation wave front in the video imagery and is the cosine of the cycle angle, as described by Equation 67. At the left and right hand sides of the annulus there were fewer pixels per angle than in the center. Uncertainty in the detonation wave front location by a single pixel had a much larger error at these edges where each pixel represented multiple degrees of azimuth than at the center of the image where a single pixel represented a fraction of a degree of azimuth. Since the error within the cycle due to measurement artifacts like this is removed by the linear regression of Equation 68, this error produces no contribution to the error or uncertainty of the phase angle. By not including the edges of the detonation channel in the average, the circular effect of phase angle averaging was also minimized.

A bias error was also be introduced by assuming that the field of view was isometric rather than perspective. This error was introduced by assuming that the edge of the inner and outer walls of the detonation channel were orthographically at 90° to the focal plane, and that 180° may be measured between the tangent lines at the left and right

portions of the cylinder. In reality, the camera experienced a perspective view. The ratio of the detonation channel width to camera distance was approximately 1:10, giving an angular field of view of about 3° and restricted the field of view on the front of the RDE centerbody to approximately 177° rather than 180° . This effect produced no uncertainty on the phase since the phase angle model was built across multiple laps but appeared as a non-linear trend in the residuals when plotted as a function of phase angle. It also introduced lateral averaging uncertainty on the order of one degree.

A 60° sector was selected for inclusion since the conversion from rectangular to cylindrical coordinates followed a sine distribution. Thus, using the small angle approximation, as described in Section 3.3 of this chapter, the azimuth from the center of the sector was easily computed as the column from the center. This method avoided the need to re-sample but introduced a small error, as depicted in Figure 75. Errors in the cycle average are introduced by saving 60° of azimuth without re-sampling the edges to combine multiple columns. This places the columns beyond 25° from the center into columns further from the center than they belong in, and thereby introduces

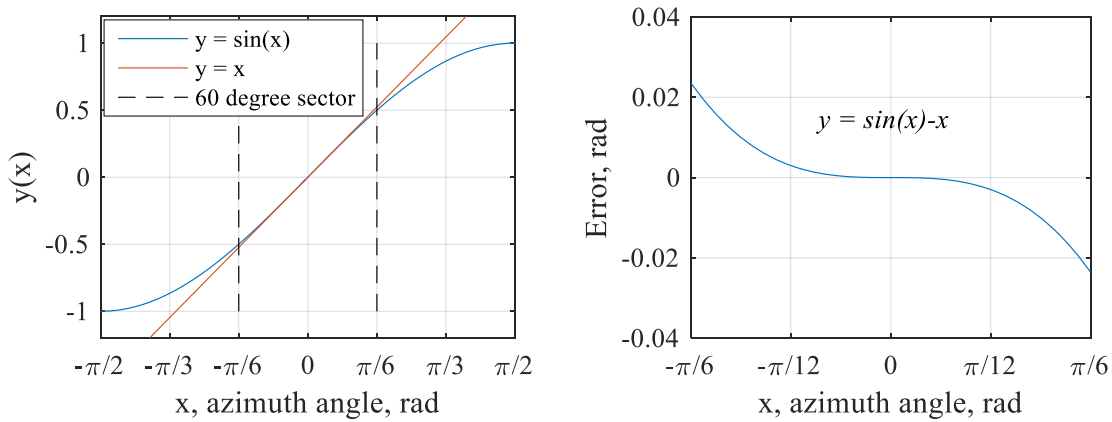


Figure 75. Cycle azimuth error is introduced by using the small angle approximation; cycle azimuth error is approximately 1.35° at 30° off azimuth, or about 0.4%

approximately 1.35° of phase averaging in the edges last column of sector image. This is a small error that represents approximately 1% of the cycle and far less than the uncertainty in the cycle phase angle model.

The exposure time of the camera introduced its own phase angle averaging. While the photosensor gate is open, it integrated the photons reaching the sensor, but the detonation wave continued to move. At a frame rate of 40,000 fps and a detonation cycle frequency of 2,000 Hz, the detonation moved through one twentieth of a cycle, $\pi/10$ radians, or about 18° . The effect of the integration time on uncertainty was greatly reduced by always tracking the leading edge of the detonation. The video camera maintained a frame rate of 40,000 fps with an exposure time that was close to $1/40,000^{\text{th}}$ of a second. The RDE cycle frequencies were usually about 2,000 Hz, so that the video imagery always showed a detonation zone that a single video frame time averaged the detonation across $1/20^{\text{th}}$ of the cycle or about 18° of azimuth. Since the integration time is constant and the wave front tracking methodology consistently seeks to track the leading edge, the integration time averaging does not introduce uncertainty into the phase angle model. Only the detonation is moving at 2000 Hz. The remainder of the flow field translates much slower and produces only about 10% to 30% of the lateral averaging when compared with the detonation wave. The anticipated result is that the image will have a broad 18° band that shows detonation, while the remainder of the cycle will have features that can be resolved to between 1.8° and 6° of phase angle.

The uncertainty in phase angle due to the model uncertainty, small angle errors, and estimated variability in wave front shape are summarized in Table 5. The uncertainty of the detonation wave intensity due to lateral averaging is also shown in Table 5 and

represents the root mean square of the total phase angle uncertainty from the tracking model with the 18° of uncertainty associated with the video camera integration time. The imagery taken with the CH filter showed the worst phase angle averaging and phase angle uncertainty due to detonation wave speeds varying during the sampled period. The imagery taken with the C-C filter showed the least variability in phase angle position and lateral averaging, and this lower uncertainty produced a steeper gradient at the leading edge of the detonation front and a slightly narrower time-averaged band of chemiluminescence.

Table 5. Uncertainties for wavefront phase angle with a 95% confidence level

Filter	Model Uncertainty	Small Angle Uncertainty	Wavefront Shape	Total Phase Angle Uncertainty	Total Lateral Averaging Uncertainty
OH	$\pm 12^\circ$	$\pm 1.35^\circ$	$\pm 1.8^\circ$	$\pm 12.2^\circ$	$\pm 22^\circ$
CH	$\pm 18^\circ$	$\pm 1.35^\circ$	$\pm 1.8^\circ$	$\pm 18.1^\circ$	$\pm 26^\circ$
C-C	$\pm 8^\circ$	$\pm 1.35^\circ$	$\pm 1.8^\circ$	$\pm 8.3^\circ$	$\pm 20^\circ$

The single cycle image in Figure 66 showed deflagration structures within the moving flow field. These structures were interpreted as deflagrating reactants, and were seen in the video imagery to be turbulent structures which both gyrated and expanded as they translated from the feed system to the channel exit at the top of the image. The time averaging of this turbulent flow field inevitably washed out the contrast between a dark inert gas and the more intense combustion. In the effort to understand what the dark band issuing from the plenum was, it should not be forgotten that the dark band itself will, to some degree, become lost as the turbulent portion of the flow field is averaged over multiple cycles.

4. Results and Discussion

The premixed ethylene-air RDE emitted a bright blue zone of combustion as seen in Figure 76. Premixed fuel and oxidizer flowed from a feed plenum at the bottom of the image toward the detonation channel exit at the top with a mass flow rate of 0.33 kg/s and equivalence ratio of 1.05 while the detonation passed from the left of the image toward the right. The exposure for the image was approximately 1/8200 s during which time the detonation moved approximately 90 degrees of phase inside the annulus. The wave front was last captured in the center of the image and had left a bright trail of chemiluminescence burned into the video frame as it moved. The blue coloration of the flame is typical of the Swan band emission in the visible wavelengths from diatomic carbon. Horizontal bands were seen between the bright bands of combusting reactants. The dark band persisted even in the region on the left of the image where the detonation has moved through approximately one fourth of the annular channel as it moved from left to right. The high speed video camera was sensitive to ultraviolet through visible red wavelengths,



Figure 76. Full color imagery of an ethylene-air premixed RDE configured with a quartz outerbody and showing the distinctive blue hues of Swan band emission captured with an exposure of 122 μ s, or approximately 1/4th of a cycle

but only emissions in the green, blue, and violet bands were present. This corroborates the spectra of Figure 68 taken during a separate run. Detection of active combustion radicals in the dark band was attempted with three additional high speed videos that were collected using band pass filters. The settings for the camera and flow settings for each of the images created from the videos is detailed in Table 6.

4.1. Hydroxyl (OH*) Bandpass Image

One of the prime indicators of combustion is the Hydroxyl (OH*) radical.

Hydroxyl emits from the $A^2\Sigma^+ - X^2\Pi_i$ electronic transition between the wavelengths of

Table 6. Summary of time averaged image conditions

Image	Radical	Emission Band (nm)	Band Pass* (nm)	Exposure (ns)	Gain (%)	Cycles (#)	Phase Uncertainty
Figure 66	OH	303-323	300-342	500	65	1	N/A
Figure 77	OH	303-323	300-342	500	65	28	$\pm 12.2^\circ$
Figure 79	CH	424-436	419-452	500	63	25	$\pm 18.1^\circ$
Figure 82	C-C	545-564	555-567	500	65	26	$\pm 8.3^\circ$

* Filter limits taken at full-width half maximum

(Table 6 Continued)

Image	Radical	Mass Flow Rate (kg/s)	ϕ	D, Detonation Wave Speed (m/s),	Cycle Time (μ s)	β_1 , Phase Rate (rad/frame)
Figure 66	OH	0.320	1.11	1040	487	0.322395
Figure 77	OH	0.320	1.11	1040	487	0.322395
Figure 79	CH	0.382	0.992	1011	502	0.312946
Figure 82	C-C	0.374	1.03	1019	498	0.315514

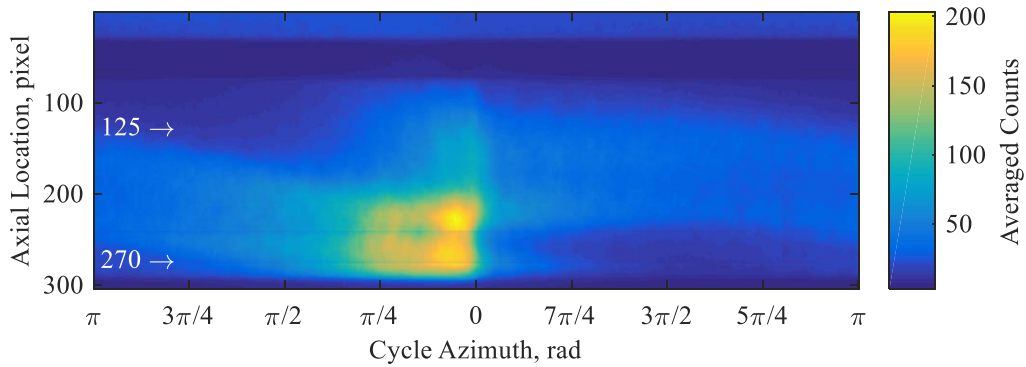


Figure 77. Hydroxyl (OH*) emission from time averaged filtered high speed video of an ethylene-air premixed RDE operating at 0.320 kg/s total mass flow, $\phi = 1.11$

300 nm and 320 nm. Figure 77 shows the time averaged emission of hydroxyl over the course of 28 cycles. The RDE was operating at an equivalence ratio of 1.11 and a mass flow rate of 0.320 kg/s. Because this imagery was collected with slightly rich conditions, not all reactants were consumed.

The hydroxyl chemiluminescence showed the characteristic sharp gradient of a detonation wave traveling from the left to the right in the image. The chemiluminescence had a bright band approximately 23° of azimuth wide, which matched the anticipated 18° of detonation wave travel during the video frame exposure time added in quadrature with 12.2° of model error. The 95% confidence interval for total phase angle uncertainty for the detonation wave was reported in Table 5 as approximately 22° . This provided an indication that the model performed at the reported residual error. The hydroxyl emission left a sweeping trail to the left of the detonation wave that extended the full cycle as it gradually decayed.

The detonation front extended from the injection slots, which were obscured at the bottom of the image, to the detonation channel at the top of the exit. The primary reaction zone for the detonation front brightly emitted between axial location 300 and 210 as it passes through the premixed refill zone. A secondary zone extends from axial location 210 to 110 where it was obscured by the opaque band holding the quartz outerbody in place. The secondary zone did not emit as brightly, and, based on the path lines in Figure 67, this was a result of a reactant depletion from the primary detonation. Figure 78 shows cross sections taken from two horizontal lines in Figure 77 at the axial locations of 125 and 270. The data from location 270 passed through the primary detonation zone, while the data from line 125 passed through a secondary pressure-wave

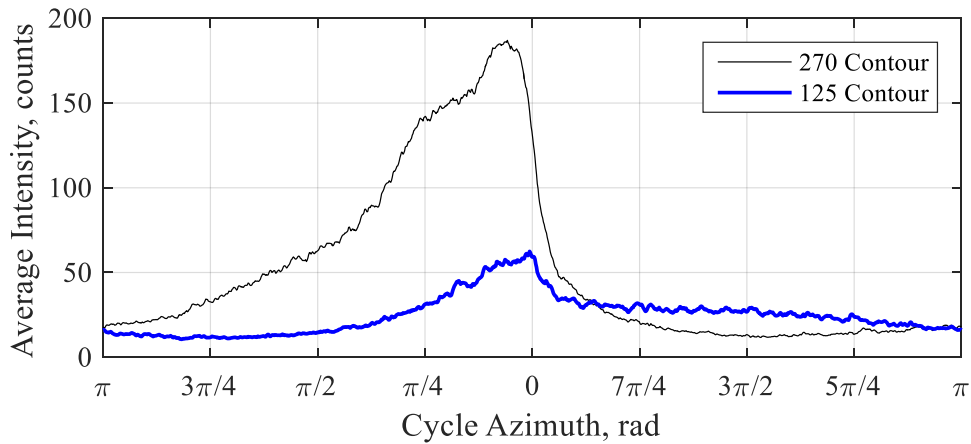


Figure 78. Cross section of the average OH intensity at the 270 pixel axial location

combustion zone. The trailing hydroxyl emissions behind the primary detonation zone gradually decayed as the cycle progressed from left to right and wrapped around. The cross section at 270 also passed through a low-emission zone between π and $7\pi/4$ radians cycle azimuth. The time-averaged low emission zone corresponded to the dark band referred to in the introduction of this chapter and was the zone of primary interest.

Emission persisted throughout the time-averaged trail of detonated products trailing the detonation wave, and the time-averaged data of from Figure 77 never showed a location where there was zero emission, in contrast with the zero-emissions features seen in individual frames of the video imagery. The chemiluminescent structures were seen to rotate and translate in the flow, and each detonation cycle resulted in slight variances to the movement. The variation, in turn, created a time-averaged image that had regions of relatively lower emission but not regions of zero emission. Also, chemiluminescent emission persisted at some level throughout the remainder of cycle, indicating that the detonation wave in this RDE did not result in complete combustion with the first passing of the detonation wave. Instead, combustion was completed in a

flow field where pressure constantly varied with time and position as the products expanded by a second passing of the detonation front as noted above. Subsequently, while the dark band still existed, it was washed out by the time-averaging and was represented in the time averaged images as the low-emission zones preceding, penetrating, and trailing the combustion zone.

There was a region of hydroxyl emission to the right of the detonation wave in Figure 77 that was not predicted in the computational models of Schwer et al. (21). The emission zone resides between $3\pi/2$ rad and 0 rad phase angle and between 250 pixel and 290 pixel in the axial location in the time averaged image. The pathline of this inflow emission zone is next to that of the low-emission zone discussed above and time delayed from the low-emission flow. From the detonation wave's frame of reference, this new zone is associated with the inflow of fresh reactants from the feed plenum at the bottom of the image. The hydroxyl image marked the initiation of a deflagration combustion at the reactant feed slot between passages of the detonation wave. As the partially reacted fluid passed into the detonation wave, it produced the most intense region of chemiluminescence in the entire cycle. Assuming that the fresh reactants were releasing energy as they began the reaction, the chemiluminescence preceding the detonation in the cycle was an indicator of increased temperature and pressure in addition to a different chemistry than in the feed plenum. The observations taken from the chemiluminescence imagery supports the conclusion of Chapter V that the detonation wave property calculations need to include variations in the temperature and chemistry when evaluating real RDE.

4.2. Methylidyne (CH) Bandpass Image

Similar to the effort and results described in Section 4.1, the high speed imagery was filtered for methylidyne during a separate test where the RDE operated at 0.392 kg/s and $\phi = 0.992$, as described in Table 6, to generate Figure 79. Although attempting to run with the same conditions as the previous imagery, the mass flow rate was slightly higher and the equivalence ratio notably less than for the hydroxyl imaging. Again the detonation wave front is shown just to the left of 0 rad cycle azimuth, extending from the mixture injection plane at the bottom of the image to the detonation exit channel at the top of the image. Parallel to the hydroxyl image, the detonation zone still shows a primary detonation zone in the lower center portion of the image, a secondary combustion zone in the upper half, a region of low emission trailing the detonation wave and passing through the remaining cycle, and a predetonation combustion zone feeding the brightest region within primary detonation zone.

Unlike the data for Figure 77, the linear regression of the phase angle showed a peculiar heteroscedasticity with time, as seen in the top plot of Figure 80. The variation of the mean of the residual with time indicated that the rotation frequency of the

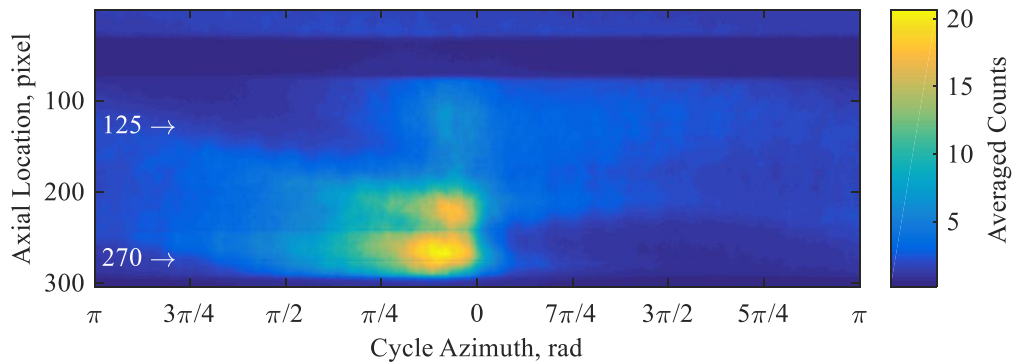


Figure 79. Methylidyne (CH) emission from time averaged filtered high speed video of an ethylene-air premixed RDE operating at 0.382 kg/s total mass flow, $\phi = 0.992$

detonation wave was shifting slightly throughout this data set. The result was azimuthal averaging over more phase angle than the hydroxyl image of Section 4.1 that was manifest in Figure 79 as a broader zone of intensity than was seen in Figure 77. The variation that accurately described the phase angle variation was the residual error between -30° and $+30^\circ$ phase angle in the lower plot of Figure 80. The uncertainty in this region was the appropriate descriptor of the model error for two reasons; first, the model was constructed from the wavefront location in the laboratory frame of reference and, second, the phase angle and the laboratory frame of reference were synonymous for the lower residual plot in Figure 80. The time-averaged imagery only used the information within the -30° to $+30^\circ$ sector as shown in Figure 70, so only the residual error from that sector is retained. The model uncertainty was reported in Table 5 as $\pm 18^\circ$ for the methylidyne image, which compared very well with the detonation wave averaging seen in Figure 79, reaffirming the stated accuracy of the plot.

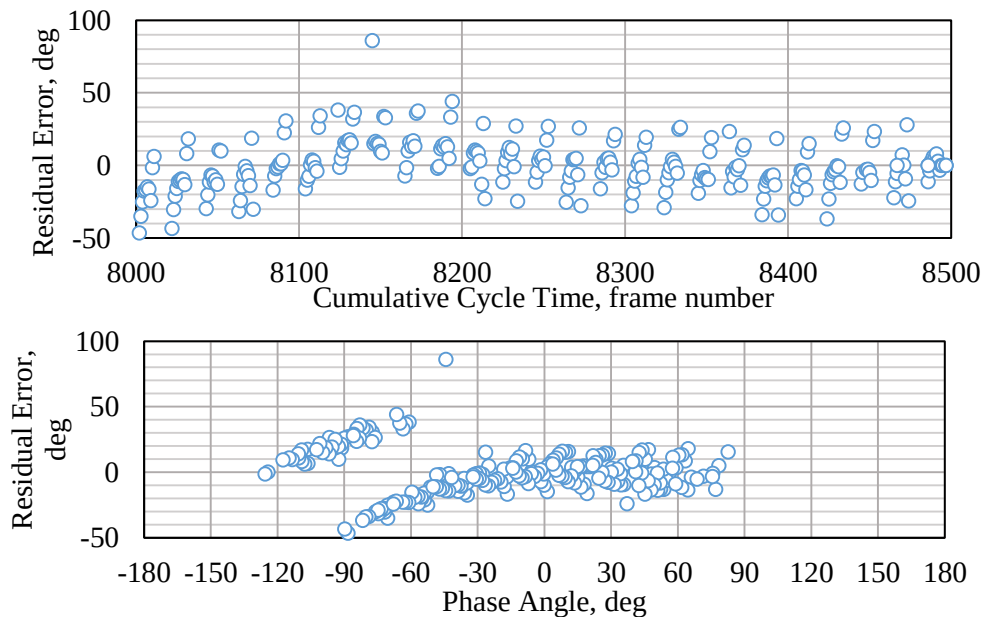


Figure 80. Residual error for the linear fit of cycle phase rate for the CH image showing variable phase rates and cyclic measurement error, the linear fit removes the cyclic measurement error but not the variable phase rate

A cross section plot from the 270 pixel axial location of Figure 79 is shown in Figure 81. Just as with the hydroxyl, the emission decays behind the detonation wave. The emission decay is comparable to that of the OH emission. Although it is tempting to make an assessment based on the differences in the shape of the contours, it must here be noted that the imagery comes from two different runs, and, therefore, the changes in equivalence ratio may be the root cause of the difference in radical production and relaxation. The differences in mixture ratios is an effect that cannot be separated within this data set. Ideally, a binocular system would be constructed that allows simultaneous imagery of an identical field of view through two separate filters so that the assessment can be accurately made. With such a system, both time-accurate and time-averaged offsets in radical production and relaxation could be made. The presence of time offsets would inform the chemical-kinetic models for detonation combustion, and pursuit of such an effort is a recommended follow-on to the present work.

Like hydroxyl, methylidyne is an intermediate product of combustion; an intermediary step between an ethylene molecule and the final products of water and

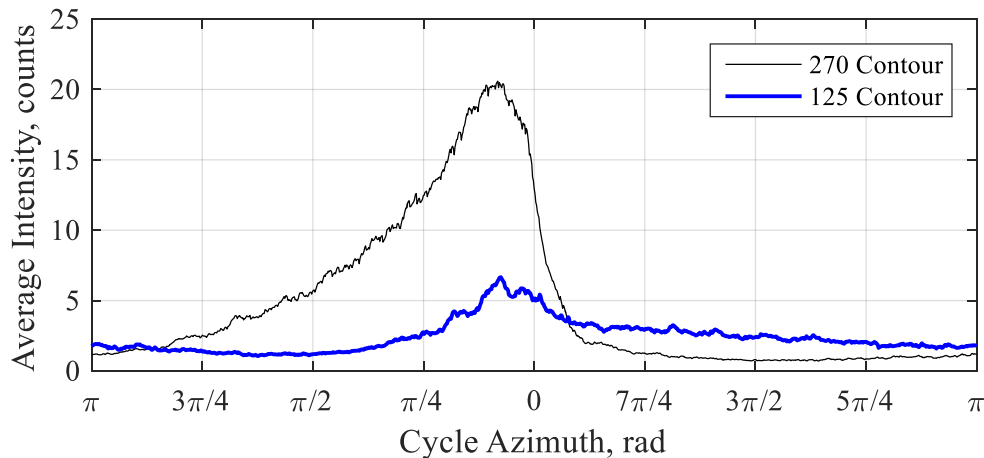


Figure 81. Cross section of the CH filtered average intensity taken at the 270 pixel and 125 pixel axial location

carbon dioxide. The emission trailing the detonation both on the first and second pass indicated that in this engine the combustion chemical processes had not progressed to completion within the span of one detonation cycle. This may or may not be indicative of all hydrocarbon fuels in an RDE, but it is an area of interest. If the CFD community intends to model RDE with accuracy, the real timescales of the combustion need to be quantified and modeled correctly. Inability to combust completely within the detonation wave denies a detonation some of the potential chemical energy. Furthermore, one of the underlying assumptions of the Chapman-Jouguet detonation model is that the combustion process completes all reactions to equilibrium. A detonation that fails to unlock the full chemical potential within the reactant mixture will always have a lower wave speed compared to the calculation of a Chapman-Jouguet detonation.

A multi-spectral system with associated analysis that can provide the insight into production and consumption of the combustion radicals, temperature, or pressure profiles would inform the computational community. With such a system, the chemistry models could be built and verified, and the initial assumptions for the one-dimensional Chapman-Jouguet calculations could be correctly applied.

4.3. Ethenediylidene or Bicarbon (C-C) Bandpass Imagery

Emission of the ethenediylidene, or bicarbon, within the flow is shown in Figure 82 and was captured in an identical method to the hydroxyl and methylidyne emissions discussed in Sections 4.2 and 4.3 of this chapter. Because the available filter had such poor transmission, as noted in Figure 68, the signal passed to the sensor was relatively less than the other imagery while the same noise existed. The time averaged image shown

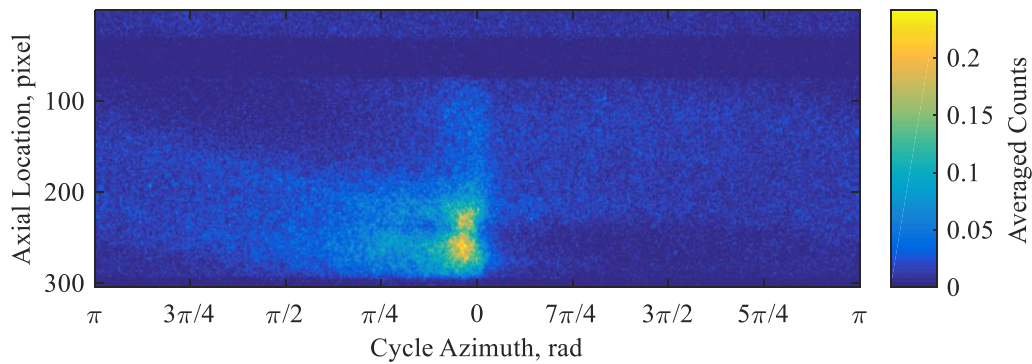


Figure 82. Time averaged emission from ethenediylidene (C_2), filtered high speed video of an ethylene-air premixed RDE operating at 0.374 kg/s total mass flow, $\phi = 1.03$

in Figure 82 displays the characteristic hallmark of a low signal-to-noise ratio: a grainy image. Time averaging helped to smooth the image out but did not completely ameliorate the effects of an overly aggressive filter. Future work with this imagery should consider finding a better bandpass filter or imaging one of the other Swan bands, such as the $\Delta v = 0$ peak between 502 nm and 520 nm.

Despite the lower signal-to-noise ratio, the wave front phase rate model performed better, with only $\pm 8^\circ$ of uncertainty. The small uncertainty in the model resulted in a “sharper” peak in the cross section plot of Figure 83. The total phase angle

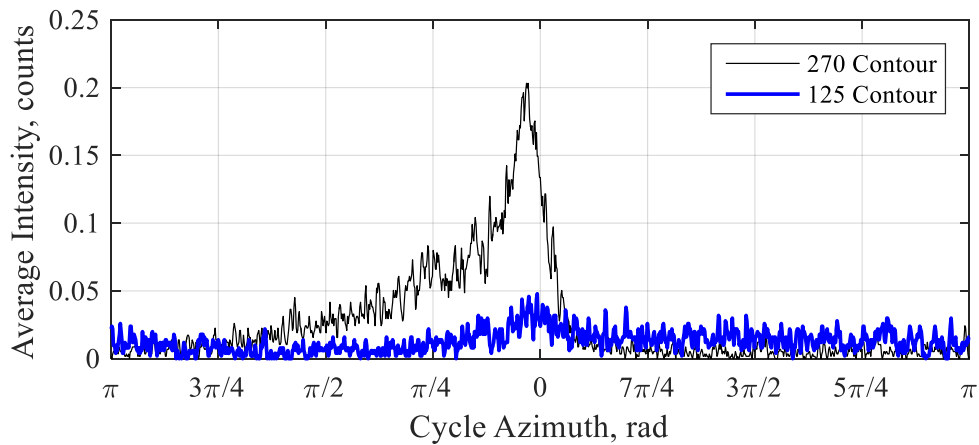


Figure 83. Cross section plot of the C-C filtered time-averaged image at the 270 pixel axial location

uncertainty of the detonation wave was reported in Table 5 as $\pm 22^\circ$ and corresponds well with the phase angle width displayed in both Figure 82 and Figure 83.

The cross sections shown in Figure 83 were taken at the axial locations of 270 and 125. These cross sections appeared to indicate a faster decay and less production than for either the hydroxyl or methylidyne radicals. The cross section plot also displayed the influence of a decreased signal to noise with an intensity line that varied rapidly over the range of a small angle and a much lower intensity count than the other filtered images. At this point in the analysis, the signal-to-noise became a real issue, since it appeared that there was a zone of increased C-C emission at $\pi/4$ azimuth, but the relative variation near the feature prevented definitive identification. No additional insights were noted based on the ethenediylidene imagery beyond those of the previous images.

4.4. False Color Multi-Spectral Image

The three time-averaged images in Figure 77, Figure 79, and Figure 82 were super-imposed with false-color to create Figure 84, as described in Section 3.4 of this chapter. In this figure, the three detonation waves traveled from left to right, while the premixed reactants flowed from the bottom of the image toward the detonation channel exit at the axial location 30 pixels from the top of the image. The cycle azimuths of each filtered image were shifted slightly from previous figures in an attempt to match the sharp intensity gradient of the chemiluminescence associated with the detonation wave. There was no evidence that suggested the luminescent regions were equidistant from the leading shock wave, so this becomes an assumption.

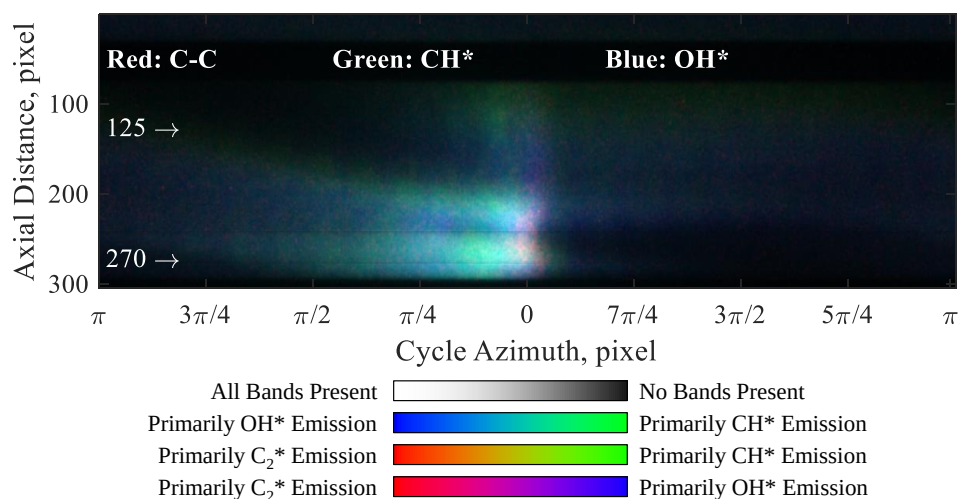


Figure 84. Emission of multi-spectral high-speed imagery cycle-averaged from different runs of an ethylene-air RDE with similar conditions, each filtered image was normalized before combination

Figure 84 aggregated information taken from three separate test events whose flow conditions were not identically matched. Equivalence ratios varied from 0.99 to 1.1, while mass flow rates varied from 0.32 to 0.38 kg/s, as described in Table 6. These variations introduced independent flow field and chemistry variability which could not be isolated in this limited data set. Since the influence of chemistry and mass flow rate could not be isolated, a rigorous quantitative comparison of the images cannot be made.

A qualitative approach provides some insights to the detonation mode for this premixed ethylene-air RDE. First, all three bands are present in the region determined to be the detonation wave, as seen by the white region at approximately 0 radians of cycle azimuth. Further, the detonation front stretches the entire length of the channel but produced much less emission between the axial position of 90 to 200 than between 200 and 300. A portion of the refill zone immediately to the right of the detonation front was seen to be chemiluminescent, indicating deflagration was anchored at the premixed feed

system. This zone initiates combustion before the detonation arrives, and the highest radical emission is noted where the preburned zone passes through the detonation wave.

The dark band noted in Chapter IV was less apparent in the time averaged imagery. As discussed previously, the non-emitting zone flowed into the detonation channel behind the detonation wave, mixed with chemiluminescent structures, and moved toward the exit as the detonation cycle progressed. In the time averaged images of this chapter, these zones, which show no-emission in real time, become averaged out and appear as lower-emission zones in what would be expected to be a uniform field. The low emission zones were shown in the time-averaged imagery collected from the ultraviolet and visible spectrums. Omission of chemiluminescence in this band, even in the presence of an active detonation wave, indicated that the OH, C-C, and CH radicals are both less prevalent over time (and assumed not present in real time) and not produced in this zone. In an RDE that provided premixed fuel and oxidizer directly into the channel, this persistent band tied to the detonation cycle could not be reactants since they do not produce the chemiluminescent radicals when subjected to the detonation wave. The quenched combustion products would not emit, and the premixed feed system was designed to arrest flashback by feeding the detonation through very narrow slots that quenched the combustion as it is forced back into the system. The conclusion is that the dark band was inert combustion products that appeared in the time-averaged imagery as low-emission zones.

The dark band was surrounded by bands of chemiluminescent flow with which it turbulently mixed as noted in Figure 66. Time averaging the cycles consistently showed that the band persists. The false-color image in Figure 84 represented a comparative

contour of the detonation cycle OH, CH and C-C radicals. A cross section of the contour was taken at axial locations 125 and 270 and was shown in Figure 85. The false color image collected the cross section plots of Figure 78, Figure 81, and Figure 83. All lines showed that the detonation wave front was correlated to a sharp rise in the emission in all spectral bands. As the detonation cycle progressed, the intensity decreased exponentially until it reached an emission floor somewhere above zero and probably created by underlying black-body radiation of carbon compounds.

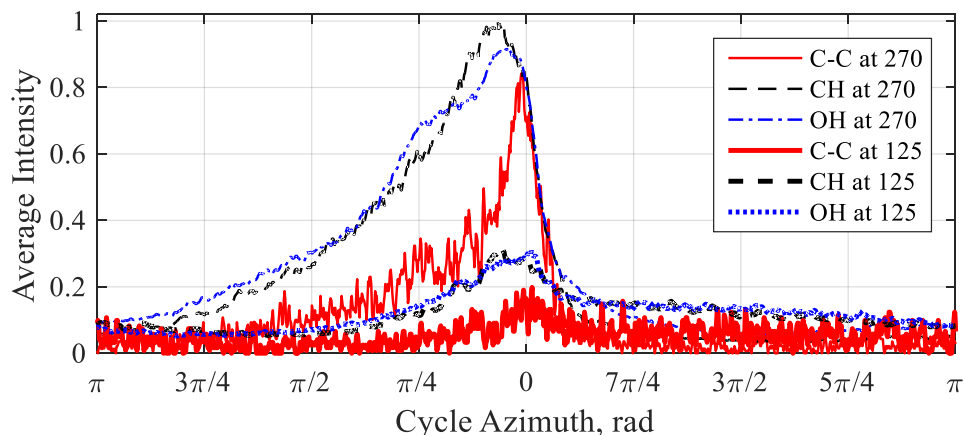


Figure 85. Cross sections from the normalized false-color multi-spectral imagery at the axial locations of 270 and 125

5. Conclusions from Multi-Spectral Imagery

A premixed ethylene-air RDE was configured with an optically accessible outerbody. High speed multi-spectral video was collected with a filtered high-speed camera connected to a filtered intensifier. The time-averaged cycle imagery distilled from the video footage showed a dark band that persisted throughout the cycle and mixed in a turbulent manner with deflagrating reactants feeding into the plenum. Lack of emission from the ultra-violet and visible spectrum indicated that the dark band did not contain

excited OH, CH, or C-C radicals, nor the ingredients to produce those radicals in the presence of either a detonation wave or deflagration.

The deduction that the dark band consisted of inert combustion products showed that the thermal and chemical quenching mechanisms within a premixed RDE are important, and should be modeled in CFD simulations. Furthermore, the emission from the OH, CH, and C-C radicals is seen to decay over an extended period of time within the detonation cycle, indicating that CFD codes need to have an accurate combustion mechanism that have not been so oversimplified that reaction is completed in a single step across the detonation wave. Although such a model might be appropriate for a pulsed detonation engine where the detonated gases continue to reside within the tube for a finite period of time allowing the combustion to move toward completion and reach equilibrium, the dwell time in an RDE combustor is much shorter, disallowing complete combustion and equilibrium.

VI. Conclusions and Recommendations

1. Motivation

The time and spatial delay in mixing fuel and oxidizer were implicated as the root causes that created the difference between computational and experimental wave speeds and specific impulse. While most CFD RDE simulations assume a premixed fuel and oxidizer injected through an idealized scheme of infinitely small holes distributed evenly across the injection face, experimental RDE inject separate fuel and oxidizer injection streams such that mixing occurs at the base of the detonation channel. A good comparison between experimental results and CFD results using the premixed assumption required construction and operation of an experimental premixed RDE. Operating a premixed RDE required overcoming both the problem of unstart when the detonation consumed all the reactants too quickly and the hazard of flashback into the mixing chamber when the detonation pushed combustion back through the feed plenum. This research effort successfully applied adjustments to traditional burner stability theory to describe a premixed feed geometry that arrested flashback while it supplied an RDE with fresh reactants for continuous operation.

2. Objectives and Achievements

The desire to construct and operate a premixed RDE that avoided flashback and supported continuous detonation was guided by four objectives. These objectives were met, as described here:

2.1. Objective 1

The first objective was: “Discover the flow conditions that halt flashback into a premixed feed system exposed to a transient detonation.” Flow conditions that halted flashback were discovered when experimental results showed that long narrow slots could successfully arrest flashback, that flashback occurred at the speed of sound in the reactants, and that the velocity gradient method of determining flashback limits was applicable, but that adjustments needed to be made. The long narrow slots identified that a compressible friction flow regime that exchanged stagnation pressure for bulk velocity was key to arresting flashback. The fluid properties constrained by the geometries define the flow conditions. The flow conditions are generally summarized by the boundary layer velocity gradient and theoretical quenching distance figures of merit.

2.2. Objective 2

The second objective was: “Characterize the correlations between flashback in a premixed flow exposed to a transient detonation front and traditional burner stability parameters, such as; quenching distance and critical boundary layer velocity gradient as a function of the temperature, pressure, equivalence ratio, mass flow rate, and fuel.” The characterization involved the collection of experimental data sets where premixture was fed into an operating detonation engine through long narrow slots. Both hydrogen-air and ethylene-air mixtures were injected into a pulsed detonation engine. During a second set of tests, premixture was fed into an operating RDE while the same parameters were varied.

The slot length, slot height, mass flow rate, and equivalence ratio were varied during both tests, and the feed system was monitored for flashback to identify those combinations of variables where flashback did and did not occur. The collected data were compared to the traditional burner stability parameters of quenching distance and critical boundary layer velocity gradient. The boundary layer velocity gradients were calculated using the premixed plenum feed conditions and Equations 36, 37, and 39 and adjusted back to the conditions referenced in traditional burner stability diagrams using Equation 46. These adjustments required both laminar flame speed and quenching distance calculations from models. Since the estimate was based on the highest pressure location in the feed plenum, it provided the most conservative (lowest) velocity gradient that was seen for the entire length of the feed slot. After adjustment, the conservative estimates were found to agree qualitatively with the published burner stability diagrams.

A premixed detonation feed design method was formulated based on the experimental data for premixed ethylene-air. The method first used an equation that related the maximum flashback length that could be tolerated to support a rotating detonation cycle with an assumed operating frequency so that slot length could be bounded (Equation 61). Next, an equation that related slot height to slot length required to arrest flashback (Equation 51 and 52) defined the feed geometry. Finally, minimum mass flow rate thresholds were related to the maximum flashback velocity gradients using Equation 46, while feed pressure and number of slots were treated as independent variables.

2.3. Objective 3

The third objective was: “Explore the ability of traditional burner stability design principles to effectively arrest flashback in a premixed rotating detonation engine.” The relationships and characterizations from Objective 2 led to a design that would arrest flashback in less than 2.5 cm with a 0.5 mm slot height using ethylene as the fuel and air as the oxidizer. Hundreds of runs using the slot height of 0.5 mm resulted in no flashback events, and the slot height was increased to 0.8 mm where flashback was also not seen. The full range of the available slot height has not been tested. The author concludes that the principles and adjustments discussed for Objective 1 and Objective 2 and used to design the premixed RDE feed system were effective for the construction of a system that successfully fed the detonation but where flashback was not evident.

2.4. Objective 4

The fourth objective was: “Experimentally characterize the operation of a premixed rotating detonation engine.” This objective was met by building an operating map for the premixed RDE and exceeded by comparisons with non-premixed RDE, CFD results, and the efforts to understand the operating mode with multi-spectral imagery.

An operating map was built for the premixed RDE that varied the mass flow rates and fuel-to-air equivalence ratio. The operating map was compared to a non-premixed RDE and found that premixed RDE detonation occurred within a narrower band of equivalence ratios. The narrower range of premixed RDE detonation suggests that a non-premixed RDEs operate with a localized region of reactants at a minimum ignition energy over wider ranges of equivalence ratios. Premixing the fuel and oxidizer ensures

that the reactants presented to the detonation front are at a specified equivalence ratio without variation, and if those reactants are not at the minimum ignition energy, then detonation operation is inhibited by the higher ignition energy and larger cell size. Wave speeds were between 40% and 60% of Chapman-Jouguet predictions calculated with standard one-dimensional algorithms and assuming that the mixture feeding the initial conditions is at the global equivalence ratio with no dilution due to mixing and no heating.

Panchromatic video imagery of premixed RDE operation showed combustion anchored at the mixture injection and indicated that initial conditions for computational sources need to include the effects of deflagration and product-reactant mixing in RDE calculations and simulations. The presence of combusted products was confirmed through multi-spectral imagery that captured chemiluminescent emissions of hydroxyl (OH), ethenediylidene (C-C), and methylidyne (CH) radicals in the detonation channel.

3. Unique Contributions

This research provides the first detailed description of design and operation of an air breathing premixed rotating detonation engine. The first theory that described how to adjust the detonation engine flashback conditions to traditional burner stability diagrams is shown with Equation 46. This adjustment led to a methodology for designing a premixed RDE that ensured fresh reactants supported a continuous detonation cycle while simultaneously arresting flashback, using Equations 51, 52, and 61. These equations describe the critical fed slot parameters that allowed the construction of the premixed RDE described in Chapter IV, Section 2.1. Experimental data from this

premixed RDE showed no signs of flashback, thereby demonstrating the theory and methodology were sufficient. This device has opened the door to study how the fuel-oxidizer mixing delay influences the operation of an RDE.

The premixed RDE required mixtures near stoichiometric ratios of fuel and air, as opposed to non-premixed RDE, and exhibited different detonation properties than had been expected. Wave speeds were much slower than CFD or one-dimensional calculations and suggested that the experimental wave speeds are influenced by the multi-dimensional variations in the mixtures and not the mixing time delay seen in non-premixed RDE. Operating maps constructed by varying mass flow rate and equivalence ratio showed that the premixed RDE achieved detonation only at equivalence ratios closer to one while similar non-premixed RDE operated with equivalence ratios between 0.6 and 1.5. The difference in operating maps led to the conclusion that variation in the mixture across physical space was contributing to slower detonation wave speeds in experimental RDE.

Multi-spectral imagery captured deflagration co-existing with the detonation cycle inside the detonation channel. This multi-mode combustion provided evidence that the ethylene-air rotating detonation was reliant on the combustion to preheat the reactants. Dark regions within the flow field were noted, and, upon further investigation, were concluded to be inert combustion products.

4. Significance

These results identify that accurate modeling of a practical RDE will require the ability to calculate the deflagration reactions as well as the detonation within the RDE.

Further, accurate modeling will require capturing the separate stream or finite injection geometries so that the effects of mixing or flashback may be accurately modeled.

Simplifications that negate the variation in mixture across the detonation wave front and remove the time-varying flow into the detonation channel cannot capture the detonation cycle accurately and will always provide overly optimistic estimates of performance.

Further, in a premixed system, the effects of quenching a chemical reaction in the feed system was shown experimentally to be a fundamental physical process that should be modeled.

5. Recommendations for Future Work

Various aspects of this work could be improved upon or studied further. The characterization of the flashback in a narrow slot was a means to an end. While sufficient to meet the objectives, a better understanding of the phenomenon should be pursued. Pursuit of a theory that explains the slot height to length requirements based on measured parameters of feed pressure, detonation channel cycle pressures, and mixture chemistry would eliminate the tedious process of repeating the single injector tests described in Chapter III, Sections 3.1 and 3.2.

It is anticipated that the pressure profile of the detonation engine will drive the flashback profile. The relationship between the detonation engine operating point and flashback would be more apparent if a test section with multiple high speed pressure sensors could be constructed to characterize the feedback pressure wave movement as a function of time. The high speed pressure data would inform any theory that attempted to describe the ability of a slot to arrest flashback since the data would provide evidence

regarding how the feed slot changes the shape of the flashback pressure wave and how any expansion wave might be affecting the pressure wave.

Minimization of deflagration in the detonation channel is another area in which to pursue further research. The premixed RDE operated with continuous detonation only at equivalence ratios near one. The subsequent operating map was fairly small and restricted to mass flow rates below 0.9 kg/s. It would be desirable to seek a configuration where the RDE operated at higher mass flow rates. This could be done by minimizing the flame holding at the mixture injection point or adding additional pressurization to the channel to slow the reactants through the detonation channel. Premixed operation without anchored flame should provide an opportunity to compare wave speeds and operating maps in a rotating detonation that is presented with a nearly uniform mixture.

Appendix I Experimental Analogue of a Premixed Rotating Detonation Engine in Plane Flow

This paper was presented in 2015 at the AIAA Aerospace Sciences Meeting in Kissimmee, Florida and contains the initial results for attempted premixing. The experiment was designed to test the ability of a small hole feed system with an expansion step to arrest flashback. Two predet initiators were intended to be fired sequentially so that two detonation waves passed across the feed plenum in an analogue of an RDE. Upon firing, the predetonator detonation never coupled into the premixed reactants in the channel, so the primary objective could not be met directly. Close observation of the flashback phenomenon in this optically accessible setup provided the insight that small holes were insufficient to halt flashback and that the feed geometry halted the detonation wave but not the deflagration from entering the premixed plenum.

Experimental Analogue of a Premixed Rotating Detonation Engine in Plane Flow

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The mixing effects of fuel and oxidizer in the operation of non-premixed rotating detonation engines (RDE) are not well understood. This experiment explores feed systems for premixed RDE operation. A linear detonation test section was constructed that closely replicates the conditions of a proposed rotating detonation engine. Optically accessible walls facilitate velocity measurements as the detonation travels along a 0.038 cm (0.15 inch) x 15.2 cm (6.0 inch) x 61.0 cm (24 inch) channel. Premixed hydrogen and air are injected into the channel from a mixing plenum with a series of 160 expansion nozzles featuring throat diameters of 0.43 mm (0.017 inches) or 1.04 mm (0.041 inches). Choked flame is only maintained across the field of view during the final test case. Emission of shock waves from a combustion zone are observed and linked to turbulent flow. Shock waves are not seen propagating back into the mixing plenum. Even in the absence of choked flame, six test events experienced flashback, indicating that a small nozzle throat diameter is insufficient to prevent flashback in a premixed detonation engine.

Nomenclature

a	= speed of sound, m/s
d_i	= shock front location at time $i-1/2$, m
f	= video frame rate, s^{-1}
h	= height, m
i	= time index
L_p	= pixel to meter conversion factor
$\dot{m}$	= mass flow rate, kg/s
V_i	= Velocity of shock front at time $i-1/2$, m/s
x_i	= horizontal pixel measurement, pixels
ϕ	= mass fraction fuel to air equivalence ratio

1. Introduction

Premixing fuel and oxidizer removes mixing effects from detonation experiments. For several years, the Detonation Engine Research Facility at Wright-Patterson Air Force

Base has studied and operated rotating detonation engines (RDE) utilizing non-premixed fuel and air injection schemes. It has been shown (102,140) that the rotating detonation is sensitive to the size, quantity and positioning of the fuel and air feed holes. Placement of the fuel and air holes affect mixing, and it is hypothesized that incomplete mixing inhibits the rotating detonation. Mixing of the fuel and oxidizer prior to introducing it into the detonation channel provides an ideally mixed system. With a premixed fuel stream, basic research on the effects of mixing may be carried out (15). However, a system that provides premixed fuel and oxidizer into the detonation chamber may also allow the high pressure detonation to feed back into the mixing plenum. Fire in the plenum will prematurely terminate the test and result in a destructive flashback (1). This research explored feed system geometries for preventing the upstream detonation.

Focused pressure waves passed from the detonation channel into the mixing plenum provide another avenue for a destructive flashback. Previous detonation experiments (141,142) showed that detonation waves tend to propagate as roughly planar waves that diffract at sharp external corners. Within the diffracted portion of the detonation wave, the combustion decouples from the pressure wave and transitions to deflagration. When physical geometries such as internal corners focus pressure waves, detonation may re-ignite. Computational fluid dynamics simulations (75,92) consistently predict that detonations generate overpressure waves that flow into feed plenums, where internal corners tend to focus them and allow re-ignition. Previous research (115) has also shown that attempting to prevent plenum feedback by increasing feed plenum surface area relative to flow volumes reduces the chain branching reactions that drive detonations. To better understand the flow phenomena of a bottom pressure fed RDE

engine, this research included experiments with geometries that implement both favorable surface area (quenching diameter) and geometries intended to inhibit overpressure propagation. The experiment examined whether the feed nozzles quenched the chemical reaction, limited the overpressure waves, and avoided re-ignition.

1.1. Experimental Setup

A pair of predetonator initiators enabled two sequential detonations to pass through the detonation channel during operation. The first wave, as shown in Figure A1.1, was intended to prepare the detonation channel by consuming the unburned reactants in the chamber. The continuous flow of premixed fuel and air from the mixing chamber created a binary zone of combustion products and unburned reactants in the detonation channel. The second detonation was timed to follow the first and detonated into the lower zone containing only unburned reactants.

A linear detonation test section was constructed that closely approximated a small arc of an axial-azimuthal feed system in an RDE (Fig. 1) while enabling schlieren

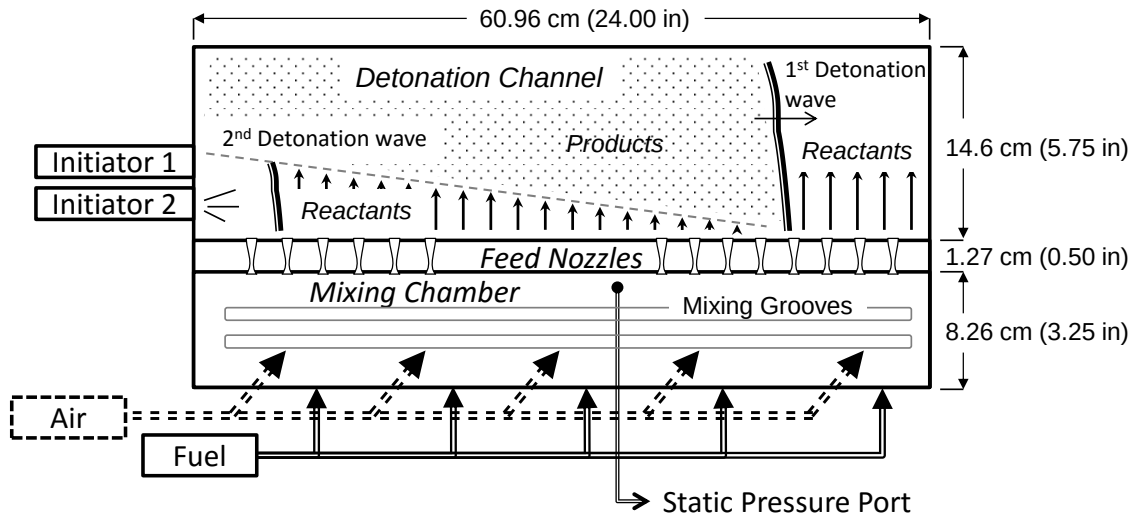


Figure A1.1 Schematic of the linear test section showing fluid streams and ideal detonation mechanics

videography. The device consisted of polycarbonate walls, steel end plates, a pair of predetonators, and a bank of supersonic feed nozzles that separated the mixing plenum from the detonation chamber. The detonation chamber had a channel width of 3.81 mm (0.15 inch), approximating the annulus width of an RDE. The bottom feed plenum was optically accessible and pressure instrumented.

The operating parameters of mass flow rate and equivalence ratio were controlled remotely. Fuel feed pressures were controlled with a pressure dome loader and metered upstream of the mixing plenum with a choked nozzle. Fuel then fed into the plenum through 5 ports of 5.48 mm (0.216 inches) diameter. Air was also controlled and metered upstream with a separate dome loader and choked nozzle, and fed into the plenum from side ports with diameters of 9.5 mm (0.375 inches). Fuel and oxidizer jets entering the mixing chamber were aligned at 90 degrees so that they impinged to promote mixing. Two 2.54 mm (0.1 inch) by 6.35 mm (0.25 inch) grooves in the side of the mixing chamber walls periodically expanded the fuel and oxidizer as it flowed through the channel. The grooves equalized pressure along the length of the chamber and promoted mixing.

A steel bar separated the combustion reactants in the mixing plenum from the combustion reaction in the detonation channel. The bar contained 160 expansion nozzles that choked the flow. The nozzles were grouped in 8 banks of 20 nozzles. Each nozzle bank was 61.09 mm (2.4 inches) long as shown in Fig. 2, and each bank was separated from the next by 11.75 mm (0.46 inches) to allow a bolt to pass through the test section for assembly. The nozzles were oriented to feed the mixture vertically into the detonation chamber. Figure A1.2 shows a two view detail drawing of the expansion nozzles. The

nozzles were not contoured, rather they were free expansion nozzles (143) cut with simple drill bits. Fuel-air mixtures were fed continuously through the nozzles into the detonation channel while the initiators fired. Constant spacing of the walls was established by using the nozzle bar as a spacer, fastening the steel end plates, inserting spacers along the top exit, and bolting the assembly together. The detonation channel was open to ambient conditions along the top and the side opposite the initiators. Once initiated, the detonation wave was intended to travel horizontally through the detonation channel from left to right in Figure A1.1.

Over the course of testing, the modifications in Table A1.1 were made to the feed nozzles and channel inlet in an effort to achieve detonation for the full length of the detonation channel. The original throat and exit diameters of the expansion nozzles were 0.43 mm (0.017 inches) and 1.2 mm (0.047 inches), respectively, with a resulting area ratio of 7.65, and a design Mach number of 3.63. The original throat diameters were selected based on the minimum quenching distance (115, p. 287) of 0.6 mm (0.23 inches) for premixed hydrogen and air at an equivalence ratio of 1.0 and a pressure of 1 atm. To

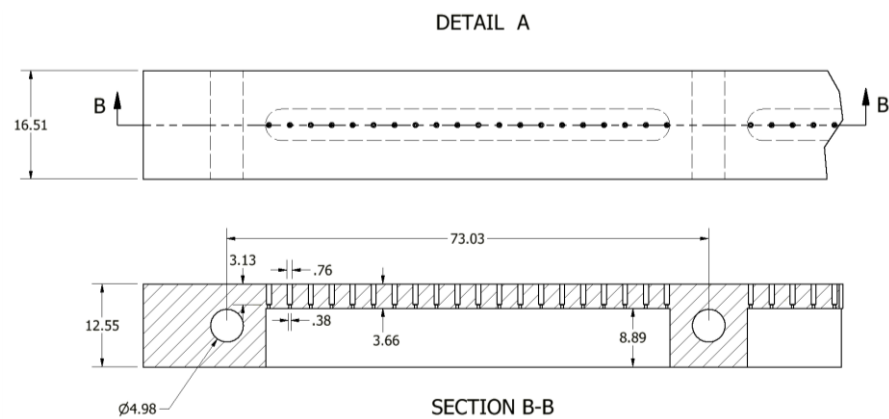


Figure A1.2 Detail drawing of the feed nozzle bar. Nozzles were not contoured. Dimensions are in mm

increase the mass flow rate into the channel, the throat areas were enlarged to 1.04 mm (0.041 inches) for the final two tests, with a resulting area ratio of 1.33 and design Mach number of 1.7. Feed pressures measured with a pressure transducer located in the side wall of the mixing plenum, 6.35 mm (0.25 inches) below the nozzle bank verified choked flow out of the mixing plenum. Additionally, the predetonators fed into the channel through separate 8.25 cm (0.325 inch) diameter pipes. Originally, no effort was made to allow a smooth transition from the circular pipe to the rectangular detonation channel with a 3.8 mm (0.15 inch) gap. Consequently, the detonation front immediately encountered decreased area and sharp corners at the exact point where it was intended to couple with the premixed gases. Two modifications, as shown in Figure A1.3, were made to the predetonator interface to improve detonation entry into the channel. First, a conical groove was filed into the polycarbonate walls of the channel to remove the sharp corner. Second, steel plates were inserted into the channel to form a two dimensional diffuser with a 7.5 degree half-angle that would slowly expand the detonation cross-section. The diffuser unintentionally shortened the effective channel length and obstructed a portion of

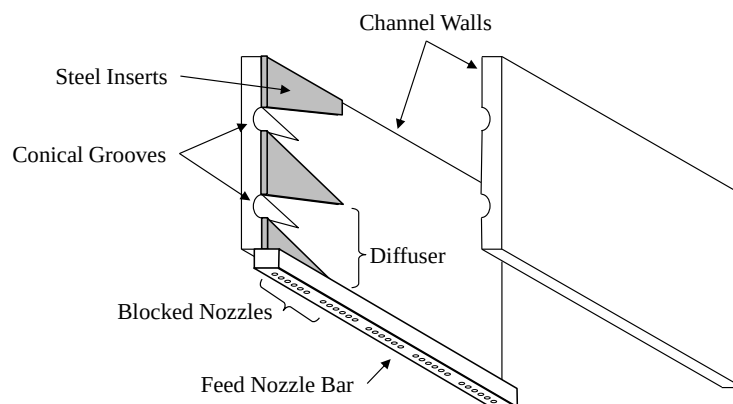


Figure A1.3 Diagram showing conical grooves and steel inserts to create a diffuser in the detonation channel

Table A1.1 Test section configurations

Configuration	Tests	Nozzle Throat mm (in)	Nozzle Exit mm (in)	Quantity of Nozzles	Detonation Entry Modification
1	A – F	0.43 (0.017)	1.2 (0.047)	160	None
2	G, H	0.43 (0.017)	1.2 (0.047)	160	Conical Groove
3	I - L	0.43 (0.017)	1.2 (0.047)	140	Conical Groove and Diffuser
4	M, N	1.04 (0.041)	1.2 (0.047)	140	Conical Groove and Diffuser

the expansion nozzles. The modifications to the feed nozzles and predetonator interface resulted in the four configurations listed in Table A1.1.

High speed schlieren imagery was collected using a Vision Research Phantom VR0711 high speed camera with a Nikon AF NIKKOR 80-200 mm 1:2.8D zoom lens. The two optical paths, shown in Figure A1.4, were used on separate test events with different effects. For both layouts, the camera's aperture was maintained full open at 2.8, with focus set near infinity and zoom was varied slightly. The light source for both was a 24 V, 250 W halogen lamp with a nominal output of approximately 800 lumens. The schlieren configurations employed two Z-folded beam paths (144) to accommodate space

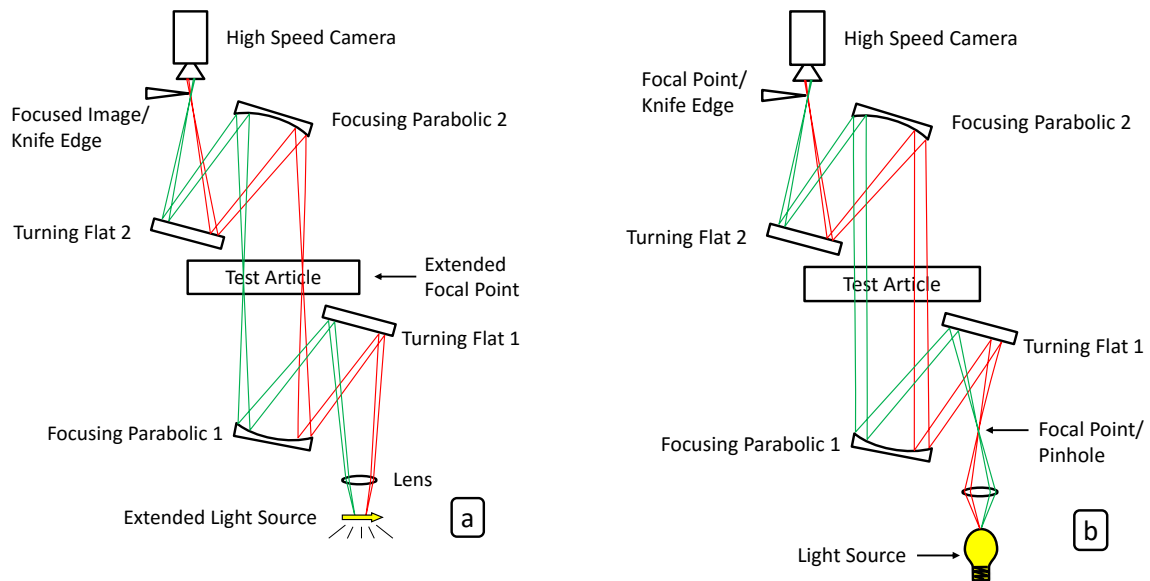


Figure A1.4 Diagram of the two schlieren optical paths for this experiment, a) focused schlieren, b) parallel beam schlieren

limitations. For the focused schlieren (144) of Figure A1.4a, a simple focusing optic at the light source was employed to control the divergence of the beam. Alternatively, it focused the light on a pinhole to create a point source for the traditional parallel-beam schlieren(144) of Figure A1.4b.

2. Methodology

2.1. Test Control

Computer control systems operated the test section timing to produce two detonations. Test flow was intended to occur in two phases: I) Preparation of the detonation channel and II) Mimicked RDE operation. The preparation phase established steady state reactant flow into the detonation channel and created a binary zone of unburned reactants and combusted products as shown in Figure A1.1. The test preparation cycle began with the command to open the high pressure dry air valve. The air flow was allowed to establish steady state flow through the test section (approximately 2 seconds), then the hydrogen fuel valve was activated and hydrogen gas flow was allowed to come to steady state (approximately 2 additional seconds). After hydrogen flow reached steady state, the firing sequence was triggered.

As shown in Figure A1.5, three separate systems were connected with a trigger signal, and the two test phases were separated chronologically by the second detonation event. The firing sequence was commanded from the National Instruments data collection system and sent to both the high speed camera and the signal generator for the predetonators. The high speed camera centered image collection on the trigger signal. After the test sequence completed, the imagery was briefly reviewed for key test events, then transferred from the camera to other computer systems for post-processing. Post

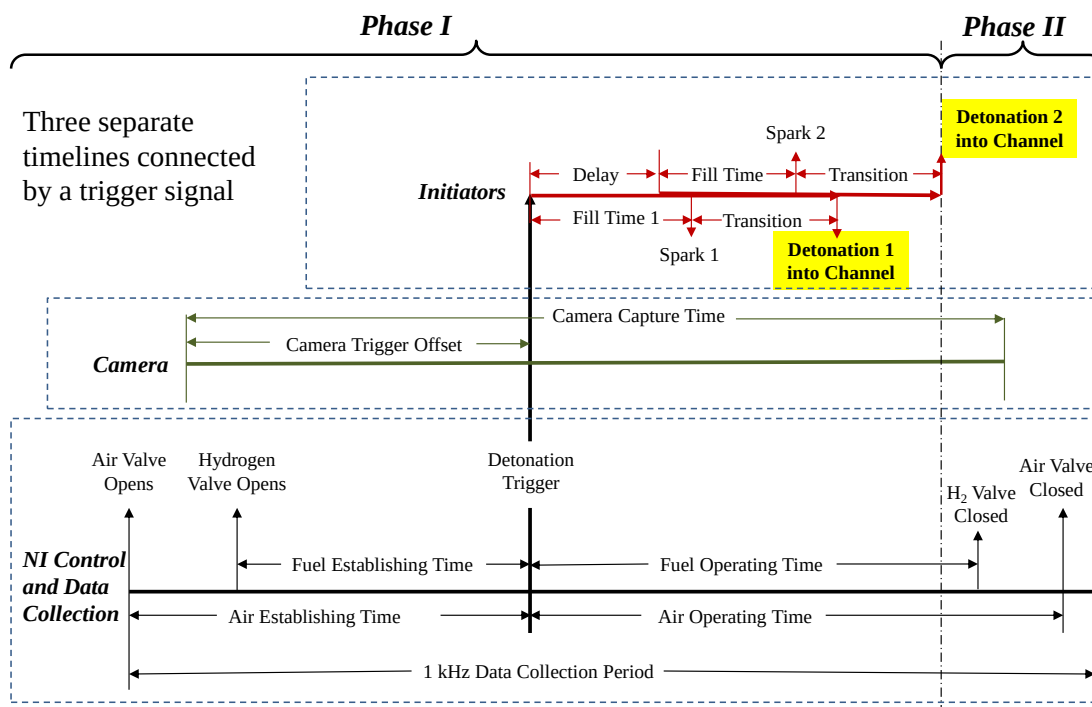


Figure A1.5 Test section timeline diagram. Three separate timelines were tied to a central trigger while the test was separated into two phases by the initiation of the second detonation

processing involved calculating shock velocities, evaluating decoupling of detonation, looking for flashback into the mixing plenum, and observing detonation related events.

2.2. Test Section Function

Upon receiving the trigger signal, the signal generator sent two time-sequenced commands to the predetonators. The predetonators were mounted together at the entrance of the detonation channel. The initial detonation wave propagated into the detonation channel as depicted in Figure A1.1, roughly perpendicular to the injector mass flow, and ignited the reactants. A continuous flow of fresh reactants into the mixing chamber was designed to blow off the flame and to create a binary zone of combusted gas and unburned reactants. The second detonation was timed to follow the first in the lower

binary zone containing only unburned reactants. The second detonation was designed to mimic the continuous detonation cycle seen in an RDE.

2.3. Data Collection

Characterizing events against mass flow rates and equivalence ratios was important to interpreting test results. Pressure measurements were collected at 1000 Hz both upstream and downstream of the metering nozzles and in the mixing plenum. The data were post-processed to determine global mass flow rates and equivalence ratios.

2.4. Imagery Processing

Imagery was post processed to determine shock wave speed, identify flashback, identify blowoff, and to observe any detonation related phenomena. Measured wave speeds were determined with a centered finite difference scheme.

$$V_1 \approx \frac{\Delta x}{\Delta t} A_p = (x_2 - x_1) f L_p, \quad (\text{A1.1})$$

where x_1 and x_2 are horizontal distances from a reference point measured in pixels, and f is the frame rate of the video segment. Multiple physical features from the channel walls were identified in each video, and the number of pixels that these features traversed was divided by the known length to produce a conversion factor L_p . Distances of the wave speeds with the same data points as

$$d_1 = \frac{x_1 + x_2}{2} L_p \quad (\text{A1.2})$$

Since there were many optical elements that could shift slightly between tests, calibration of the video imagery was necessary for each video segment of interest. Figure

A1.6 illustrates the velocity measurement technique using two sequential video images separated by $30\ \mu\text{s}$. Each image in Figure A1.6 comes from test J in configuration 3 (Table A1.2) with background subtraction. Dark portions of the figure represent density

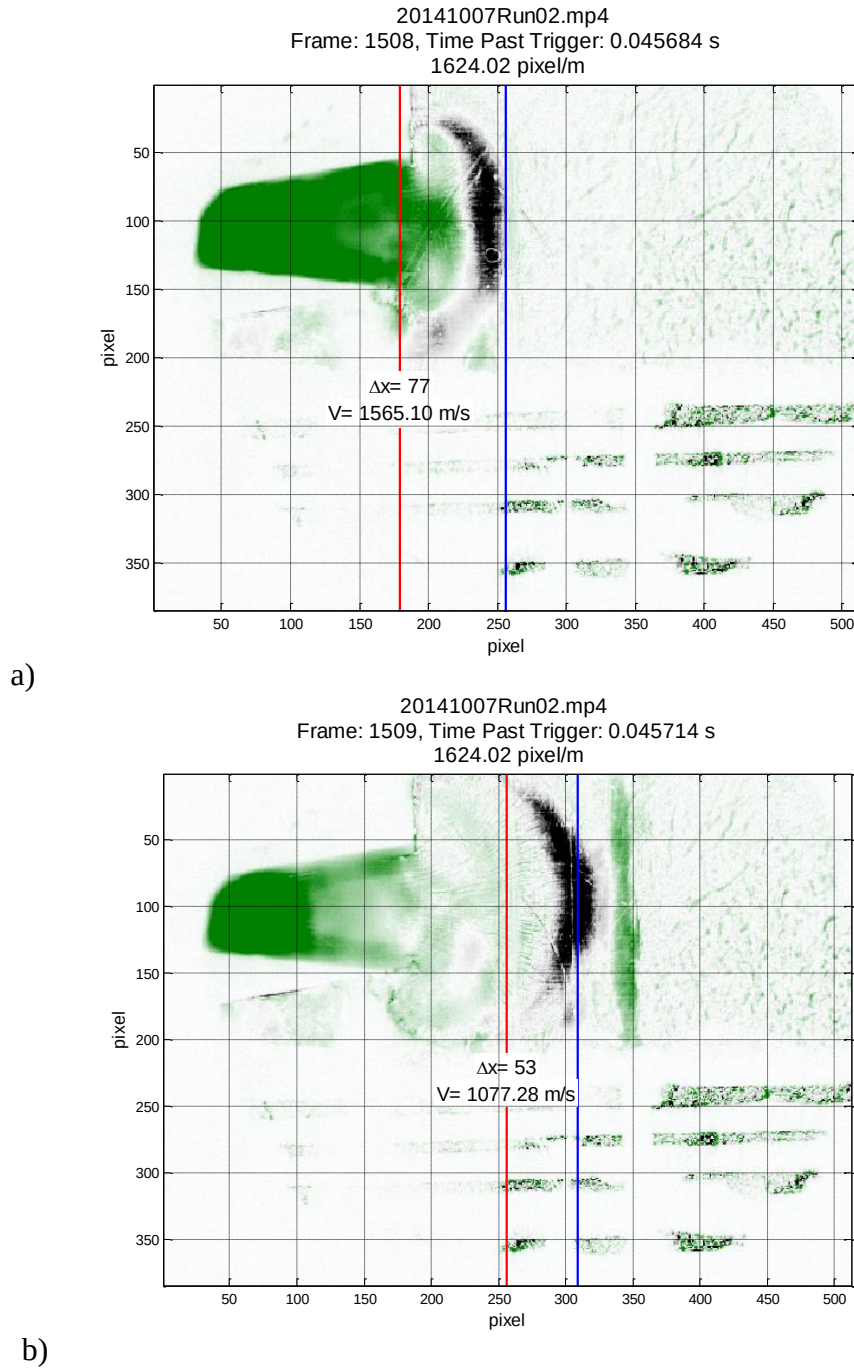


Figure A1.6 Position measurements between sequential images, $\Delta t = 30\ \mu\text{s}$, from test J were combined with frame rate and length calibration factors to generate velocity measurements

gradients. The detonation channel is in the upper right hand corner of each image between $y = 0$ and $y = 205$ and to the right of $x = 185$. The diffusers for the initiators extend to the left of the detonation channel between $x = 30$ and $x = 185$. The upper and lower edges of the diffuser define the trapezoidal region in both Figure A1.6a and A1.6b. A second diffuser for the second initiator may be seen in Figure A1.6b. The optically opaque nozzle bar stretched across the entire image between $y = 205$ and $y = 230$. The mixing plenum extends from $y = 230$ to $y = 384$. Bands below the nozzle bank correspond to mixing grooves.

Two thin vertical overlay lines colored red and blue in each of the subfigures correspond to position measurements. The left-most overlaid vertical line represents the location of the shock front in the previous image (x_1), while the right-most overlaid vertical line represents the location of the shock front in the current image (x_2). The shock velocity (V_1) is calculated as the finite difference in the shock location divided by the time between frames. The location of the velocity (d_1) is simply the time average of the two locations.

This method of velocity measurement had some analytical benefits. With only one set of feature measurements for each video segment, analysis was simplified. Each velocity measurement shared a distance measurement (x_i) with the previous and subsequent velocity measurements, so that if a distance was selected incorrectly for one point it affected two velocity measurements, but in opposite directions (one will be high and the other low). Thus, when attempting to attach trends to accumulated data, errors in measurements were normally distributed about the mean.

The focused schlieren technique (Figure A1.4a) using an extended source produced higher quality images. It allowed more light to reach the sensor, thereby shortening the shutter speed from 10 or 20 μs down to 0.4 μs . Focused schlieren also allowed the focal depth of the image to be restricted to immediately around the test section, eliminating significant amounts of background noise. The camera operated at either approximately 22,000 fps or 33,000 fps, depending on the image size captured.

For the purposes of this research, successful phase I operation required combustion coupled with a shock at sonic velocities or higher relative to the combustion products (choked flame). Validation of success against this definition required evaluation of imagery to determine coupling and quantitative data for velocity measurements. The shock speed measurements were compared with the Chapman-Jouget detonation speed, and the speed of sound (a) in both the premixed reactants and the combusted products. Figure A1.7 shows the predicted values for the detonation and sonic speeds as calculated in CEA (137) as a function of equivalence ratio (ϕ). The prediction assumed the premixed

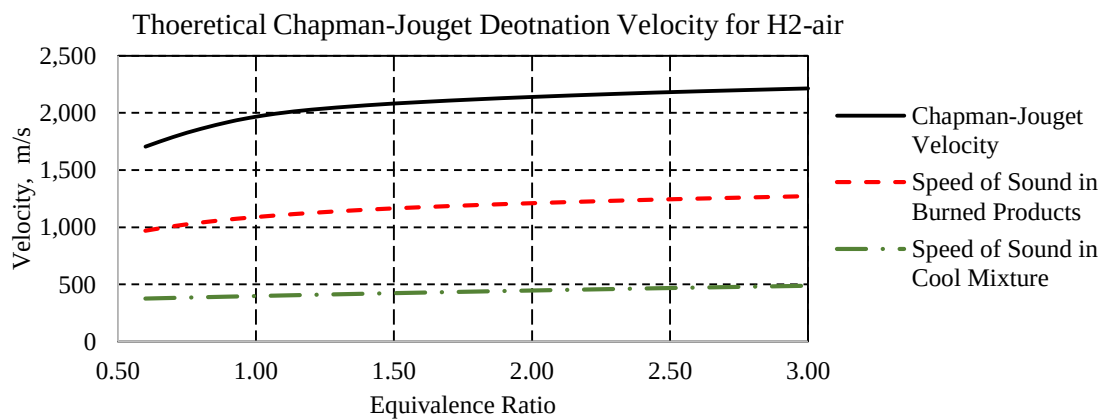


Figure A1.7 Illustration of theoretical Chapman-Jouget Detonation and sonic velocities for hydrogen-air combustion as a function of equivalence ratio as computed with NASA's CEA (137)

reactants were at 285 K and 1 atm. The span of ϕ in Figure A1.7 corresponds to the values in the experimental data set and produced a band of possible velocities when compared to the joint data set.

The predetonators operated with propane and NO_2 , but the detonation velocity was similar to that of the test section. As seen in Figure A1.6, portions of the initiator were optically accessible and available for position and velocity measurements when the diffuser was used. Tests with modifications 3 and 4 (Table A1.1) included velocity measurements in the diffuser section. Assuming reactants at 1 atm and 285 K, the Chapman-Jouget detonation velocity for the initiator was predicted as approximately 2300 m/s, with a sonic speed of 1230 m/s in the combusted products. These values correspond well with the hydrogen-air velocities and no attempt was made to delineate the transition of the detonation from the predetonator to the test section.

Not all measurements were quantitative. Each video was reviewed for evidence, as seen in Figure A1.8, that the combustion zone had decoupled from the shock. Figure

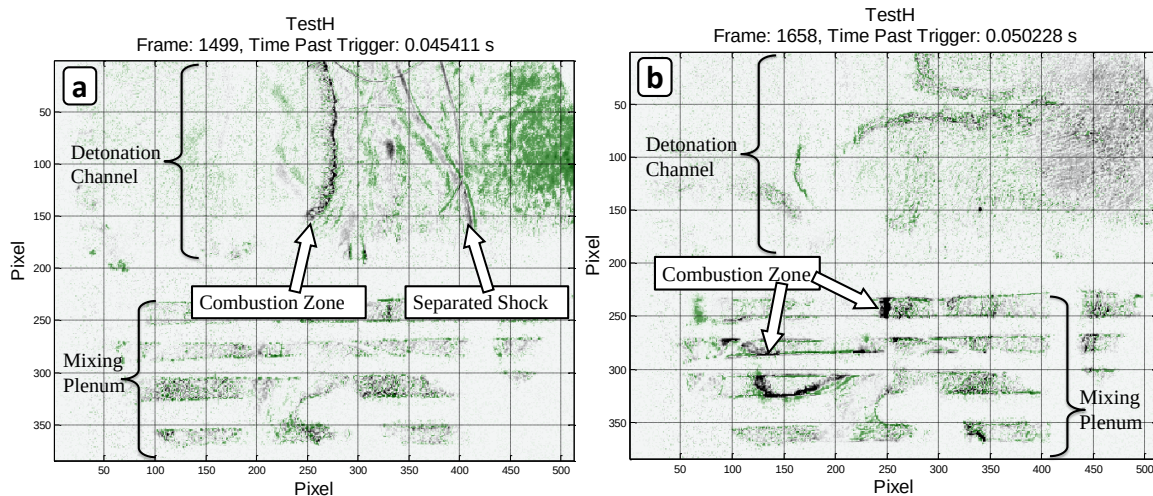


Figure A1.8 Two frames showing qualitative measurements of a) decoupling of the shock in the detonation channel and b) combustion in the mixing plenum during test H

A1.8 contains two background subtracted images from test H. In each image the detonation channel fills the width of the field of view and from $y = 0$ to $y = 200$ (the top half of each image). The mixing plenum stretches from $y = 225$ to $y = 384$ (the bottom half of each image). The image in Figure A1.8a shows typical decoupling where the combustion zone appeared as a scalloped fan and trailed the shock. From frame to frame, the combustion zone fan was seen to decelerate and move at a significantly slower velocity than the shock. Flashback was easily identifiable as a combustion zone which first appeared on the lower side of the feed bar and expanded to fill the mixing plenum. The combustion zone of Fig. 8b was pushed into the plenum by the second shock 0.048774 s after the trigger signal, and progressed approximately 7.6 cm during the intervening 1.45 ms. The time-averaged velocity of approximately 50 m/s was higher than laminar flame speed, estimated at 6 m/s in a 4 atm mixing chamber, indicating turbulent flame.

3. Results

This test achieved only secondary goals since no test adequately completed phase I. Either the first detonation produced flames that anchored on the feed bar and consumed the fuel-air mixture as it flowed into the detonation channel, or the second detonation decoupled rapidly upon introduction into the detonation channel. Despite failure to achieve phase II operation, there were some important lessons learned.

3.1. Choked Flame in the Detonation Channel

Successfully maintaining a choked flame in the test section was hampered by low mass flow rates. After applying safety factors for assembly bolt loads, test section operation was limited to plenum pressures less than 5 atm. For configurations 1, 2, and 3,

the pressure limit of 5 atm restricted flow to about 0.025 kg/s of mixture into the detonation channel. This is about one tenth of the flow that a non-premixed RDE with analogous geometry requires to operate (19). Enlarging the throat of the feed bar nozzles allowed a mass flow rate of 0.158 kg/s in test N (Table A1.2) and choked flames were achieved in the detonation channel.

Table A1.2 contains a description of the test points attempted and the key results for flashback and blowoff. Table A1.2 also catalogues the fact that detonation was seen in two tests (G and N). The oxidizer valve failed to open for test G, and the result was that the detonation channel filled with detonable gases from the predetonators while the mixing plenum filled with pure hydrogen. Although a portion of the detonation wave de-

Table A1.2 Summary of test conditions and results

Test Event Identification	Configuration	Flashback?	Blowoff?	Detonation in Channel achieved?	Equivalence Ratio	$\dot{m}$, kg/s
A	1	N	N	N	1.2 ± 0.11	0.020 ± 0.003
B	1	N	N	N	1.8 ± 0.15	0.020 ± 0.003
C	1	N	N	N	2.9 ± 0.25	0.020 ± 0.003
D	1	N	N	N	2.9 ± 0.25	0.020 ± 0.003
E	1	N/A	N/A	*†	∞	0.001 ± 0.0002
F	1	1st	N	N	1.6 ± 0.13	0.019 ± 0.003
G	2	N/A	N/A	Y*	∞	0.001 ± 0.0002
H	2	2nd	N	N	1.15 ± 0.10	0.021 ± 0.003
I	3	Y†	N/A†	†	0.83 ± 0.07	$0.035 \pm 0.005^{\ddagger}$
J	3	1st	N	N	0.82 ± 0.07	$0.024 \pm 0.004^{\ddagger}$
K	3	N	Y	N	0.69 ± 0.06	$0.026 \pm 0.004^{\ddagger}$
L	3	N	Y	N	0.73 ± 0.064	$0.024 \pm 0.004^{\ddagger}$
M	4	1st	N	N	1.13 ± 0.06	0.110 ± 0.004
N	4	1st	N	Y	1.40 ± 0.08	0.158 ± 0.006

* - The air valve did not open during this test and the detonation channel filled with gases from the initiator and H₂

† - Schlieren imagery for this test was not captured, assessment of flashback is derived from plenum pressure data

‡ - Mass flow rate through the detonation channel was affected by mixing plenum leaks during this test event.

coupled upon entry into the channel, other portions near the floor of the channel were able to maintain a combustion reaction coupled with shocks. Tests showed that detonation decoupling in the chamber was not a function of geometry and that the test section was capable of supporting a detonation. Without a premixture to refill the channel, phase II operations were not possible.

The second successful choked flame (Test N) was verified by measuring the detonation wave speed. Shock position was carefully recorded from all schlieren videos to generate time averaged shock velocity as a function of distance from the channel inlet. Data from all test events are plotted in Figure A1.9. Although some tests had shock velocities that reached theoretical detonation velocities, only two test events (G and N) maintained velocities higher than the speed of sound relative to the combustion products across the field of view. The remainder of the tests showed that detonation decoupled into a leading shock wave followed by deflagration within the first 30 cm (12 inches) of

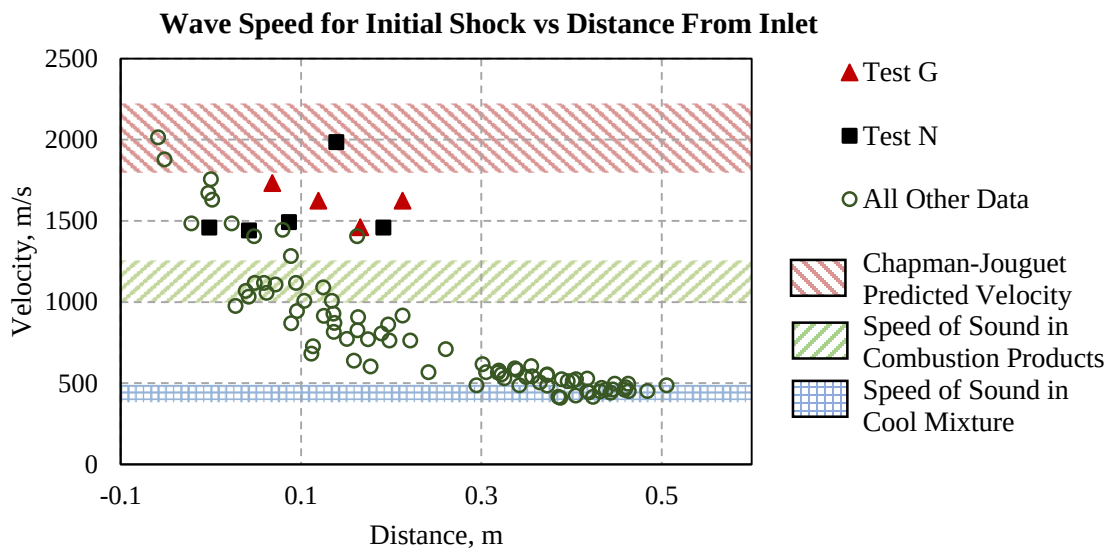


Figure A1.9 Compendium of velocity measurements from high speed schlieren video. The data from -0.1 to 0.28 m were collected using a different field of view than data at distances greater than 0.28 m

entering the detonation channel. The leading shock was seen to decelerate to sonic velocities relative to the cool reactants. Flashback accompanied the first detonation during test N, and the resulting fire in the plenum broke the test section. The fire in the plenum also consumed the premixture and prevented phase II operations.

Previous experimentation (19) has shown that there are operating conditions where an RDE will not function. When mass flow rates are below a set threshold, the RDE fails to maintain detonation and transitions to deflagration. This phenomenon is seen in the data set where only test M and N achieved mass flow rates that were comparable to successful operating regions in an analogous RDE, and test N was the only successful premixed detonation. Slight variations in the feed geometries or the degree of mixing may account for the failure of test M to detonate.

3.2. Detonation Decoupling and Shock Velocities

It should be noted that the data in Figure A1.9 represent the accumulated data from all tests. As noted in the figure caption, the imaging field of view was shifted from mid test section to the beginning of the test section after the first set of tests (A-D). Simultaneously, the schlieren set-up was changed from the focused schlieren, shown in Figure A1.4a, to the more traditional layout shown in Figure A1.4b. Velocity measurements in the subsequent tests (E-M) showed the deceleration of the shock wave as it decoupled from combustion. It is significant that varying the equivalence ratio and mass flow rate had little or no effect on the deceleration trend until the mass flow rate reached 0.158 kg/s.

3.3. Detonation Related Phenomenon

During the initial tests, when the imaging field of view was between 25 cm (10 inches) and 50 cm (20 inches) from the initiator inlet, shock waves created when the first predetonator fired were observed traveling at the speed of sound relative to the cool reactants, followed by a combustion front. A shock from the second predetonator was seen to arrive 1.2 ms later.

In between the shocks generated by the predetonators, the combustion front was seen to emit shock waves (Figure A1.10) that traveled ahead of it. This provided an excellent visualization of deflagration to detonation phenomena. Figure A1.10 is a six-

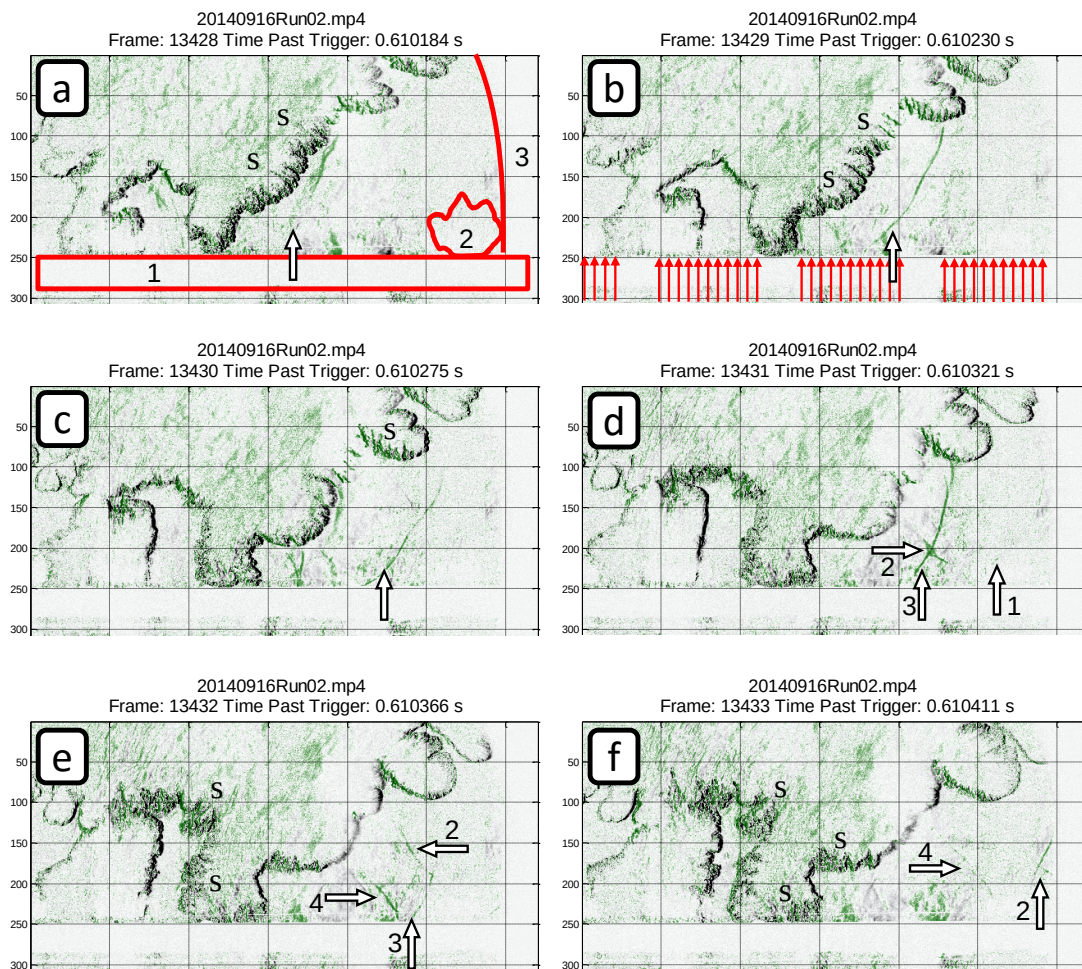


Figure A1. 10 Time sequenced schlieren of shock waves emanating from a combustion front into the cool reactants during test event B

image sequence starting 2.45 ms after the density wave from the first failed detonation attempt had already passed and spanning 0.227 ms. It shows the emission of two waves from the combustion zone. All images were background subtracted to improve signal-to-noise ratios. Three optically opaque regions were labeled as 1, 2, and 3 in Figure A1.10a; 1) the feed nozzle bar, 2) a scorch area from a previous test, and 3) a region clipped by the mirrors. The location of the banks of 20 nozzles through which the premixed reactants enter the detonation chamber is highlighted in Figure A1.10b as arrays of arrows. Grouping the nozzles into banks of 20 caused reactant flow in the detonation channel to be both turbulent and non-uniform. The combustion front produced a severe density gradient that may be seen in each of the subfigures of Figure A1.10 as a heavy black curved and convoluted line. This hydrogen-air combustion front was not coupled with a shock wave, and is deflagration. The deflagration is moving much slower than the speed of sound, and is seen in videos to surge or accelerate in small regions over 3 to 4 frames, then pause for 3 to 4 frames. It had progressed across half of the field of view before Figure A1.10a and became anchored along points of the feed bar between the banks of feed nozzles. The schlieren video showed the deflagration surges into turbulent flow issuing from the feed nozzles with a corresponding emission of a shock wave.

The combustion front during a surging period was markedly different from the normal combustion. The deflagration appeared to send out fingers along the combustion region in Figure A1.10, resulting in a band of combustion that looks like a river delta. Regions showing these characteristics of a surge are marked with the letter 'S' in Figure A1.10a, b, c, e, and f. After a few frames (approximately 200 to 400 μ s) the fingers appear to pause and the trailing valleys catch up. Visually, the deflagration now looks

relatively smooth, like the region above Arrow 2 in Figure A1.10d. The schlieren video sequences clearly showed that the surging and shock emission occurred over the turbulent jets of reactant, and that these surging regions are correlated to the emission of shock waves.

The emitted s waves are identified with arrows in Figure A1.10, and are similar to those required for transition from deflagration to detonation. The arrow in Figure A1.10a corresponds to the initial signs of the pressure wave due to a surging region identified with the letter 'S' in the center of the image. In Figure A1.10b and 10c, the wave is seen traveling away from the combustion front at an approximate velocity of 500 m/s. A minor surge in the center of Figures A1.10a, b, and c generates a second wave seen in Figure A1.10d at arrow (3), while the first wave (1) has traveled almost completely out of the field of view and is obscured behind the opaque regions. The tail was reflected off of the floor of the detonation chamber and was still seen at arrow (2). These waves continue in Figure A1.10e, where the tail of the second wave gets reflected (4). The second wave was last imaged in Figure A1.10f just before it exited the field of view.

3.4. Engineering Design Considerations

The test section design needed to consider three key failure modes; leaks, flashbacks, and sidewall failure. Evidence of the three failure modes may be seen in the portion of the sidewall shown in Figure A1.11. Leaks in the mixing plenum added uncertainty to the mass flow rate into the detonation channel for several tests in Table 2. Leaks primarily occurred where holes for assembly bolts were located close to the mixing chamber. A sign of leakage may be seen in the lower left hand corner of Figure A1.11 as discoloration in the red RTV sealant between the polycarbonate side wall and fuel



Figure A1.11 Flame erosion and sidewall fracturing of the polycarbonate mixing plenum sidewall at the sealed joint with the fuel plenum, following test H

plenum. With only 3 mm (0.125 inch) between the holes and the mixing chamber, new leaks appeared and existing leaks tended to get worse with each violent impact associated with a test attempt. During several tests, combustion from the detonation channel was able to reach and ignite the plumes of mixture flowing from the leaks. Plume ignition enlarged the leaks as it eroded the polycarbonate when the flame burned back toward the mixing plenum. Several times, combustion entered the mixing plenum through the ignited plume. Combustion in the plenum caused rapid overpressure events which increased the size and number of leaks. More frequently, combustion was driven backward through the feed nozzles into the mixing plenum, and the ensuing deflagration progressed toward an explosion. Flashback during test event H expanded the mixing plenum and fractured the polycarbonate at the point where the air inlet was attached (shown in the center of Figure A1.11). Future test facilities will employ external steel frameworks and increased sealing distance around assembly holes.

3.5. Feedback

Another key finding was that pressure waves from the detonation channel were not seen traveling into the mixing plenum. This may be due to limitations resulting from schlieren through polycarbonate, nozzle throat size successfully limiting shocks, or pressure waves so weak that they could not be visualized with the schlieren technique. Four panes of polycarbonate were inserted in the beam path: two for the sidewalls, and two for shielding optics in the event of failures. During the manufacturing process the polycarbonate naturally experiences some density gradients. This can be seen throughout the schlieren imagery set as dark vertical bands. Additionally, each pane of polycarbonate reflects some of the light passing through it, decreasing the amount of light at the focal plane of the camera. The result is that the entire schlieren system is much less sensitive in those regions.

3.6. Flashback

Flashback into the plenum was a key finding of this experiment. Although most test events did not have a sustained detonation in the channel, Table A1.2 shows that flashback still occurred on 6 test runs (4 with the first detonation, 1 from the second detonation, and 1 undetermined). Flashback did not occur on 8 test runs, most of which had equivalence ratios below 0.8 or greater than 1.5. Although the summary of test results in Table A1.2 did not identify any clear trend for flashback, test H highlighted the fact that simple quenching distance geometries are insufficient to support continuous premixed RDE operation.

Video showed two modes of flashback: flashback from firing the first predetonator and delayed flashback on the second predetonator firing. Flashback

occurred without delay for all test events with the configuration featuring 1.04 mm (0.041 inches) nozzle throats and for some tests (Table A1.2) when nozzle throat diameters were 0.43 mm (0.017 inches). During these tests, the detonation wave was seen to expand to the nozzle bar, followed several frames later by a deflagration front progressing into the mixing plenum. The un-delayed ignition occurred only in the regions closest to the initiators.

The first detonation ignited the combustible gases and the flame anchored on the nozzle bar in the detonation channel in all tests except K and L. Delayed flashback occurred when the second detonation pushed anchored flames through the nozzle bar. Again deflagration was noted a few frames after the detonation had encountered the nozzle bar. Detonation did not travel directly into the plenum for any test.

4. Conclusions

Valuable lessons were learned from these experiments. Choked flame in the linear test section was shown to analogue RDE mass flow rate requirements. For the geometry utilized in this test, choked flame occurred with equivalence ratios near 1.0 and mass flow rates greater than 0.11 kg/s. A deflagration combustion zone was clearly seen to emit shock waves in turbulent flows.

Utilizing throat diameters sized for quenching distances was insufficient to prevent flashback into the mixture plenum. Though free expansion nozzles effectively limited pressure wave propagation back into the plenum, they were insufficient to prevent flashback. We suggest that if nozzle length were sufficient to act as a capacitor during the transient passage of the detonation wave, and nozzle design supported blowoff, flashback into the mixing plenum might be avoided.

5. Acknowledgments

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Appendix II Uncertainty Analysis for Mass Flow Rate and Derivatives

Knowing the range of possible values for each reported datum provides insight into trends and gives perspective on the conclusions that may be drawn from a set of data. This work involved calculation of those ranges (also known as uncertainties) for mass flow rates (of fuel, oxidizer, and premixture), equivalence ratio, velocity, and boundary layer velocity gradients. Each uncertainty is tied to the calculation formulae and the uncertainty of the measured (or tabulated) values. Each of these formulae are considered individually, and algebraic formulations for total uncertainty due to measurement error are developed where possible.

1. Mass Flow Rates

1.1. Fuel

Mass flow rate for flow through a choked orifice is completely governed by the universal flow function:

$$\frac{\dot{m}_f}{A_f} \left(\frac{\sqrt{T_0 R_f}}{P_0} \right) = M \sqrt{\gamma_f} \left(1 + \frac{\gamma_f - 1}{2} M^2 \right)^{\frac{-(\gamma_f + 1)}{2(\gamma_f - 1)}} \quad (\text{A2.1})$$

where $\dot{m}_f$ is the mass flow rate for fuel, A_f is the throat area of the nozzle for fuel, T_0 is the stagnation temperature, R_f is the gas-specific constant for the fuel, P_0 is the stagnation pressure, M is the Mach number at a given location (defined as 1 at the choke point), and γ_f is the specific heat ratio for fuel. The gas-specific constant can be further broken into:

$$R_f = \frac{R_u}{\bar{M}_f} \quad (\text{A2.2})$$

where R_u is the universal gas constant, and $\bar{M}_f$ is the molar-averaged weight of the fuel.

The total fuel nozzle choke area is generally calculated based on a throat diameter d using the standard formula for the area of a circle:

$$A_f = \frac{\pi d^2}{4} \quad (\text{A2.3})$$

Pressure and temperature are measured with electronic sensors, and what the data signal actually recorded is a voltage level. The formula for stagnation pressure is:

$$P_0 = V_{P_0} C_P + P_{amb} \quad (\text{A2.4})$$

where V_{P_0} is the voltage from the pressure sensor, C_P is a conversion constant for the sensor, and P_{amb} is the ambient pressure (if the sensor reports gauge instead of absolute pressure). The stagnation temperature formula is given as:

$$T_0 = V_{T_0} C_T \quad (\text{A2.5})$$

where V_{T_0} is the voltage from the thermocouple and C_T is the conversion constant for the thermocouple.

After re-arranging and substituting the above relations, Equation A2.1 takes on the following form for calculating mass flow of the fuel:

$$\dot{m}_f = \frac{\pi d^2}{4} (V_{P_0} C_P + P_{amb}) M \sqrt{\frac{\gamma_f \bar{M}_f}{V_{T_0} C_T R_u} \left(1 + \frac{\gamma_f - 1}{2} M^2 \right)^{\frac{-(\gamma_f + 1)}{2(\gamma_f - 1)}}} \quad (\text{A2.6})$$

Measurement and property uncertainties are summarized in Table A2.1.

Table A2.1 Measurement property uncertainty for gaseous fuel

Term	Description	Measurement Uncertainty, Δ	Nominal Measurement	Note
M	Mach	0	1	
π	Constant	1×10^{-6}	3.1415926	
R_u	Universal Gas Constant	1.0	8313.219	kJ/(kg K)
γ_f	Ratio of specific heats for fuel (H_2)	0.01	1.41	
V_{P_0}	Upstream Stagnation Pressure Voltage	+/- 0.01 V nominal (varies)	1.5 V	Measured in a low Mach section of pipe
C_P	Pressure transducer constant	1%	$\frac{2000 \text{ psi}}{5 \text{ V}}$	Instrument is set to within 1%.
T_0	Upstream Stagnation Temp Voltage	+/- 0.01 V nominal	1.5 V	Assumed facility temperature when not measured
C_T	Thermocouple constant	1%	$300 \frac{K}{V}$	
$\bar{M}_f$	Molecular weight of fuel	.05 g/gmol	2.0 g/gmol	
d	Inside diameter of nozzle throat	0.0127 mm (0.005 in)	.016 in	Machining tolerance is 30% error here...

1.2. Oxidizer (Air)

The formulae for oxidizer look similar to those of fuel, with oxidizer subscripts substituted in:

$$\frac{\dot{m}_o}{A_o} \left(\frac{\sqrt{T_0 R_o}}{P_o} \right) = M \sqrt{\gamma_o} \left(1 + \frac{\gamma_o - 1}{2} M^2 \right)^{\frac{-(\gamma_o + 1)}{2(\gamma_o - 1)}} \quad (A2.7)$$

and,

$$R_o = \frac{R_u}{\bar{M}_o} \quad (A2.8)$$

and,

$$A_o = \frac{\pi d^2}{4} \quad (A2.9)$$

and,

$$P_0 = V_{P_0} C_P + P_{amb} \quad (\text{A2.10})$$

and finally:

$$T_0 = V_{T_0} C_T \quad (\text{A2.11})$$

which may be substituted back into Equation A2.7 to arrive at:

$$\dot{m}_o = A_o (V_{P_0} C_P + P_{amb}) M \sqrt{\frac{\gamma_o \bar{M}_o}{V_{T_0} C_T R_u}} \left(1 + \frac{\gamma_o - 1}{2} M^2 \right)^{\frac{-(\gamma_o + 1)}{2(\gamma_o - 1)}} \quad (\text{A2.12})$$

The underlying measurements and the uncertainty for oxidizer measurements and constants is listed in Table A2.2.

Table A2.2 Measurement uncertainty values for gaseous oxidizer

Term	Description	Measurement Uncertainty, Δ	Nominal Measurement	Note
M	Mach	0	1	dimensionless
π	Constant	$< 1 \times 10^{-6}$	3.1415926	Circle circumference to diameter ratio
R_u	Universal Gas Constant	1	8313.219	kJ/(kg K)
γ_o	Ratio of specific heats for oxidizer (air)	0.01	1.4	dimensionless
V_{P_0}	Upstream Stagnation Pressure Voltage	+/- 0.01 V nominal (varies)	1.5 V	Measured in a low Mach section of pipe
C_P	Pressure transducer constant	1%	$\frac{2000 \text{ psi}}{5 \text{ V}}$	Instrument is set to within 1%.
T_0	Upstream Stagnation Temp Voltage	+/- 0.01 V nominal	1.5 V	Assumed facility temperature when not measured
C_T	Thermocouple constant	1%	$300 \frac{K}{V}$	
$\bar{M}_o$	Molecular weight of oxidizer	1	28.8	g/gmol
d	Inside diameter of nozzle throat	0.0127 mm (0.005 in)	.787 mm (0.031 in)	Machining tolerance, mm (in.)

1.2.1. Total Mass Flow Rate Uncertainty Overview

The uncertainties are calculated as the partial differential of Equation A2.12 with respect to the measurement values. The individual measurement errors are combined in quadrature to obtain the total measurement error:

$$\begin{aligned}\Delta \dot{m}^2 = & \left(\frac{\partial \dot{m}}{\partial \gamma} \Delta \gamma \right)^2 + \left(\frac{\partial \dot{m}}{\partial \pi} \Delta \pi \right)^2 + \left(\frac{\partial \dot{m}}{\partial R_u} \Delta R_u \right)^2 + \left(\frac{\partial \dot{m}}{\partial \bar{M}} \Delta \bar{M} \right)^2 + \left(\frac{\partial \dot{m}}{\partial P_0} \Delta P_0 \right)^2 \\ & + \left(\frac{\partial \dot{m}}{\partial T_0} \Delta T_0 \right)^2 + \left(\frac{\partial \dot{m}}{\partial M} \Delta M \right)^2 + \left(\frac{\partial \dot{m}}{\partial n} \Delta n \right)^2 + \left(\frac{\partial \dot{m}}{\partial d} \Delta d \right)^2\end{aligned}\quad (\text{A2.13})$$

where n is the number of nozzles and has no uncertainty for the fuel and oxidizer flow rates, which have exactly 1 nozzle. For other choked flow locations (specifically the feed nozzles described in Appendix I that connected the mixing plenum to the detonation channel), there may be many small choke points. Uncertainty in the number is introduced for two reasons: 1) some of the feed nozzles may become clogged and 2) the mass flow equation may be re-arranged to obtain an equivalent choking area (or number of nozzles) if the mass flow rate is known.

1.2.2. Specific Heat Ratio

The uncertainty term for the specific heat ratio, γ , is the most involved:

$$\begin{aligned}
\frac{\partial \dot{m}}{\partial \gamma} \Delta \gamma = & \frac{\pi d^2}{4} P_0 M \sqrt{\frac{\gamma \bar{M}}{T_0 R_u}} \left[\frac{\left(1 + \frac{\gamma-1}{2} M^2\right)^{\frac{-(\gamma+1)}{2(\gamma-1)}}}{2\gamma} \right. \\
& - \ln \left(1 + \frac{\gamma-1}{2} M^2\right) \left(\frac{1}{2(\gamma-1)} - \frac{2(\gamma+1)}{(2\gamma-2)^2} \right) \left(1 + \frac{\gamma-1}{2} M^2\right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \\
& \left. + \frac{M^2(\gamma+1) \left(1 + \frac{\gamma-1}{2} M^2\right)^{\frac{-(\gamma+1)}{2(\gamma-1)}}}{2 \left(1 + \frac{\gamma-1}{2} M^2\right) 2(\gamma-1)} \right] \Delta \gamma \quad (A2.14)
\end{aligned}$$

Collecting the universal flow function simplifies the problem a little.

$$\begin{aligned}
\frac{\partial \dot{m}}{\partial \gamma} \Delta \gamma = & \frac{\pi d^2}{4} P_0 M \sqrt{\frac{\gamma \bar{M}}{T_0 R_u}} \left(1 + \frac{\gamma-1}{2} M^2\right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \\
& \cdot \left[\frac{1}{2\gamma} - \ln \left(1 + \frac{\gamma-1}{2} M^2\right) \left(\frac{1}{2(\gamma-1)} - \frac{2(\gamma+1)}{(2\gamma-2)^2} \right) \right. \\
& \left. + \frac{M^2(\gamma+1)}{2 \left(1 + \frac{\gamma-1}{2} M^2\right) 2(\gamma-1)} \right] \Delta \gamma \quad (A2.15)
\end{aligned}$$

Recognizing that the terms in front of the bracket are a generic form of Equation A2.1 or Equation A2.7 that has been solved for the mass flow rate, $\dot{m}$, a substitution changes Equation A2.15 into:

$$\begin{aligned}
\frac{\partial \dot{m}}{\partial \gamma} \Delta \gamma = & \dot{m} \left[\frac{1}{2\gamma} - \ln \left(1 + \frac{\gamma-1}{2} M^2\right) \left(\frac{1}{2(\gamma-1)} - \frac{2(\gamma+1)}{(2\gamma-2)^2} \right) \right. \\
& \left. + \frac{M^2(\gamma+1)}{2 \left(1 + \frac{\gamma-1}{2} M^2\right) 2(\gamma-1)} \right] \Delta \gamma \quad (A2.16)
\end{aligned}$$

which is a fairly complex formulation. Often the ratio of specific heats, γ , is assumed to be a constant with no uncertainty and with no contribution to the total uncertainty of the mass flow rate. In reality, the specific heat ratio varies with temperature, and uncertainty of models can be as high as 2%. The percent error in mass flow rate due to uncertainty of specific heat ratio, $\left(\frac{\partial \dot{m}}{\partial \gamma}\right) \left(\frac{\Delta \gamma}{\dot{m}}\right)$, is plotted in Figure A2.1. The plot shows that the uncertainty of the specific heat ratio is amplified by the mass flow rate equation so that a 1% uncertainty for a specific heat ratio of 1.2 will produce a 5% uncertainty component for the mass flow rate. The amplification is inversely proportional with the value of the specific heat so that the error decreases with increasing specific heat ratio.

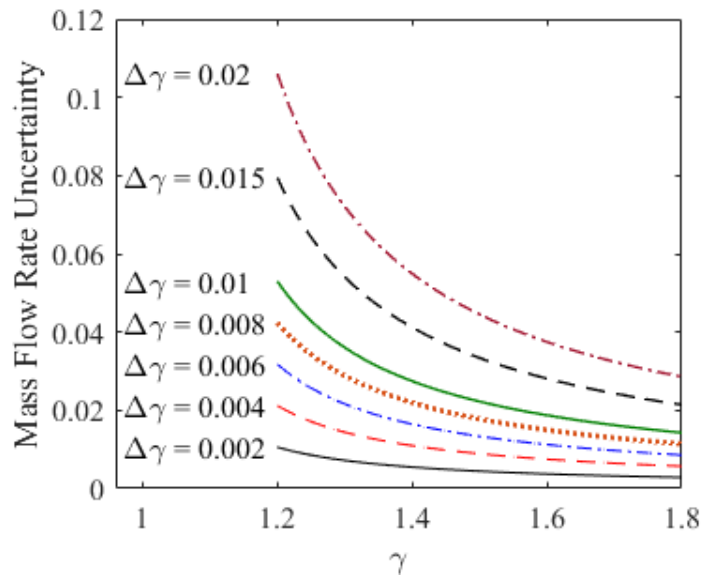


Figure A2.1 Plot of the contribution of the specific heat ratio uncertainty to the total mass flow rate error as a function of the specific heat ratio, and initial uncertainty

1.2.3. The Uncertainty of Pi

The value of π is carried with an accuracy of less than 1×10^{-6} by most computer codes, and the (double precision) error is really so small it could be ignored.

The uncertainty stated mathematically is:

$$\frac{\partial \dot{m}}{\partial \pi} \Delta \pi = \frac{\dot{m}}{\pi} \Delta \pi \quad (\text{A2.17})$$

which says the contribution to the total mass flow uncertainty due to uncertainty of π is on the order of the accuracy of π , which for a double precision number, is approximately 1×10^{-16} . This is so small that it may be ignored since the total error is multiple orders of magnitude greater than the uncertainty error due to truncating π .

1.2.4. The Uncertainty of the Universal Gas Constant

The universal gas constant has been measured and reported to 6 significant digits of accuracy. Error due to this term is included here for thoroughness:

$$\frac{\partial \dot{m}}{\partial R_u} \Delta R_u = \left(\frac{1}{2R_u} \right) \frac{\pi d^2}{4} n P_0 M \sqrt{\frac{\gamma \bar{M}}{T_0 R_u}} \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \Delta R_u \quad (\text{A2.18})$$

Substituting in for the mass flow equation:

$$\frac{\partial \dot{m}}{\partial R_u} \Delta R_u = \frac{-\dot{m}}{2R_u} \Delta R_u \quad (\text{A2.19})$$

Since $R_u \gg \Delta R_u$ this term will be insignificantly small, buried beneath the leading terms and it may generally be ignored.

1.2.5. The Uncertainty of Molecular Weight

The contribution of the uncertainty of molecular weight is:

$$\frac{\partial \dot{m}}{\partial \bar{M}} \Delta \bar{M} = \frac{\dot{m}}{2 \bar{M}} \Delta \bar{M} \quad (\text{A2.20})$$

The uncertainty of this term may be considered small if using a measured value (such as that for dry air), or it may grow larger if attempting to calculate the average molecular weight from the constituents of some mixture. Molecular weights are generally accurate on the order of 10^{-4} and may be neglected.

1.2.6. The Uncertainty of the Pressure Transducer

If stagnation pressure were measured directly, the contribution to the total error would be:

$$\frac{\partial \dot{m}}{\partial P_0} \Delta P_0 = \frac{\dot{m}}{P_0} \Delta P_0 \quad (\text{A2.21})$$

For the experimental setups, pressure transducers were used which generated a voltage reading when presented with a pressure. There is uncertainty associated not only with the voltage reading, but also with the constant used to make the linear conversion from voltage to pressures. Additionally, when the gauge is designed to generate a gauge measurement instead of an absolute measurement, there is some uncertainty associated with the ambient pressure. The result is that the uncertainty contribution of total pressure must be written as:

$$\frac{\partial \dot{m}}{\partial P_0} \Delta P_0 = \dot{m} \left(\left(\frac{\Delta V_{P_0}}{V_{P_0}} \right)^2 + \left(\frac{\Delta C_P}{C_P} \right)^2 + \left(\frac{\Delta P_{atm}}{P_{atm}} \right)^2 \right)^{\frac{1}{2}} \quad (\text{A2.22})$$

1.2.7. The Uncertainty of the Thermocouple

Stagnation temperature takes on the same form of uncertainty as the universal gas constant. It becomes:

$$\frac{\partial \dot{m}}{\partial T_0} \Delta T_0 = \frac{-\dot{m}}{2T_0} \Delta T_0 \quad (\text{A2.23})$$

Since $\Delta T_0 \ll 2T_0$ this term will be small. Although not the preferred method for the tests with the linear test section, upstream stagnation temperatures were neither monitored nor stored. Instead, the uncertainty was assigned a nominal value for the temperature of the test bay, and temperature variations on the order of +/- 10 K were presumed. This contributes about 3% error to those measurements. For other experiments, upstream temperature is generally available as a thermocouple reading and is recorded or at least monitored. For these measurements, the temperature uncertainty may be stated as:

$$\frac{\partial \dot{m}}{\partial T_0} \Delta T_0 = \frac{-\dot{m}}{2} \left(\left(\frac{\Delta V_{T_0}}{V_{T_0}} \right)^2 + \left(\frac{\Delta C_T}{C_T} \right)^2 \right)^{\frac{1}{2}} \quad (\text{A2.24})$$

The assumption is that the thermocouple measures a stagnation temperature, which it does not in reality do. Instead the thermocouple measures the recovery temperature, which is a temperature somewhere between the static temperature and stagnation temperature (145,146, p. 710). When the fluid is moving slowly there is little difference between the static and stagnation temperatures. The isentropic relations described in texts such as Anderson (33) show that the stagnation and static temperatures differ by only 1.8% when the flow is moving at Mach 0.3, and the difference decreases as the Mach number drops. Further, Fernelius and Gorrell (147) showed that for a small thermocouple, the recovery factor may be as high as 0.85, reducing the error significantly. For the purposes of this research, flow was constantly designed to be moving below Mach 0.3 in the region of thermocouple measurements and the bias

between the recovery temperature measured with the thermocouple and the stagnation temperature were ignored.

1.2.8. The Uncertainty of Mach Number

The formula for the individual contribution of uncertainty of Mach is:

$$\begin{aligned} \frac{\partial \dot{m}}{\partial M} \Delta M = & \left(\frac{1}{M} \frac{\pi d^2}{4} n P_0 M \sqrt{\frac{\gamma \overline{M}}{T_0 R_u}} \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \right. \\ & \left. + \left(\frac{2M \left(\frac{\gamma-1}{2} \right)}{\left(1 + \frac{\gamma-1}{2} M^2 \right) 2(\gamma-1)} \right) \frac{\pi d^2}{4} n P_0 M \sqrt{\frac{\gamma \overline{M}}{T_0 R_u}} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \right) \Delta M \end{aligned} \quad (\text{A2.25})$$

Again, the mass flow rate of the form found in Equations A2.1 and A2.6 is embedded within this formula. Substituting the mass flow rate simplifies the Mach uncertainty to:

$$\frac{\partial \dot{m}}{\partial M} \Delta M = \dot{m} \left(\frac{1}{M} + \left(\frac{2M \left(\frac{\gamma-1}{2} \right)}{\left(1 + \frac{\gamma-1}{2} M^2 \right) 2(\gamma-1)} \right) \right) \Delta M \quad (\text{A2.26})$$

further simplification yields:

$$\frac{\partial \dot{m}}{\partial M} \Delta M = \dot{m} \left(\frac{1}{M} + \left(\frac{M}{2 \left(1 + \frac{\gamma-1}{2} M^2 \right)} \right) \right) \Delta M \quad (\text{A2.27})$$

Since there is no uncertainty in Mach (flow calculations require that the flow is defined as choked, such that $M \equiv 1$), the uncertainty of 0 cancels out the remaining portion and this term is ignored. Mathematically the statement becomes:

$$\frac{\partial \dot{m}}{\partial M} \Delta M = \frac{\partial \dot{m}}{\partial M} 0 = 0 \quad (\text{A2.28})$$

1.2.9. The Uncertainty with the Number of Nozzles

For hydrogen and air, only one nozzle existed. It is an integer with 0 uncertainty.

$$\frac{\partial \dot{m}}{\partial n} \Delta n = 0 \quad \text{iff} \quad \Delta n = 0 \quad (\text{A2.29})$$

The feed bar described in Appendix 1 had multiple holes. It was desired to calculate the mass flow rate through the nozzles so that an estimate of leak rates in the plenum could be performed. At some point during operation, silicone adhesive and Teflon tape blocked some of the 160 nozzles during tests, so it is necessary to calculate the mass flow rate uncertainty due to uncertainty in the number of nozzles as:

$$\frac{\partial \dot{m}}{\partial n} \Delta n = \frac{\dot{m}}{n} \Delta n \quad (\text{A2.30})$$

which would contribute an error on the order of the percentage of blocked holes.

1.2.10. The Uncertainty of the Nozzle Throat Diameter

The uncertainty contribution of the diameter of the nozzle is:

$$\frac{\partial \dot{m}}{\partial d} \Delta d = 2 \frac{\dot{m}}{d} \Delta d \quad (\text{A2.31})$$

If the uncertainty is due to machining tolerances (say ± 0.005 in.), this error can be one of the largest contributors to the total, especially when the diameters are small. Care must be taken to ensure that the uncertainty in the nozzle diameter is properly accounted for.

1.2.11. Total Mass Flow Rate Uncertainty in Detail

Combining all the terms of Equations A2.14 through A2.31, the total uncertainty initially described in Equation A2.13 becomes:

$$\begin{aligned}
\Delta \dot{m} = & \left(\left(\dot{m} \left[\frac{1}{2\gamma} - \ln \left(1 + \frac{\gamma-1}{2} M^2 \right) \left(\frac{1}{2(\gamma-1)} - \frac{2(\gamma+1)}{(2\gamma-2)^2} \right) \right. \right. \right. \\
& \left. \left. + \frac{M^2(\gamma+1)}{2 \left(1 + \frac{\gamma-1}{2} M^2 \right) 2(\gamma-1)} \right] \Delta \gamma \right)^2 + \left(\frac{\dot{m}}{\pi} 0 \right)^2 + \left(\frac{-\dot{m}}{2R_u} \Delta R_u \right)^2 \\
& + \left(\frac{\dot{m}}{2\bar{M}} \Delta \bar{M} \right)^2 + \dot{m} \left(\frac{\Delta V_{P_0}}{V_{P_0}} \right)^2 + \dot{m} \left(\frac{\Delta C_P}{C_P} \right)^2 + \dot{m} \left(\frac{\Delta P_{atm}}{P_{atm}} \right)^2 + \dot{m} \left(\frac{\Delta V_{T_0}}{2V_{T_0}} \right)^2 \\
& \left. + \dot{m} \left(\frac{\Delta C_T}{2C_T} \right)^2 + \left(\frac{\partial \dot{m}}{\partial M} 0 \right)^2 + \left(\frac{\dot{m}}{n} \Delta n \right)^2 + \left(2 \frac{\dot{m}}{d} \Delta d \right)^2 \right)^{\frac{1}{2}}
\end{aligned} \tag{A2.32}$$

Using the distributive property of multiplication, the mass flow rate term, $\dot{m}$, is moved outside the brackets to obtain:

$$\begin{aligned}
\Delta \dot{m} = & \dot{m} \left(\left(\left[\frac{1}{2\gamma} - \ln \left(1 + \frac{\gamma-1}{2} M^2 \right) \left(\frac{1}{2(\gamma-1)} - \frac{2(\gamma+1)}{(2\gamma-2)^2} \right) \right. \right. \right. \\
& \left. \left. + \frac{M^2(\gamma+1)}{2 \left(1 + \frac{\gamma-1}{2} M^2 \right) 2(\gamma-1)} \right] \Delta \gamma \right)^2 + (0)^2 + \left(\frac{-\Delta R_u}{2R_u} \right)^2 \\
& + \left(\frac{\Delta \bar{M}}{2\bar{M}} \right)^2 + \left(\frac{\Delta V_{P_0}}{V_{P_0}} \right)^2 + \left(\frac{\Delta C_P}{C_P} \right)^2 + \left(\frac{\Delta P_{atm}}{P_{atm}} \right)^2 + \left(\frac{\Delta V_{T_0}}{2V_{T_0}} \right)^2 \\
& \left. + \left(\frac{\Delta C_T}{2C_T} \right)^2 + (0)^2 + \left(\frac{\Delta n}{n} \right)^2 + \left(2 \frac{\Delta d}{d} \right)^2 \right)^{\frac{1}{2}}
\end{aligned} \tag{A2.33}$$

The most significant terms are identified by examining which of the largest uncertainties are paired with the smallest values. Inevitably it is the last term, d , the nozzle throat

diameter that has the largest uncertainty and smallest value – making it the most significant contributor to the uncertainty of the calculated mass flow rate.

1.3. Premixture Combined Flow Rates

When the fuel and oxidizer streams are combined to form a premixture, another formula is used to combine them:

$$\dot{m}_{mix} = \dot{m}_f + \dot{m}_a \quad (\text{A2.34})$$

Subsequently, the mixture mass flow rate uncertainty must take on the uncertainties of both the fuel and the oxidizer as described above:

$$\Delta \dot{m}_{mix} = \dot{m}_{mix} \left(\left(\frac{\Delta \dot{m}_f}{\dot{m}_f} \right)^2 + \left(\frac{\Delta \dot{m}_a}{\dot{m}_a} \right)^2 \right)^{\frac{1}{2}} \quad (\text{A2.35})$$

1.4. Equivalence Ratio

Frequently, the mixture of a fuel and oxidizer is described in terms of a mass ratio called the equivalence ratio. This ratio compares the actual amount of fuel mixed with an oxidizer to the amount of fuel it would require to stoichiometrically balance the reaction. It may be written as:

$$\phi = \frac{\left(\frac{f}{a} \right)}{\left(\frac{f}{a} \right)_{stoich}} \approx \frac{\left(\frac{\dot{m}_f}{\dot{m}_a} \right)}{\left(\frac{f}{a} \right)_{stoich}} \quad (\text{A2.36})$$

where ϕ is called the equivalence ratio, f is the mass of fuel in the mixture, a is the amount of air (oxidizer), $\dot{m}_f$ is the fuel mass flow rate, and $\dot{m}_a$ is the air mass flow rate.

The uncertainty for this calculation becomes:

$$\Delta\phi = \phi \left(\left(\frac{\Delta f}{f} \right)^2 + \left(\frac{\Delta a}{a} \right)^2 + \left(\frac{\Delta \left(\frac{f}{a} \right)_{stoich}}{\left(\frac{f}{a} \right)_{stoich}} \right)^2 \right)^{\frac{1}{2}}$$

$$\approx \phi \left(\left(\frac{\Delta \dot{m}_f}{\dot{m}_f} \right)^2 + \left(\frac{\Delta \dot{m}_a}{\dot{m}_a} \right)^2 + \left(\frac{\Delta \left(\frac{f}{a} \right)_{stoich}}{\left(\frac{f}{a} \right)_{stoich}} \right)^2 \right)^{\frac{1}{2}}$$
(A2.37)

Since $\left(\frac{f}{a} \right)_{stoich}$ is taken from the stoichiometric equation, which is theoretical, the uncertainty revolves around the molecular weights for the reactants, which is relatively small when compared to the uncertainty of the mass flow rates, and it may be ignored.

1.5. Mixture Gas Constant (R_{mix})

When the fuel and oxidizer streams combine into a new mixture, the thermochemical properties adjust with the molarity. The mixture gas constant, R_{mix} , has been seen to be important to our mass flow calculation and needs to be considered.

$$R_{mix} = R_u \left(\frac{\frac{f}{\bar{M}_f} + \frac{a}{\bar{M}_a}}{f + a} \right)$$
(A2.38)

where f and a are the mass fractions for fuel and air respectively and may be replaced by substitution with the mass flow rates of fuel ($\dot{m}_f$) and oxidizer ($\dot{m}_o$) respectively.

$$R_{mix} = R_u \left(\frac{\frac{\dot{m}_f}{\bar{M}_f} + \frac{\dot{m}_o}{\bar{M}_o}}{\dot{m}_f + \dot{m}_o} \right)$$
(A2.39)

$$R_{mix} = R_u \left(\frac{\frac{\dot{m}_f}{\bar{M}_f} + \frac{\dot{m}_o}{\bar{M}_o}}{\dot{m}_f + \dot{m}_o} \right)$$

The mixture uncertainty then becomes:

$$\begin{aligned} \Delta R_{mix} = R_{mix} & \left(\left(\frac{\Delta \bar{R}_u}{\bar{R}_u} \right)^2 + \left(\frac{\Delta \bar{M}_f}{\bar{M}_f} \right)^2 + \left(\frac{\Delta \bar{M}_o}{\bar{M}_o} \right)^2 \right. \\ & + \left(\Delta \dot{m}_f \left(\frac{1}{\bar{M}_f \left(\frac{\dot{m}_f}{\bar{M}_f} + \frac{\dot{m}_o}{\bar{M}_o} \right)} - \frac{1}{\dot{m}_f + \dot{m}_o} \right) \right)^2 \\ & \left. + \left(\Delta \dot{m}_o \left(\frac{1}{\bar{M}_{ox} \left(\frac{\dot{m}_f}{\bar{M}_f} + \frac{\dot{m}_o}{\bar{M}_o} \right)} - \frac{1}{\dot{m}_f + \dot{m}_o} \right) \right)^2 \right)^{\frac{1}{2}} \end{aligned} \quad (A2.40)$$

The uncertainty associated with the universal gas constant is negligible and is ignored.

Likewise the uncertainty associated with the molecular weights of fuel and oxidizer should be relatively small, leaving the uncertainty of the mixture gas constant on the order of the total mass flow rate. It would also be possible to replace all the fuel-to-air ratios with something in terms of the equivalence ratio and come up with a similar formulation for the error. Mass flow rates are expected to remain the predominant terms and would not significantly change the uncertainty.

1.6. Area from Mass Flow Rate

At times, the linear test section experienced some leakage. With a known mass flowing into the system, an upstream pressure measurement, and an approximate stagnation temperature, the mass flow formula repeated here:

$$\frac{\dot{m}}{nA} \left(\frac{\sqrt{T_0 R_M}}{P_o} \right) = M \sqrt{\gamma} \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \quad (\text{A2.41})$$

can be solved for the choke area:

$$A = \frac{\dot{m}}{nMP_0} \sqrt{\frac{T_0 R_{mix}}{\gamma}} \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\frac{\gamma+1}{2(\gamma-1)}} \quad (\text{A2.42})$$

and there will be significant uncertainty associated with this calculation.

The initial cut at the uncertainty produces 7 terms:

$$\begin{aligned} \Delta A = A \left(\left(\frac{\Delta \dot{m}}{\dot{m}} \right)^2 + \left(\frac{-\Delta P_0}{P_0} \right)^2 + \left(\frac{\Delta T_0}{2T_0} \right)^2 + \left(\frac{\Delta R_{mix}}{2R_{mix}} \right)^2 + \left(\frac{\Delta n}{n} \right)^2 + f(M)^2 \right. \\ \left. + f(\gamma)^2 \right)^{\frac{1}{2}} \end{aligned} \quad (\text{A2.43})$$

where the partial differentials of the area formula with respect to Mach and specific heat ratio have not been expanded. Leveraging the analysis of previous sections, it was recognized that the uncertainty of both Mach:

$$f(M) = \frac{\partial A}{\partial M} = A \left(\frac{2MA(\gamma + 1) \left(\frac{\gamma - 1}{2} \right)}{\left(1 + \frac{\gamma - 1}{2} M^2 \right)} - \frac{1}{M} \right) \Delta M \approx 0 \quad (\text{A2.44})$$

and specific heat ratios:

$$\begin{aligned} \frac{\partial A}{\partial \gamma} \Delta \gamma = A \left(\ln \left(1 + \frac{\gamma - 1}{2} M^2 \right) \left(\frac{1}{2(\gamma - 1)} - \frac{2(\gamma + 1)}{(2(\gamma - 1))^2} \right) \right. \\ \left. + \frac{M^2(\gamma + 1)}{2 \cdot 2(\gamma - 1) \left(1 + \frac{\gamma - 1}{2} M^2 \right)} - \frac{1}{2\gamma} \right) \cdot \Delta \gamma \approx 0 \end{aligned} \quad (\text{A2.45})$$

would be insignificant and they were dropped from the analysis.

$$\Delta A = A \left(\left(\frac{\Delta \dot{m}}{\dot{m}} \right)^2 + \left(\frac{-\Delta P_0}{P_0} \right)^2 + \left(\frac{\Delta T_0}{2T_0} \right)^2 + \left(\frac{\Delta R_{mix}}{2R_{mix}} \right)^2 + \left(\frac{\Delta n}{n} \right)^2 \right)^{\frac{1}{2}} \quad (\text{A2.46})$$

Leaving only terms that can be found in the analysis from Sections 1.1 through 1.3 of this appendix.

2. Velocity

Velocity measurements taken between two frames of a stop-motion video are based off of the calculation

$$V = \frac{x_2 - x_1}{t_2 - t_1} \xi_p = \frac{(x_2 - x_1) x}{nf d} \quad (\text{A2.47})$$

where V is the velocity, $x_2 - x_1$ is the change in the pixel location, $t_2 - t_1$ is the elapsed time between frames, ξ_p is a pixel-to-distance conversion. The time between frames can be written as $t_2 - t_1 = nf$, where n is the number of elapsed frames, and f is the frame rate. The pixel-to-distance conversion is made by dividing the number of pixels, x , between two points whose physical separation, d , is known. The total uncertainty for the velocity becomes:

$$\Delta V = V \left(\left(\frac{\Delta x_1}{x_1} \right)^2 + \left(\frac{\Delta x_2}{x_2} \right)^2 + \left(\frac{\Delta x}{x} \right)^2 + \left(\frac{\Delta n}{n} \right)^2 + \left(\frac{\Delta f}{f} \right)^2 + \left(\frac{\Delta d}{d} \right)^2 \right)^{\frac{1}{2}} \quad (75)$$

Generally, the number of frames is a known integer with 0 error, and the frame rate is accurate to 6 significant digits. The uncertainty of the distance d is also generally less than 1% and is ignored. The result is that identifying the locations of the features becomes critically important. The calibration pixel separation (x) is repeated several times, and each feature location (x_1, x_2) are carefully made to minimize error.

3. Velocity Gradient Estimate Uncertainty

Grumer et al. (30) used the velocity gradient in the laminar boundary layer to normalize all of their stability diagrams. The boundary velocity gradient ($\frac{du}{dy}$, or g) for the near-wall laminar boundary layer is related to the pressure drop along the channel (l , or Δx) with:

$$\mu g 2\pi r = \left(\frac{\Delta p}{\Delta x} \right) \pi r^2 \quad (A2.48)$$

where μ is the dynamic viscosity, g is the laminar boundary layer velocity gradient normal to the flow, r is the tube radius, Δp is the differential pressure, and Δx is the axial distance along flow between pressure points of Δp . Solving for g , the boundary layer velocity gradient, Equation A2.48 becomes:

$$g = \left(\frac{\Delta p}{\Delta x} \right) \left(\frac{r}{2\mu} \right) \quad (A2.49)$$

In this fundamental form, the uncertainty for the velocity gradient (Δg) due to measurement precision errors would be:

$$\begin{aligned}
(\Delta g)^2 = & \left(\frac{\partial g}{\partial(\Delta p)} \Delta(\Delta p) \right)^2 + \left(\frac{\partial g}{\partial(\Delta x)} \Delta(\Delta x) \right)^2 + \left(\frac{\partial g}{\partial(r)} \Delta(r) \right)^2 \\
& + \left(\frac{\partial g}{\partial(\mu)} \Delta(\mu) \right)^2
\end{aligned} \tag{A2.50}$$

After performing the partial differentials, the previous equation to reduces to

$$\left(\frac{\Delta g}{g} \right)^2 = \left(\frac{\Delta(\Delta p)}{\Delta p} \right)^2 + \left(\frac{\Delta(\Delta x)}{\Delta x} \right)^2 + \left(\frac{\Delta r}{r} \right)^2 + \left(\frac{\Delta \mu}{\mu} \right)^2 \tag{A2.51}$$

which would be a fairly simple uncertainty if Δx and Δp were known or measured.

Measurements of the pressure differential are not known, so the relationship between the pressure gradient along the direction of the flow in terms of the Darcy-Weisbach friction factor may be defined (123, p. 109) as

$$\frac{\Delta p}{\Delta x} = f_D \frac{\rho \bar{u}^2}{4r} \tag{A2.52}$$

where $\bar{u}$ is the bulk or mean velocity of the flow, and r is the radius of a tube.

Substituting this relationship into Equation A2.48, yields:

$$g = f_D \frac{\rho \bar{u}^2}{4r} \frac{R}{2\mu} \tag{A2.53}$$

There is a Reynolds number hidden in Equation A2.53 that may be defined by Equation A2.54:

$$Re = \frac{2\rho \bar{u} R}{\mu} \tag{A2.54}$$

Substituting Equation A2.54 into Equation A2.53 generates:

$$g = f_D \frac{Re \bar{u}}{16r} \tag{A2.55}$$

Assuming that the volumetric flow rate is related to the bulk velocity with $\dot{V} = \bar{u}A = \bar{u}\pi r^2$,

$$g = f_D \frac{Re \dot{V}}{16\pi r^3} \quad (\text{A2.56})$$

which is what Grumer et al. (30, p. 91). used to create the stability diagrams described in Chapter II, Section 6.

Substituting the Darcy friction factor with the Fanning friction factor, ($f_D = 4c_f$), Equation A2.56 becomes:

$$g = c_f \frac{Re \dot{V}}{4\pi r^3} \quad (\text{A2.57})$$

Equation A2.57 is the form of the equation used to calculate velocity gradients for this work. Understanding the uncertainty for the error measurement associated with this equation requires conversion to the fundamental measurements taken: temperature and pressure.

The friction factor was calculated using the transcendental Colebrook equation (123, p. 432)

$$\frac{1}{\sqrt{f_D}} = -2.0 \log_{10} \left(\frac{\frac{\epsilon}{D}}{3.7} + \frac{2.512}{Re\sqrt{f_D}} \right) \quad (\text{A2.58})$$

where f_D is the Darcy friction factor, ϵ is the surface roughness height, D is the pipe diameter or channel height, and Re is the Reynold's number. An explicit approximation for the Colebrook equation with $\pm 2\%$ error was given by Haaland (123, p. 433):

$$\frac{1}{\sqrt{f_D}} = -1.8 \log_{10} \left(\frac{6.9}{Re_D} + \left(\frac{\epsilon}{3.7D} \right)^{1.11} \right) \quad (\text{A2.59})$$

An algebraic manipulation changes the equation into a form that is easily substituted into the velocity gradient formula:

$$f_D = \left(-1.8 \log_{10} \left(\frac{6.9}{Re_D} + \left(\frac{\epsilon}{3.7D} \right)^{1.11} \right) \right)^{-2} \quad (\text{A2.60})$$

Substitute Equation A2.59 into Equation A2.58 to generate:

$$g = \left(-1.8 \log_{10} \left(\frac{6.9}{Re_D} + \left(\frac{\epsilon}{3.7D} \right)^{1.11} \right) \right)^{-2} \frac{Re \dot{V}}{16\pi r^3} \quad (\text{A2.61})$$

The volumetric flow rate is defined in terms of mass flow rate and density as:

$$\dot{V} = \frac{\dot{m}}{\rho} \quad (\text{A2.62})$$

Substitution back in gives:

$$g = \left(-1.8 \log_{10} \left(\frac{6.9}{Re_D} + \left(\frac{\epsilon}{3.7D} \right)^{1.11} \right) \right)^{-2} \frac{Re \dot{m}}{16\pi r^3 \rho} \quad (\text{A2.63})$$

The Reynolds number for a narrow slot is defined in terms of the hydraulic diameter as:

$$Re = \dot{m} \frac{D_h}{A\mu} = \frac{2\dot{m}}{w\mu} \quad (\text{A2.64})$$

where $D_h = 2h$, $r = h$, $\rho = P/RT$, and all are substituted back into Equation A2.63 to generate:

$$g = \left(-1.8 \log_{10} \left(\frac{6.9}{\frac{2\dot{m}}{w\mu}} + \left(\frac{\epsilon}{\frac{2h}{3.7}} \right)^{1.11} \right) \right)^{-2} \frac{2\dot{m}}{w\mu} \frac{\dot{m}R_g T}{P} \frac{1}{16\pi h^3} \quad (A2.65)$$

Mass flow rate, $\dot{m}$, is a derived quantity found from the summation of fuel and oxidizer mass flow rates

$$\dot{m} = \dot{m}_{fuel} + \dot{m}_{oxidz} \quad (A2.66)$$

The fuel and oxidizer mass flow rates were calculated with the choked flow equation as described in Appendix II, Sections 1.1 to 1.4. Combining terms and distributing for ease of performing a partial differentiation

$$g = \left(-1.8 \log_{10} \left(\frac{6.9}{\frac{2\dot{m}}{w\mu}} + \left(\frac{\epsilon}{\frac{2h}{3.7}} \right)^{1.11} \right) \right)^{-2} \frac{2\dot{m}^2 R_{mix} T}{wP\mu} \frac{1}{16\pi h^3} \quad (A2.67)$$

The Sutherland model for μ is within 2 percent (123, p. 28) of measured data. The gas constant of the mixture, R_{mix} , and π are assumed to be exact and contributions to the error were not tracked. One more step is taken in preparation for performing a partial differential; the constants are collected and the fraction simplified:

$$g = 0.41 \left(\log_{10} \left(\frac{6.9}{\frac{2\dot{m}}{w\mu}} + \left(\frac{\epsilon}{\frac{2h}{3.7}} \right)^{1.11} \right) \right)^{-2} \frac{\dot{m}^2 R_{mix} T}{\pi h^3 w P \mu} \quad (A2.68)$$

The contributions of error due to temperature and plenum pressure are fairly simple:

$$\frac{\partial g}{\partial T} = g \frac{\partial T}{T} = \frac{\Delta g}{\Delta T} \quad (A2.69)$$

$$\frac{\partial g}{\partial P} = g \frac{\partial P}{P} \quad (A2.70)$$

More difficult is the contribution due to surface roughness of the sidewall:

$$\frac{\partial g}{\partial \epsilon} = \frac{\frac{8.8 \dot{m}^2 R_g T}{\pi h^4 w P \mu} \left(\frac{\epsilon}{2h} \right)^{0.11}}{\left(\left(\frac{\epsilon}{2h} \right)^{1.11} + \frac{6.9}{2\dot{m}} \right) \ln^3 \left(\left(\frac{\epsilon}{2h} \right)^{1.11} + \frac{6.9}{2\dot{m}} \right)} \quad (\text{A2.71})$$

Contributions due to mass flow rate, channel width, and channel height are even more complicated to perform analytically and do not produce a form that is easily separable.

Due to the nature of the uncertainty functions, the magnitude of the uncertainty will be affected of the magnitude of all terms in the equation, not just the one that is measured.

Numeric uncertainty is significantly easier. Numeric uncertainty is calculated with

Equation A2.72:

$$\frac{\Delta g(z)}{g} = \frac{|g(z) - g(z \pm \Delta z)|}{g(z)} \quad (\text{A2.72})$$

where z may represent the channel roughness, mass flow rate, channel width, or channel height, and Δz represents the uncertainty in the measurement.

All of the uncertainties are summed in quadrature so that:

$$\begin{aligned} \Delta g = g & \left(\left(\frac{\Delta T}{T} \right)^2 + \left(\frac{\Delta P}{P} \right)^2 + \left(\frac{\Delta \mu}{\mu} \right)^2 + \left(\frac{|g(\epsilon) - g(\epsilon + \Delta \epsilon)|}{g(\epsilon)} \right)^2 \right. \\ & + \left(\frac{|g(\dot{m}) - g(\dot{m} + \Delta \dot{m})|}{g(\dot{m})} \right)^2 + \left(\frac{|g(h) - g(h + \Delta h)|}{g(h)} \right)^2 \\ & \left. + \left(\frac{|g(w) - g(w + \Delta w)|}{g(w)} \right)^2 \right) \quad (\text{A2.73}) \end{aligned}$$

This provides a viable formula and method for calculating uncertainty.

To understand the relationships that exist within the Equation A2.73, it is desirable to have the mass flow rate written in terms of pressures and temperatures. The mass flow rate is calculated from the universal flow function (148, p. 71), but assuming flow is choked across the feed plenum, a discharge coefficient could be found (135, pp. 397-403) for the plenum that allows metering the flow through the plenum using the temperature and pressure of the plenum mixture that is already in Equation A2.73. The mass flow rate would then be calculated with the equation:

$$\dot{m}_{mix} = MAC_D P_0 \sqrt{\frac{\gamma_{mix}}{R_{mix} T_0}} \left(1 + \frac{\gamma_{mix} - 1}{2} M^2 \right)^{\frac{-(\gamma_{mix} + 1)}{2(\gamma_{mix} - 1)}} \quad (A2.74)$$

where $\dot{m}_{mix}$ is the mass flow rate of mixture, M is the Mach number, A is the Cross sectional area of the feed throat, C_D is the Discharge coefficient, P_0 is the Stagnation pressure of the flowing mixture, γ_{mix} is the Specific heat ratio of the mixture, R_{mix} is the Gas constant of the mixture, and T_0 is the Stagnation temperature of the flowing mixture

Depending on where the gradient is being measured, the Mach number may be 1 if choked or less than 1 if not at the choke location. Also, the cross sectional area is $A = hw$, so the equation simplifies to:

$$\dot{m}_{mix} = hwMC_D P_0 \sqrt{\frac{\gamma_{mix}}{R_{mix} T_0}} \left(1 + \frac{\gamma_{mix} - 1}{2} M^2 \right)^{\frac{-(\gamma_{mix} + 1)}{2(\gamma_{mix} - 1)}} \quad (A2.75)$$

Substituting this equation back into the velocity gradient equation gives the relation:

$$g = 0.41 \left(\log_{10} \left(\frac{6.9}{\frac{2hwMC_D P_0 \sqrt{\frac{\gamma_{mix}}{R_{mix} T_0}} \left(1 + \frac{\gamma_{mix} - 1}{2} M^2\right)^{\frac{-(\gamma_{mix}+1)}{2(\gamma_{mix}-1)}}}{\mu w}} \right. \right. \\ \left. \left. + \left(\frac{\epsilon}{\frac{2h}{3.7}} \right)^{1.11} \right) \right)^{-2} \left(\frac{hwMC_D P_0 \sqrt{\frac{\gamma_{mix}}{R_{mix} T_0}} \left(1 + \frac{\gamma_{mix} - 1}{2} M^2\right)^{\frac{-(\gamma_{mix}+1)}{2(\gamma_{mix}-1)}}}{\pi h^3 w P \mu} \right)^2 R_g T \quad (A2.76)$$

Reducing the fractions helps a little to show

$$g = 0.41 \left(\log_{10} \left(\frac{6.9 \left(1 + \frac{\gamma_{mix} - 1}{2} M^2\right)^{\frac{(\gamma_{mix}+1)}{2(\gamma_{mix}-1)}}}{2\mu h w^2 M C_D P_0 \sqrt{\frac{\gamma_{mix}}{R_{mix} T_0}}}} \right. \right. \\ \left. \left. + \left(\frac{\epsilon}{7.4h} \right)^{1.11} \right) \right)^{-2} \frac{w P_0 \gamma_{mix} \left(1 + \frac{\gamma_{mix} - 1}{2} M^2\right)^{\frac{-(\gamma_{mix}+1)}{(\gamma_{mix}-1)}} (M C_D)^2}{\pi h \mu} \quad (A2.77)$$

Looking at the relationships between the velocity gradient, the pressure, and slot height the proportionality of the velocity gradient to the stagnation pressure may be described as:

$$g \propto c_1 \log_{10}^{-2} \left(\frac{c_2}{P_0} + c_3 \right) P_0 \quad (A2.78)$$

$$g \propto \frac{c_1}{h} \log_{10}^{-2} \left(\frac{c_2}{h} + \left(\frac{c_3}{h} \right)^{1.11} \right) \quad (A2.79)$$

where c_1, c_2 , and c_3 are constants with respect to the variables of interest, and $c_3 \ll h$ in Equation A2.79.

What is important to note on these charts is that response of the boundary layer velocity gradient to the slot height is comparable to that of the pressure, as illustrated in

Figure A2.2. There are not units associated with Figure A2.2, and the trends will hold as long as the units of A2.78 and A2.79 are consistent within themselves.

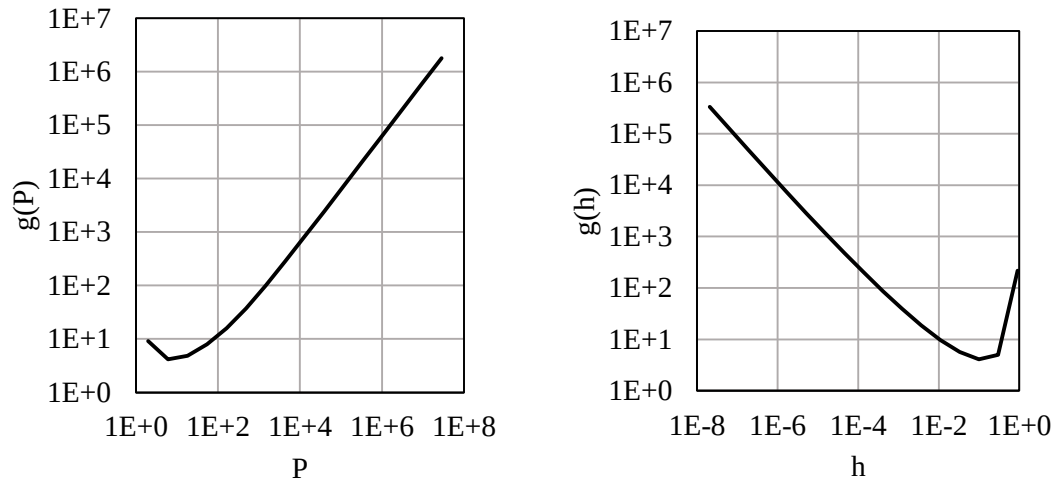


Figure A2.2 Plot of the proportional relationship between the velocity gradient and pressure (left) and slot height (right) from Equations A2.78 and A2.79 respectively

Appendix III Improving Detonation Cell Width Prediction Model

This appendix was originally written as the author's final project in the AFIT course *STAT 696: Linear Regression Analysis* in the fall quarter of 2013. A description of detonation cell width and the need for an accurate predictive model is briefly discussed. The data sets employed in the modeling are described. The current cell width model employed by AFRL is considered, transformed into a linear equation, and evaluated using simple linear regression. The model is extended through implementations of 5 additional predictor variables. One predictor variable is a transformation of equivalence ratio, while the other four are fuel types. A model for initiation energy is constructed, evaluated, and ported into the cell width data set in an attempt to extend the model. Refinements to variable transformations are proposed.

1. Background

Design of detonation machinery requires an accurate understanding of the detonation processes. Detonation progresses through a fuel-oxidizer mixture as a cascading process of small detonation cells. When the detonation passes along a sooted surface, it leaves marks, as seen in Figure A3.1.

Each of the rhomboids, which look similar to a fish scale, represent a single detonation cell. While some detonations generate uniform cell sizes, others do not, as seen in Figure A3.2 from (149).

Journal articles, conference proceedings, technical reports, and books on detonation have been surveyed and collected by Caltech in the detonation database (49).

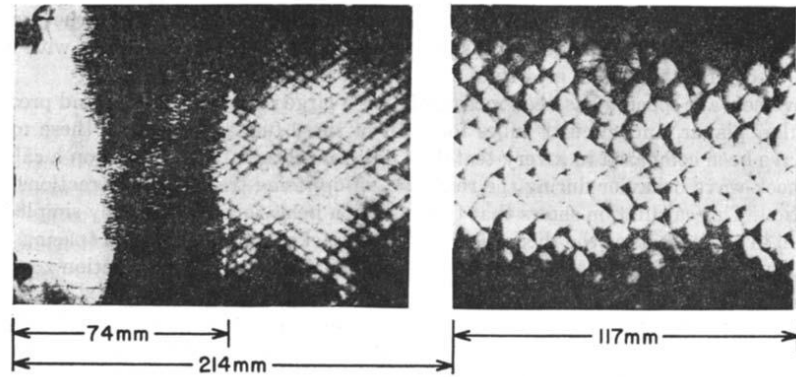


Figure A3.1 Photograph of sooted foil showing detonation cell traces (149)

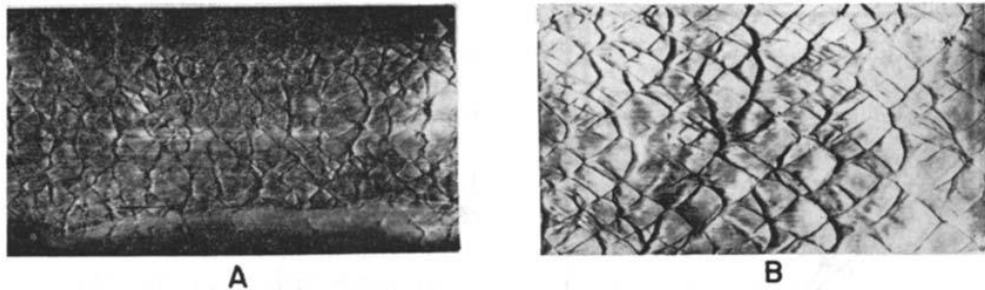


Figure A3.2 Sooted foil record of stoichiometric hydrogen and oxygen in a (A) 3.25 x 0.25 inch rectangular and (B) 2 inch circular tube (149)

This data serves as the underlying data set with over 1655 data points for cell size and 285 for ignition energy. The data includes multiple subsets of data that vary equivalence ratio (a ratio of fuel to oxidizer), initial pressure, initial temperature, fuel type, diluent type, and percent diluent.

2. Motivation

The detonation cell structure is critical to continuing detonation, and the locations where they meet create high temperature and pressure points that initiate the next cell. Detonation cell width is the parameter most commonly used to design machinery. A significant body of experimental data has been collected, and intense computational effort has been invested to understand detonation factors that affect the cell width (49). One

current model for predicting detonation cell size is described by Tucker (50). He found a correlation between the experimentally determined detonation initiation energy ($E_{initiation}$) and detonation cell width (λ) for stoichiometric detonations initiated from mixtures at standard temperature and pressure. The model is written as:

$$E_{initiation} = 3.375 \quad (A3.1)$$

which can be transformed into:

$$\lambda = \frac{2}{3} \sqrt[3]{E_{initiation}} \quad (A3.2)$$

$$\log(\lambda) = \log \frac{2}{3} + \log \left(E_{initiation}^{1/3} \right)$$

$$\log(\lambda) = -0.17609126 + \frac{1}{3} \log(E_{initiation}) \quad (A3.3)$$

which follows the general linear regression model:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i \quad (A3.4)$$

where the logarithm of cell width $\log(\lambda)$ is predicted linearly with the intercept coefficient $\beta_0 = -0.17609126$, and a slope coefficient $\beta_1 = 1/3$, for a predictor variable, X , transformed with another logarithm.

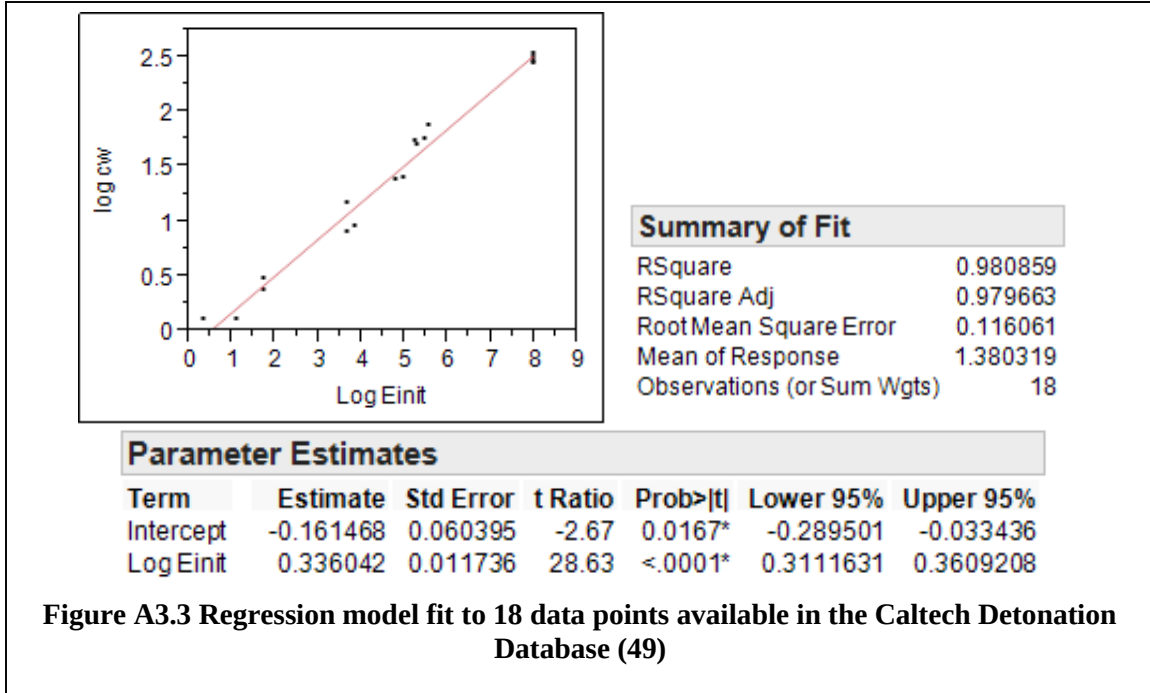
This model has served as a good rule of thumb to predict detonation cell size for stoichiometric mixtures of various fuels at standard temperature and pressure. It captured the key trend correlating cell width to initiation energy. Engineers may use the cell size information and design hardware based on the relationships for initial temperature, pressure, and diluent. The design process requires several steps and references to multiple different experimental data sets. The ultimate goal of this effort was to build a model that

included a better fit to the data and included the effects of temperature, pressure, fuel-to-air ratio (ϕ), and diluent.

The first step was to evaluate the current model, shown in Equation A3.1, using the 18 data points common between the two data sets. Within the 18 data points, four initiation energy detonation data points were repeated and paired with cell width observations at 4 closely matched conditions, and two cell width observations were paired with two closely matched initiation energy conditions. Each of the data points represent either hydrogen or a hydrocarbon fuel mixed with pure oxygen or air. All data points were selected to have a fuel-to-air mixture that allowed complete combustion of the fuel with only water and carbon dioxide as by-products (i.e. the equivalence ratio was 1). All data points were also taken for mixtures that were at 293K, and between 100 and 101.3 kPa (1 atm). Some fuels, such as CH₄, had several data points at a given mixture representing either a unique cell width observation or a unique ignition energy observation. Also, several data points were interpolated on either cell width or initiation energy to arrive at an equivalence ratio of 1 for inclusion on the chart. The linear fit of the data is shown in Figure A3.3. From the available data points, it appeared that the model was reasonable but not a perfect fit. The summary statistics of fit data also in Figure A3.3 provided a better understanding of the fit.

A statistical t-test was used to verify that the model is a linear relationship with a significance level of $\alpha = 0.05$. The significance level was selected to capture the 1/20th percentile since there are on the order of 20 data points. The test hypotheses are:

$$H_0: \beta_1 = 0 \text{ and } H_a: \beta_1 \neq 0; \quad (A3.5)$$



The rule for accepting or rejecting the null hypothesis used a two-tailed t-distribution:

$$\text{if } t^* \leq t\left(1 - \frac{\alpha}{2}; n - 2\right) = t(0.975; 16) = 2.1199, \text{ then conclude } H_0 \quad (\text{A3.6})$$

The decision statistic, t^* , for the predictor coefficient, β_1 , is shown in the Parameter Estimates table of Figure A3.3 as 28.63. The decision rule led to the conclusion of the null hypothesis, H_0 . In Table 1, the P-value is reported as <.0001, indicating that the probability that a relationship was concluded where none existed (Type I error) was less than 0.01 percent.

A more meaningful test was whether the baseline model was included in the regression model. The test hypotheses were:

$$\begin{aligned} H_{01}: \beta_0 &= -0.17609125, H_{a1}: \beta_0 \neq -0.17609125 \\ H_{02}: \beta_1 &= \frac{1}{3}, H_{a2}: \beta_1 \neq 1/3 \end{aligned} \quad (\text{A3.7})$$

When these two tests were conducted independently, the appropriate decision rules were:

$$\text{if } t^* \leq t\left(1 - \frac{\alpha}{2}; n - 2\right) = t(0.95, 16) = 2.120, \text{ then conclude } H_0 \quad (\text{A3.8})$$

where the test statistics for the independent tests were calculated as :

$$\text{For hypothesis 1: } t^* = \frac{b_0 - \beta_{0o}}{\{s\}} = 0.018710 \quad (\text{A3.9})$$

$$\text{For hypothesis 2: } t^* = \frac{b_1 - \beta_{1o}}{\{s\}} = 0.03456569$$

A more appropriate test would combine both terms into one test using the following hypotheses:

$$H_0: \beta_0 = -0.17609125 \text{ and } \beta_1 = 1/3 \quad (\text{A3.10})$$

$$H_a: \text{Not both } \beta_0 = -0.17609125 \text{ and } \beta_1 = 1/3$$

The JMP statistical software (150) was used to compute the test ratio with the following decision rule:

$$\text{if } F^* > F(0.95; 2, 16) = 3.633, \text{ then conclude } H_0 \quad (\text{A3. 11})$$

As seen in the last sub-table in Figure A3.4, the F ratio far exceeded the test statistic, so the null hypothesis, H_0 , was concluded with greater than 99% confidence that a type I error had not been committed. This indicated that the baseline model was supported by this regression model.

Custom Test		Custom Test		Custom Test	
Parameter		Parameter		Parameter	
Intercept	-0.1760913	Intercept	0	Intercept	-0.1760913
Log Einit	0	Log Einit	0.33333333	Log Einit	0.33333333
=	0	=	0	=	0
Value	0.0284331277	Value	0.1120139838	Value	0.1404471197
Std Error	0.0106351045	Std Error	0.0039119383	Std Error	0.0142334712
t Ratio	2.6735165427	t Ratio	28.633882958	t Ratio	9.8673835825
Prob> t	0.0166501795	Prob> t	3.569061e-15	Prob> t	3.3065007e-8
SS	0.0962802142	SS	11.044137053	SS	1.3115212116
Sum of Squares 0.0962802142		Sum of Squares 11.044137053		Sum of Squares 1.3115212116	
Numerator DF 1		Numerator DF 1		Numerator DF 1	
F Ratio 7.1476907041		F Ratio 819.89925323		F Ratio 97.365258765	
Prob > F 0.0166501795		Prob > F 3.569061e-15		Prob > F 3.3065007e-8	

Figure A3.4 Custom tests completed in JMP (150) testing the viability of the Baseline model given the regression of the data; all tests show statistical significance that the Baseline Model is true given the observations

Statistics for this model were computed using the JMP (150) statistical package. The Summary of Fit table in Figure A3.3 shows an R^2 value of 0.98, indicating that the model accounts for 98 percent of the variability between cell size and detonation energy for many mixtures at a stoichiometric mixing ratio at standard conditions. The root mean square error indicates some prediction variability, which is aligned with the uncertainty of using only 18 data points.

Residuals were considered in order to understand the appropriateness of the linear model. Residuals are the difference between the observed cell width and the cell width predicted by the model. In terms of the linear model shown in Equation A3.3, the residuals were calculated according to the formula found in (151):

$$e_i = Y_i - \hat{Y}_i \quad (\text{A3.12})$$

where Y_i is the observed data and $\hat{Y}_i$ is the data estimated using the same predictor variable (X_i) as the observed data. Applying this to the data set in this study, the residual represented differences between each of the 18 observed cell sizes and those calculated using Equation A3.3. The residuals helped to determine the validity of several underlying model assumptions for the model shown in Equation A3.1 (as listed in Kutner (151)).

- i. The regression function is not linear
- ii. The error terms do not have constant variance
- iii. The error terms are not independent
- iv. The model fits all but one, or a few, outlier observations
- v. The error terms are not normally distributed
- vi. One, or several, important predictor variables were omitted from the model

Each of these assumptions was considered briefly. First, the residual distribution plots were generated by the JMP statistical package (150) and shown in Figure A3.5. The plots of Figure A3.5 showed that the data approximates a normal distribution (item v). The histogram at the top identified residuals distant from the median and askew to one

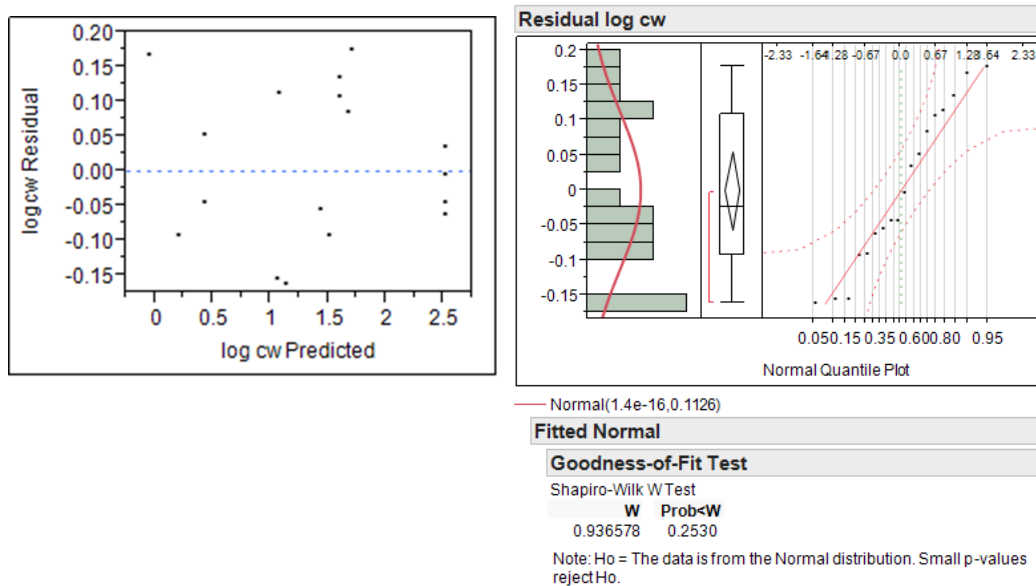
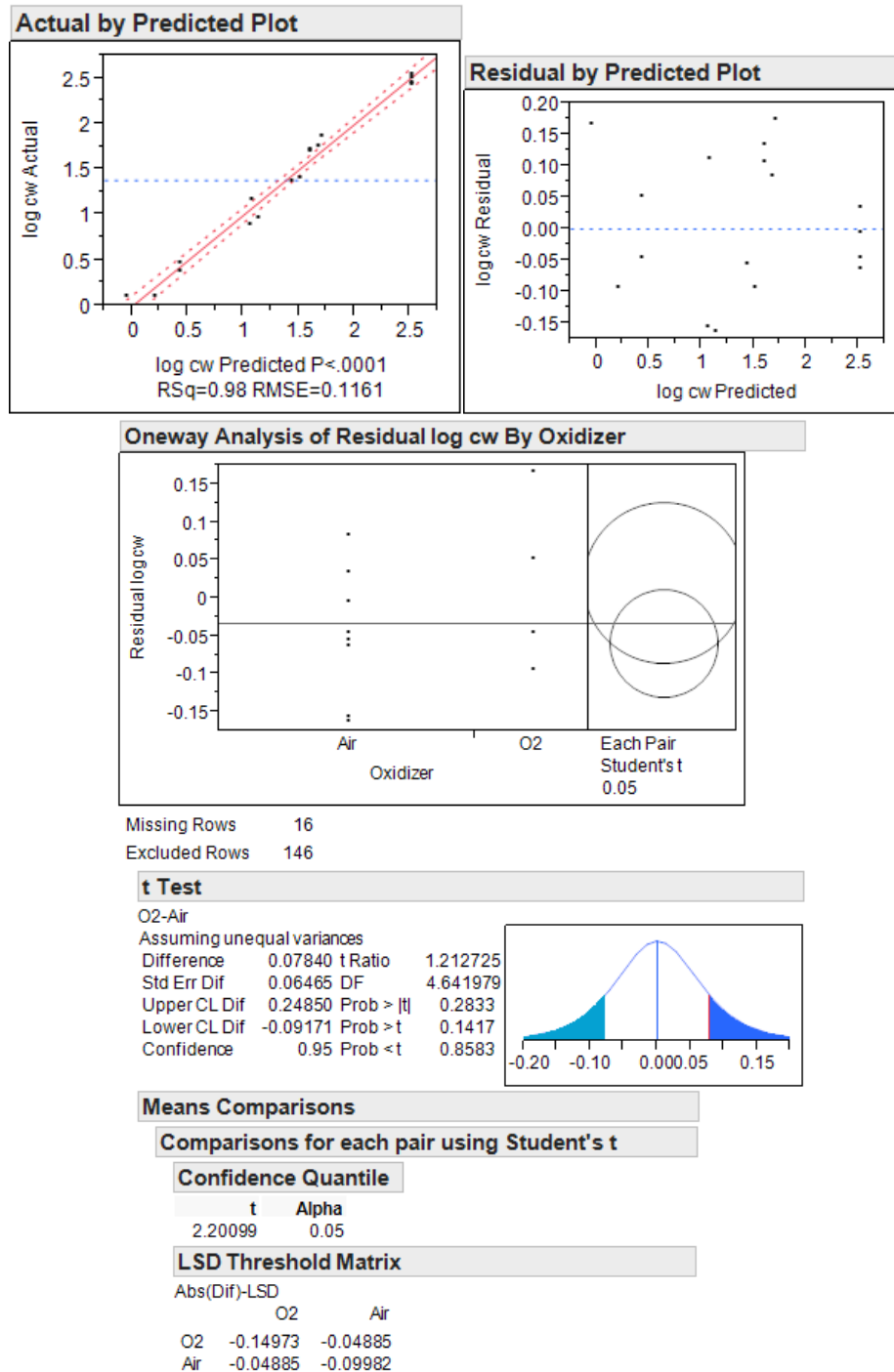


Figure A3.5 Summary of residuals for baseline model as computed by the JMP statistical package (150)

side. This was not completely unexpected since the sample size was small, consisting of only 18 data points, but provided a good starting point. The Shapiro-Wilk Goodness-of-Fit test was generated to compare the residuals and their expected values under the normal distribution assumption. The null hypothesis was H_0 : *The data is from a normal distribution*. The alternate hypothesis was H_a : *The data is not from a normal distribution*. The decision criteria was based on the P-value. For a P-value smaller than the α value, the null hypothesis should be rejected H_0 . Recall that the significance level, α , value was 0.05. Therefore the null hypothesis was concluded. Nonlinearity (item i) was suggested by the heavy-tailed trend shown in the normal-quantile plot at the top of Figure A3.5.

Figure A3.6 shows three plots. The top left plot displays the observed cell width plotted as a function of the predicted cell width. The dashed red line shows the model's



Positive values show pairs of means that are significantly different.

Figure A3.6 Test for constant variance of baseline model based on oxidizer

95% confidence band. Ideally, all the data points would lie on the red dashed line. The data points for this model showed some variance. The bottom left plot shows the residuals plotted against the transformed predictor variable, $\log(X)$. This plot indicated that the error had fairly constant variance (item ii). The conclusion of constant variance was also supported by the plot on the right which shows the means of the variance were not statistically different. Although there was a notable gap in the predictor band seen in Figure A3.3, any assertions regarding the goodness-of-fit require more data. The data are scattered at both ends of the scale, but no single value was identified as an outlier (item iv). Cell size was already known to vary dependently on the detonation mixture's temperature, pressure, and equivalence ratio and has been omitted (item vi). The data were carefully controlled for the baseline model to be orthogonal to the temperature, pressure, and equivalence ratio variations. Figure A3.5 shows a plot of the residuals grouped by oxidizer (pure O_2 or air) to check for independence (item iii). The overlapping circles show that the variance cannot be statistically separated based on type of oxidizer.

Two notes about the repeatability of this data set should be made. First, the cell width numbers reported for each data point represent a statistical average of some sort. Recall that in the background section, Figure A3.1 and Figure A3.2 showed detonation cell traces that looked like fish-scales on a sooted foil. The data collected from those tests will have a range of cell sizes. Those sizes are collected and averaged in some fashion before they are reported in a paper. With decades between this analysis and some of these tests, the cell size distribution cannot be ascertained, nor can it be determined whether the value reported was a mean or a median value. There was also little insight into how

widely the cell sizes varied within a given data set or between data sets with similar test conditions. Second, the variation is expected in the residuals when observations were repeated at similar conditions since the observations themselves have inherent variability. At this point, the baseline model serves to guide the analysis based on macroscopic trends. With that in mind, additional data points could lead to an increased confidence in the baseline model or suggest an improved model.

3. Methodology

Based on the hypothesis that the baseline model was supported as statistically significant, an attempt was made to model initiation energy and use that model to predict cell width. Careful evaluation of the experimentally observed data relating to cell width was examined and provided insight for predictor variable transforms. Subsets of the data were used at each step to improve the variable transforms and then aggregated to get a final model. Points of further exploration and study will be noted.

In general, the model was kept in the basic form of:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_n X_{in} + \epsilon_i \quad (\text{A3.13})$$

such that all the β_j terms were linear, although the X_{ij} terms may not be.

Data was imported into Excel for conglomeration from the CalTech detonation database (49). When combining data for cell size and ignition energy to evaluate the initial model, shown in Equations A3.1 and A3.2, linear interpolation was performed to get cell widths and ignition energies at matching equivalence ratios. Once a model for determining ignition energies was found, it was implemented in the cell width database and a regression was completed to take into account the effects of temperature and pressure.

4. Results

Model improvement began by combining data sets from cell width and ignition energy experiments. This data came from experiments which were carried out separately; an interpolation within a data set was required at nearly all points to match the exact conditions in the other data set. A linear interpolation introduced some small error into the data set, but it was smaller than the uncertainty of the data points themselves and was ignored. A plot with the baseline model underlying the data is shown in Figure A3.7. Running a simple linear regression on the full data set of Figure A3.7, shows that ignoring the influence of the mixture's equivalence ratio would produce a model that accounts for 84% ($R^2 = 0.84$) of the variability in cell width with initiation energy alone and supports tests showing the baseline model is statistically significant.

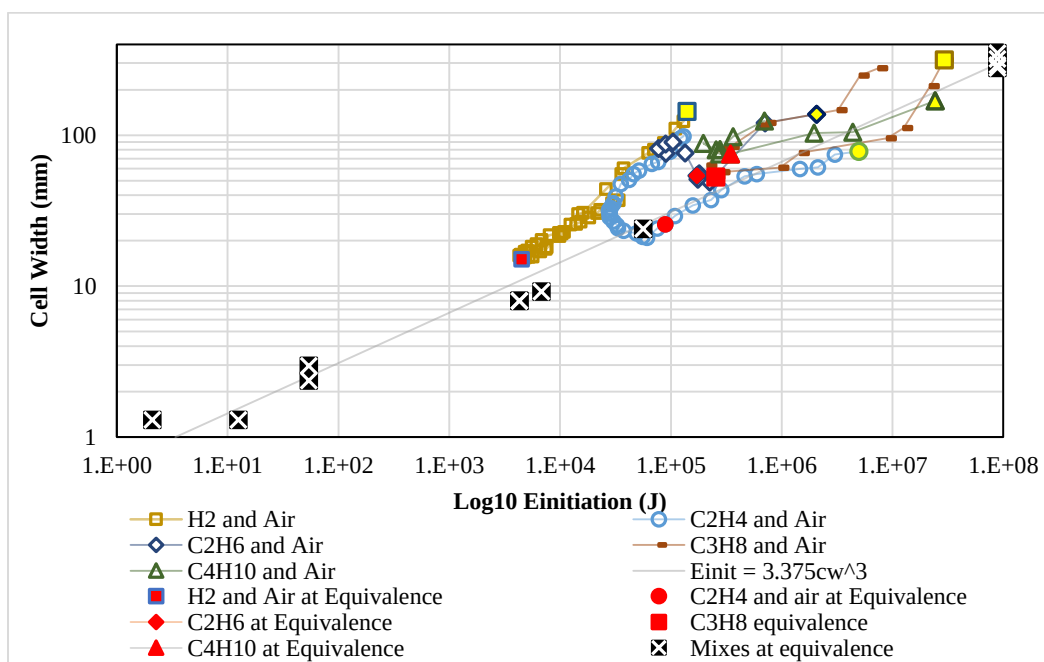


Figure A3.7 Plot of all available observed cell widths for ignition energies regardless of equivalence ratio from references from (49,51–65) catalogued in the CalTech detonation database (49) from MS Excel using a power series to project a predictor variable transformation

Since the hydrogen detonation data appeared to bias the regression to one side, and since the interest of the research organization lies with hydrocarbon detonation in air, it was removed to facilitate model evolution. It can also be noted in Figure A3.8 that each fuel species has a slightly different trend for minimum detonation energies as the equivalence ratio varies. Note that the detonation energies for the hydrocarbons follow the original model fairly closely down to their minimum (somewhere around $\phi = 1.2$) and then depart for a parallel line offset at higher values. It can be shown that a good fit for this trend is a hyperbolic cosine with an internal offset. However, the nature of that function disallows linear optimization. Instead, the approximate location of the minima was noted, and the variable transformation for the equivalence ratio was hard-coded:

$$X_i = \beta_i \cosh((\ln \phi + 0.2)\pi) \quad (\text{A3.14})$$

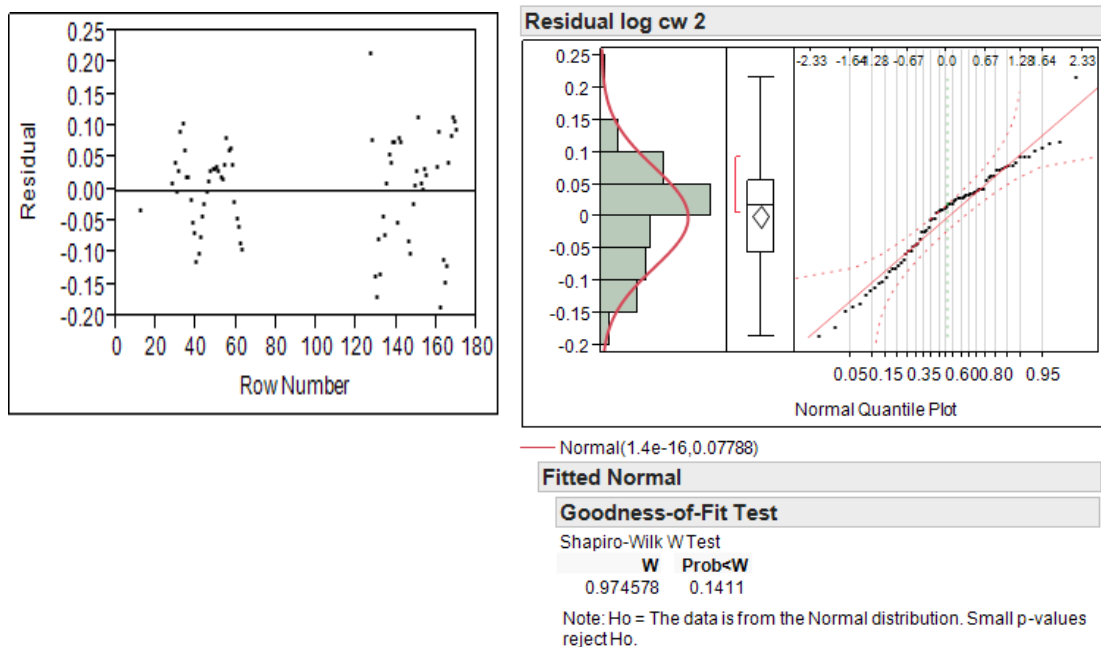


Figure A3.8 Plots of residuals vs row number for four fuel species: ethylene (C_2H_4), propane (C_3H_8), C_4H_{10} (Butane), and hydrogen (H_2) that highlight the non-linear and non-independence of the observed data, the histogram, normal quantile plot, and Shapiro-Wilk-W test show that the data does come from a normal distribution

This should facilitate modeling predictor variables that are functions of ϕ for the hydrocarbons of interest. The goal is to model the behavior of the detonations with respect to ϕ so that the prediction of cell width can be improved.

With the variable transformation coded in, a linear model was obtained in the form:

$$\log(\lambda_i) = \beta_0 + \beta_i \cosh((\ln \phi + 0.2)\pi) + \beta_3 \log(E_{init}) + \beta_4 \text{Fuel}_1 + \beta_5 \text{Fuel}_2 + \beta_6 \text{Fuel}_3 + \beta_7 \text{Fuel}_4 + \varepsilon_i \quad (\text{A3.15})$$

The details of the β values and a brief summary of the fit as computed with JMP (150), can be seen in Table A3.1. This model shows a modest improvement over ignoring equivalence ratio, accounting for 92% of the variability. An analysis of the residuals shows that the data violates some of the model assumptions: it is not linear, and it is not random, but it does follow a normal distribution, and the error is constant. This can be seen in Figure A3.8.

Table A3.1 Summary of fit and parameter estimates for an improved cell width prediction using E_{init} and equivalence ratio

Summary of Fit							
RSquare	0.920342						
RSquare Adj	0.914485						
Root Mean Square Error	0.080695						
Mean of Response	1.79173						
Observations (or Sum Wgts)	74						
Parameter Estimates							
Term	Estimate	Std Error	t Ratio	Prob> t	Lower 95%	Upper 95%	VIF
Intercept	0.3812548	0.090606	4.21	<.0001*	0.2004529	0.5620566	.
CosH((ln(phi)+.2)*pi)	0.065386	0.004902	13.34	<.0001*	0.0556036	0.0751683	1.20055
LogEinit	0.243037	0.015579	15.60	<.0001*	0.2119492	0.2741247	1.8121355
Fuel[C2H4]	-0.198554	0.017423	-11.40	<.0001*	-0.23332	-0.163787	1.7317378
Fuel[C2H6]	0.1214697	0.021271	5.71	<.0001*	0.079024	0.1639153	1.4582003
Fuel[C3H8]	0.0146834	0.020464	0.72	0.4755	-0.026152	0.0555183	1.6407589

This regression identified that significant improvement was possible over the current model by including the effects of equivalence ratio – and that by so doing the scope of the model could be extended. The success led to the next logical step, building a model to capture initiation energy and thereby utilize the rest of the data.

To develop the initiation energy model, transformations for the initiation energy variable, ϕ , and pressure variable were hard-coded into the JMP data columns. Next, a stepwise model tool in JMP (150) was employed to identify those parameters that resulted in a robust model for initiation energy. The results of this effort were conglomerated in Figure A3.9. Analysis of the residuals continued to show that the model violated the linearity and randomness terms, but the error between fuel groups was fairly constant, and normality was satisfied.

With a model for initiation energy, the next attempt was to see how well it correlated to the baseline model. The model shown in Figure A3.9 was ported into the cell width data set. The cell width observations were filtered for those fuels captured in the model. They were filtered further to show only detonations that occurred with air at standard temperature. Recalling the earlier work with predicting detonation cell width (λ) using initiation energy ($E_{initiation}$) and equivalence ratio (ϕ), the same predictors were included in the cell width model. The mediocre results can be seen in Figure A3.10. Where earlier work with the combined databases had shown an R^2 of 0.92, here only an R^2 of 0.57 was achieved. This means that 43% of the variability in cell width was not explained by this model.

While considering the model for $E_{\text{initiation}}$, it was noted that some of the fuels had fewer than 10 data points, which may have placed the verification data set outside the range of the observations used to build the model. It does not matter that the regression model for the initiation energy data accounted for 97% of the variability if the range of

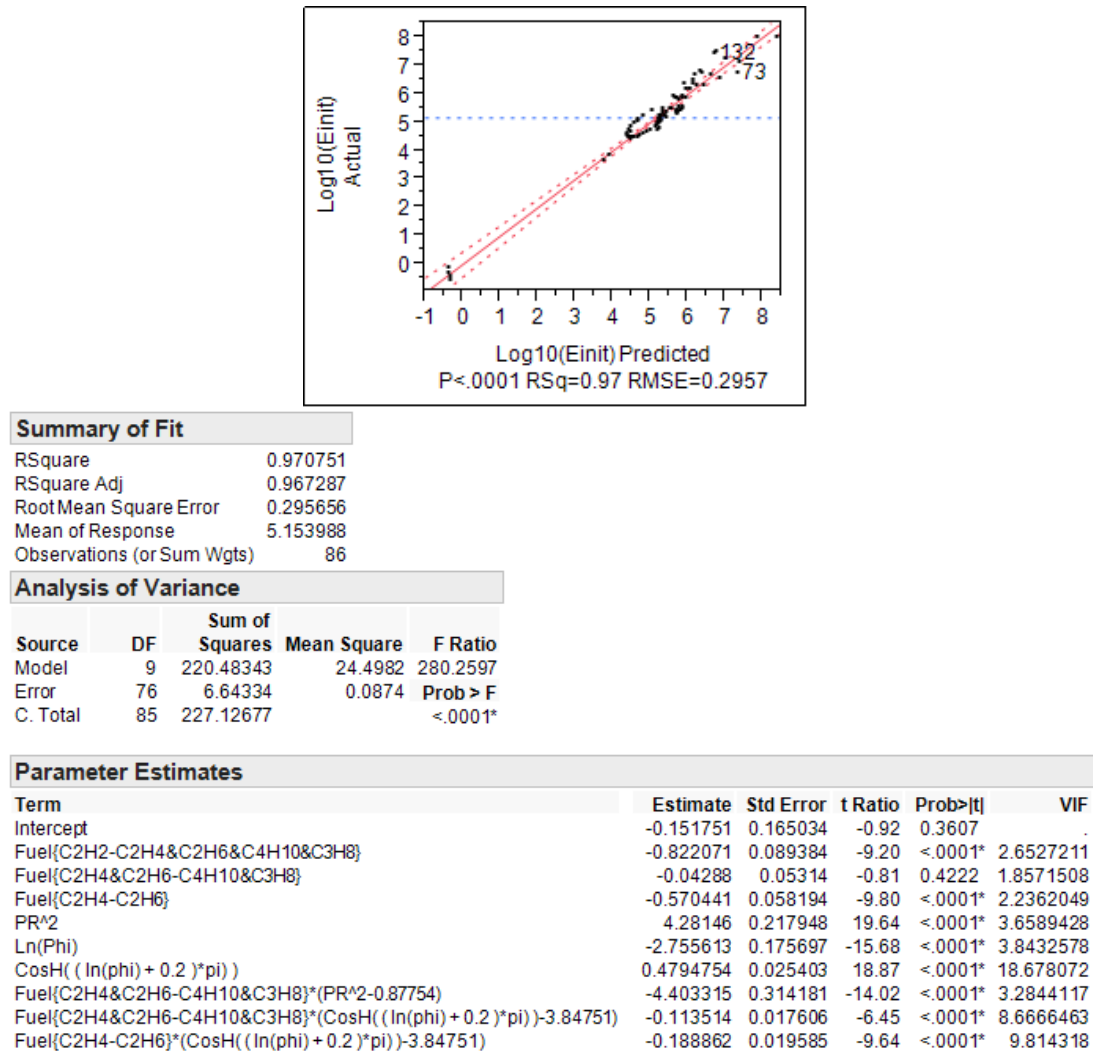


Figure A3.9 Regression model for $E_{\text{initiation}}$

predictor variables was too small to be of use. Another source of uncertainty that may not have been captured with previous models was the interaction between ϕ , P, T, Fuel type,

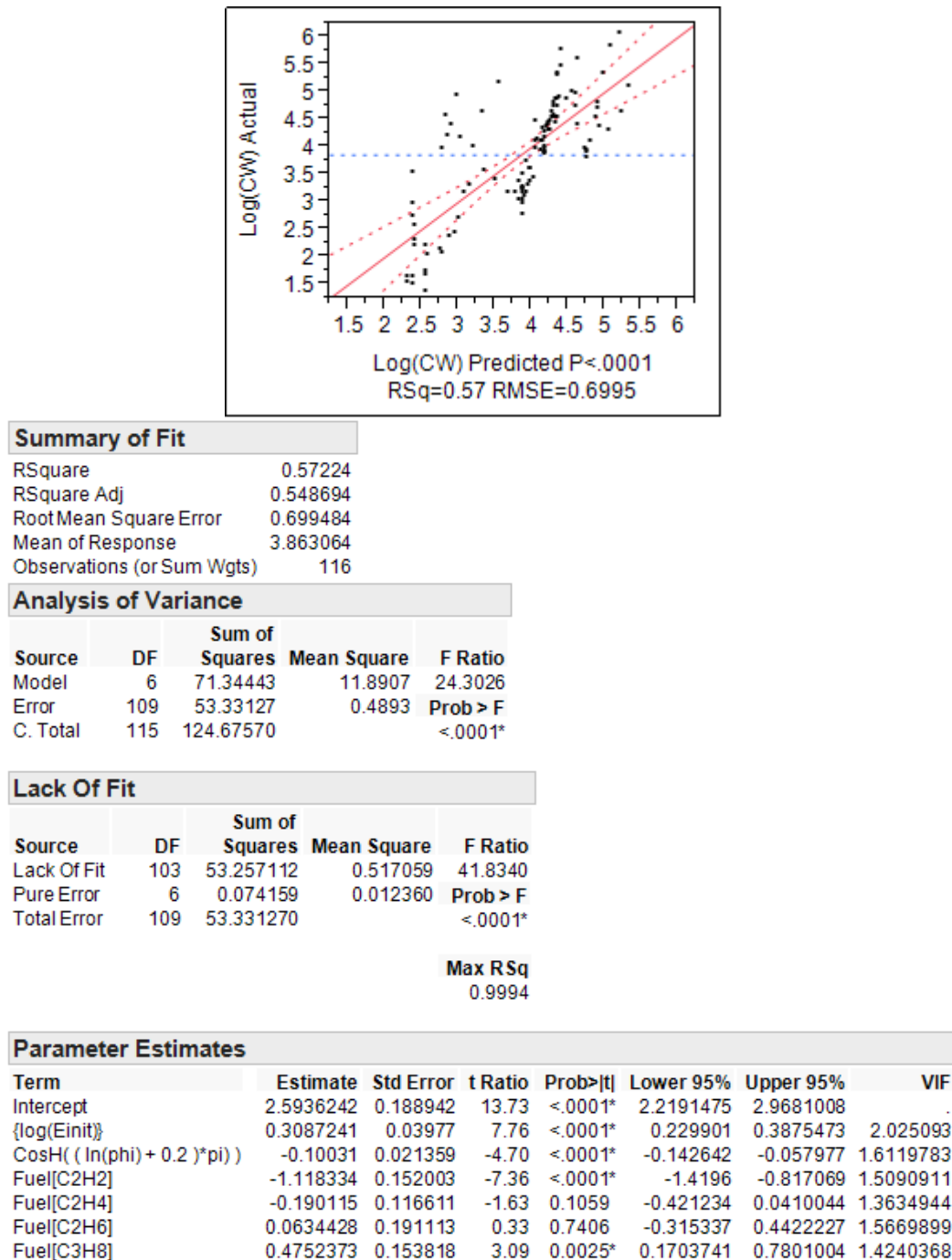


Figure A3.10 Model Verification: $E_{\text{initiation}}$ combined with Cosh(ϕ) and Fuel Type only accounts for 57% of $\log(\lambda)$

and initiation energy. A third possible explanation for the model's poor performance may lie in the hard-coding of variable transformations. It was assumed that the fuels required some shift in the ϕ - λ or ϕ - $E_{\text{initiation}}$ space, an assumption that may prove false. Also, the shift may vary with changes in pressure and temperature, requiring a regression variable on the inside of the function, and moving the modeling effort from the realm of linear regression to non-linear regression. Working through these issues should refine the variable transformations and predictor variable selections. These modifications will in turn improve the model.

The calculation of $E_{\text{initiation}}$ draws from the same predictor variables as the rest of the model shown in Figure A3.10. It does not introduce outside data; it models curves with the data that will also be utilized in cell width predictions. Rather than attempting to convolute the regression and prediction of all the variables in the model, it would be far wiser to recognize that temperature, pressure, equivalence ratio, fuel type, oxidizer type, diluent type, and percent diluent predict both initiation energy and cell width. With this knowledge, it should be possible to find the transformations of the variables or non-linear characterizations that will allow more accurate predictions of both. A proposed transformation for the ϕ data is in the form of the hyperbolic cosine:

$$\lambda = \beta_0 + \beta_1 \cosh \left((\ln(\phi) + \beta_2) \frac{\pi}{\beta_3} \right) \quad (\text{A3.1.})$$

$$\lambda = \beta_0 + \beta_1 e^{\beta_2(x+\beta_3)} + \beta_4 e^{\beta_5(x+\beta_6)} \quad (\text{A3.2.})$$

where Equation A3.16 carries the form utilized in this effort and Equation A3.17 utilizes the definition of the hyperbolic cosine function. The impact of the β terms placed at key

locations is described briefly in Table A3.2 and Table A3.3. This transform captures the modest deviations from a quadratic form that were noted when cell width values were plotted as functions of ϕ for several species. The form of Equation A3.17 as a fuel-oxidizer mixture moves from lean to rich is a decaying exponential and parallels the decrease in the mean free path between fuel molecules. However, there is also an increasing exponential as the oxidizer atoms are pushed further from each other. Addition of inert gases (diluent) will affect both of these exponentials in different ways, and the flexibility that Equation A3.17 brings should allow a more thorough exploration of the phenomena captured in the data. Glassman (115) contains other ideas for transformations.

Table A3.2 Description of beta terms for Equation A3.16

Term	Description	Assumed Value
β_0	Intercept - Shifts all λ values	none
β_1	Scaling factor for ϕ curve	none
β_2	Location from $\phi = 1$ that results in a minimum λ . May be dependent on fuel type, initial pressure, and initial temperature.	Assume $\beta_{2+} \sim -0.2$, and $\beta_3 \sim 1$.
β_3	Scaling factor for Fuel type – captures the range of ϕ	1

Table A3.3 Description of beta terms for Equation A3.17

Term	Description	Assumed Value
β_0	Intercept - Shifts all λ values	none
β_1, β_4	Offset of predicted (y-axis) values on ϕ curve	none
β_2	Positive real number describing rich mixture exponential	1
β_3, β_6	Location from $\phi = 1$ that results in a minimum λ . May be dependent on fuel type, initial pressure, percent diluent, and initial temperature.	~ 0.2 for HC fuels
β_5	Negative real number describing lean exponential	-1

5. Conclusions and Recommendations

The baseline model was shown to be a linear model through transformation of the predictor and predicted variables. The linear model was shown to be a statistically significant model of the available data for a very restricted set of conditions. The baseline

model was expanded to encompass a range of equivalence ratios for some hydrocarbon fuels and still be statistically significant but less capable of accounting for the variability in the prediction. It was shown that the baseline model's prediction of cell width for explosive mixtures outside of the restricted conditions is degraded. Various points of improvement were noted, and a non-linear transformation for the equivalence ratio was presented.

Although a combination of transformations could (and has been shown to) yield a model that accounted for over 95% of the variability in the data used in the model validation effort, it was of little practical use because it failed to describe the underlying physics of the process. Further evaluation of the raw data and subsets to identify better transformations of the predictor variables, non-linear models, and models that more accurately capture the detonation phenomena is recommended.

Appendix IV Modeling Laminar Flame Speed and Quenching Distance as a Function of Pressure and Equivalence Ratio

Descriptions of the theory for quenching flames within a narrow tube or channel may be found in many texts, such as: Lewis and von Elbe (118), Turns (108), and Kuo (38). It was desirable to have a mathematical model for these properties based on the data to increase precision with correlating detonation flashback with these phenomenon. Two mixtures were of keen interest to the work in this dissertation: ethylene-air and hydrogen-air. A third mixture of ethane-air was of minor interest. Although models for some fuels were described in (108), a simple model was not found that accounted for pressure variations. Data was found for ethylene-air flame speeds at elevated pressures (152–154) and quenching distance as a function of equivalence ratio (155). For hydrogen, data was available for quenching distances at elevated pressures (109,156) and flame speeds at elevated temperatures (157). This experimental data provided the necessary information from which simple polynomial models of flame speed and quenching distances could be formed using a linear least-squares method.

1. The Predictor Variable

It was easier and more accurate to fit a polynomial model to the data after transforming the fuel-oxidizer mass equivalence ratio (ϕ) predictor variable to a percent fuel by volume. The transformation limited the range of possible predictor variables to all real numbers between 0 and 1, instead of from 0 to infinity. Using the percentage volume, a quadratic equation modeled the data for laminar flame speed and quenching with

relatively small errors. When the mass equivalence ratio was used, the rich portion of the curve stretched from 1 to infinity and created curves that were very difficult to model.

The relation between volumetric flow rate of the fuel *by percent* for a mixture of gaseous fuel and air mixing from separate streams is:

$$\dot{V}_f = \frac{\dot{V}_f}{\dot{V}_f + \dot{V}_a} \quad (\text{A4.1})$$

where $\dot{V}_f$ is the volumetric flow rate of the fuel *by percent* of the combined total of the fuel volumetric flow, $\dot{V}_f$, and $\dot{V}_a$ is the volumetric flow rate of the oxidizer (i.e. air). Note that this equation presumes that the reactants have not mixed, where different gaseous species may combine such that the sum of the volumetric flows may not equal the total mixed volumetric flow. Assuming the gases involved are reasonably close to perfect gases, the individual volumetric flow rates may be restated in terms of the mass flow rate with the equation of state:

$$\dot{V} = \frac{\dot{m}R_uT}{\mathbb{M}P} \quad (\text{A4.2})$$

where $\dot{m}$ is the mass flow rate of a gas, R_u is the universal gas constant, T is the temperature of the gas, $\mathbb{M}$ is the molecular weight of the gas, and P is the pressure of the gas. Applying Equation A4.2 to Equation A4.1, the volumetric flow rate becomes:

$$\dot{V}_f = \frac{\frac{\dot{m}_f R_u T_f}{\mathbb{M}_f P_f}}{\frac{\dot{m}_f R_u T_f}{\mathbb{M}_f P_f} + \frac{\dot{m}_a R_u T_a}{\mathbb{M}_a P_a}} \quad (\text{A4.3})$$

Assuming that the temperature and pressure of the separate gases are equal, the equation reduces to:

$$\dot{V}_f = \frac{\left(\frac{\dot{m}_f}{M_f}\right)}{\frac{\dot{m}_f}{M_f} + \frac{\dot{m}_a}{M_a}} \quad (\text{A4.4})$$

which can be further simplified by the distribution property of addition as

$$\dot{V}_f = \frac{\dot{m}_f}{\dot{m}_f + \frac{\dot{m}_a M_f}{M_a}} = \frac{\frac{\dot{m}_f}{\dot{m}_a}}{\frac{\dot{m}_f}{\dot{m}_a} + \frac{M_f}{M_a}} \quad (\text{A4.5})$$

The equivalence ratio is defined as

$$\phi = \frac{\left(\frac{\dot{m}_f}{\dot{m}_a}\right)}{\left(\frac{f}{a}\right)_{stoich}} \quad (\text{A4.6})$$

where f is the mass flowrate of the fuel, a is the mass flow rate of the oxidizer, and

$\left(\frac{f}{a}\right)_{stoich}$ is the stoichiometric fuel to air ratio by mass. Upon substitution into Equation

A4.5, the volumetric flow rate may be written in terms of the equivalence ratio,

molecular weights of the fuel and oxidizer, and the stoichiometric mass fraction of fuel to oxidizer:

$$\dot{V}_f = \frac{\phi}{\phi + \frac{\frac{M_f}{M_a}}{\left(\frac{f}{a}\right)_{stoich}}} \quad (\text{A4.7})$$

which is what was wanted. A transformation in the opposite direction may be

accomplished by performing a reverse derivation and produces the equivalence ratio in

terms of the percent volume of a fuel as:

$$\phi = \frac{\left(\frac{\dot{V}_f}{1 - \dot{V}_f}\right) \left(\frac{M_f}{M_a}\right)}{\left(\frac{f}{a}\right)_{stoich}} \quad (A4.8)$$

Equations A4.7 and A4.8 provided the desired pathway between the infinite distribution of the mass fraction equivalence ratio, ϕ , and the percent fuel by volume, $\dot{V}_f$, which has a finite range extending from zero to one.

2. Modeling Flame Speed as a Function of Pressure and Equivalence Ratio

Laminar flame speeds are one of the fundamental properties of a combustible mixture. Combustion texts (38,108,115,118) all discuss this parameter and provide a method for estimating it. Laminar flame speeds have been shown to be proportional to the logarithm of mixture pressure (115, p. 156). When plotted as a function of percent volume, flame speeds appear to have a parabolic form.

2.1. Ethylene-Air Flame Speed

Applying a logarithmic variable transformation to pressure, and the volumetric flow transformation of Equation A4.7 to equivalence ratio, a least-squares multi-variable linear model for the ethylene air laminar flame speed data (152–154) yields the model of Equation A4.9:

$$S_{L_{C_2H_4}} = 47.71 + 259.8\dot{V}_f - 47.45E3(\dot{V}_f - 0.07054)^2 + 10.25E6(\dot{V}_f - 0.07054)^4 - 24.77 \log_{10}(P) \quad (A4.9)$$

where $S_{L_{C_2H_4}}$ is in cm/s, $\dot{V}_f$ is volumetric percentage fuel in the mixture, and P the pressure of the mixture in atmospheres.

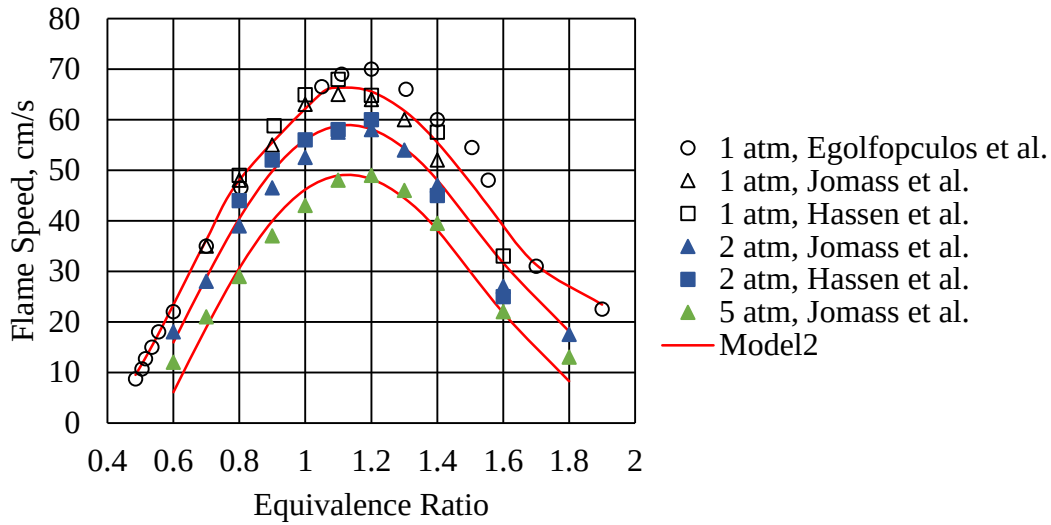


Figure A4.2 Plot of a polynomial model to data (152–154) varied by both pressure and mass equivalence ratio

The plot of this model with the underlying data is found in Figure A4.2 and shows close trending with the experimental data over the range of values reported. The plot of the residual errors, which represent the difference between the predicted and experimentally measured values, is shown in Figure A4.3. The residual errors appeared randomly distributed about the mean, indicating that there were not any non-linear trends that were not captured. A histogram and normal quantile plot of the residuals in Figure

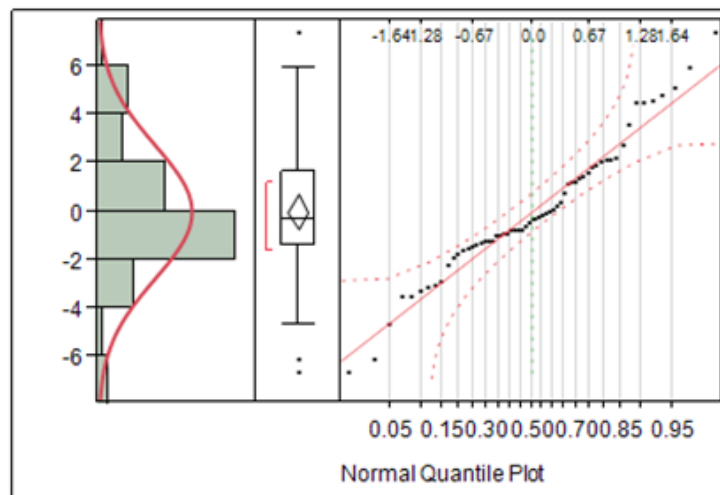


Figure A4.1 Normal quantile plot of the residuals for the initial polynomial fit to ethylene-air laminar flame speeds at elevated pressures

A4.1 indicated that residuals were normally distributed about the mean, and were not displaying non-linearity. The R^2 value of 0.976 reported in the summary of fit report in Table A4.1 showed that the model captured the overall trend. The root means squared error revealed that the standard deviation of the measured quenching distance from the numerical model was 2.8 cm/s. Referring back to Figure A4.2, it appeared that, at the equivalence ratios of 1.4 and 1.6, the model trended away from the experimentally measured values. This signaled that the flame speed was captured more accurately for the mid-range of equivalence ratios than for the rich portions. However, in Figure A4.3 the residual errors were plotted as a function of “percent by volume” and displayed errors that were distributed randomly and normally for the percent by volume predictor variable (the transformation of equivalence ratio predictor variable). The residuals at each of the

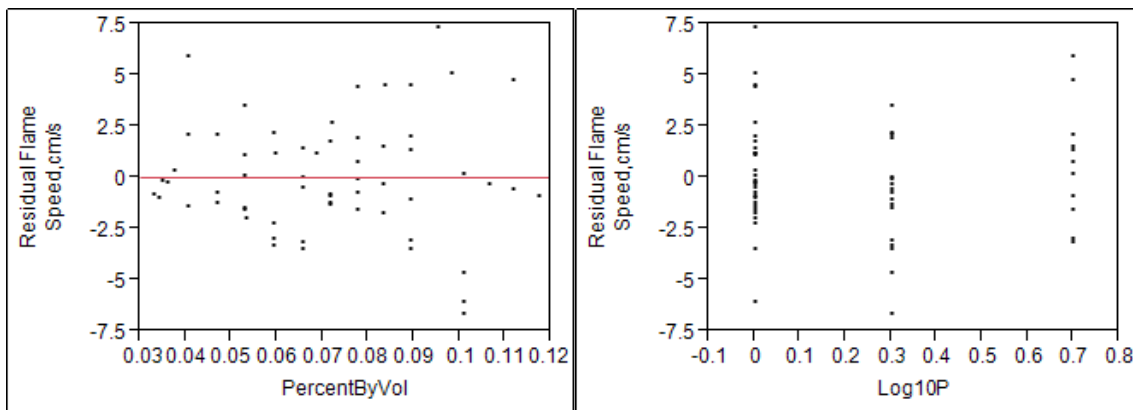


Figure A4.3 Residual errors of the ethylene-air flame speed model plotted as a function of the predictor variables percent fuel by volume (left) and initial pressure (right)

Table A4.1 Summary of fit for the ethylene-air flame speed model

Quantity	Value
R^2	0.976523
R^2_{adjusted}	0.974847
Root Mean Squared Error	2.844534
Mean of Response	43.25574
Observations (or sum of weights)	61

three pressure levels were grouped around a different mean, an effect called heteroscedasticity. This suggested that there was a non-linear effect with pressure that was not captured when it was transformed with the logarithm and which might be resolved with an additional variable transformation. Therefore, caution should be used before attempting to extrapolate this particular model to pressures outside the range of experimental data used to generate it. The specific range included pressures from 1 to 5 atm, equivalence ratios from 0.5 to 1.8, and initial temperatures at 300 K.

2.2. Hydrogen-Air Flame Speed

Laminar flame speed for hydrogen-air mixtures as a function of pressure were not found after performing a literature search, but laminar flame speed for elevated temperatures was found in a NACA technical memorandum (157). The least squares linear model constructed using the data collected at temperatures of 287 K and 317 K is:

$$S_{L_{H_2REF}} = 0.0006272(\dot{V}_f)^4 - 0.1112(\dot{V}_f^3) + 6.713\dot{V}_f^2 - 157\dot{V}_f + 1045.7 + T \quad (A4.10)$$

The resulting model is plotted in Figure A4.4 with the data from the NACA technical memo (157). For this research, the equivalence ratios of interest were between 0.6 and 1.5, which is a region that was captured fairly well with Equation A4.10. The residuals in Figure A4.5 indicated that error grows as the flame speed increased – a nonlinear effect not captured with the model. The summary of fit presented in Table A4.2 shows a coefficient of determination (R^2) to be 0.954 for this model, which was adjusted down to 0.936 after accounting for the 6 terms used for the model generation. Both the slope of

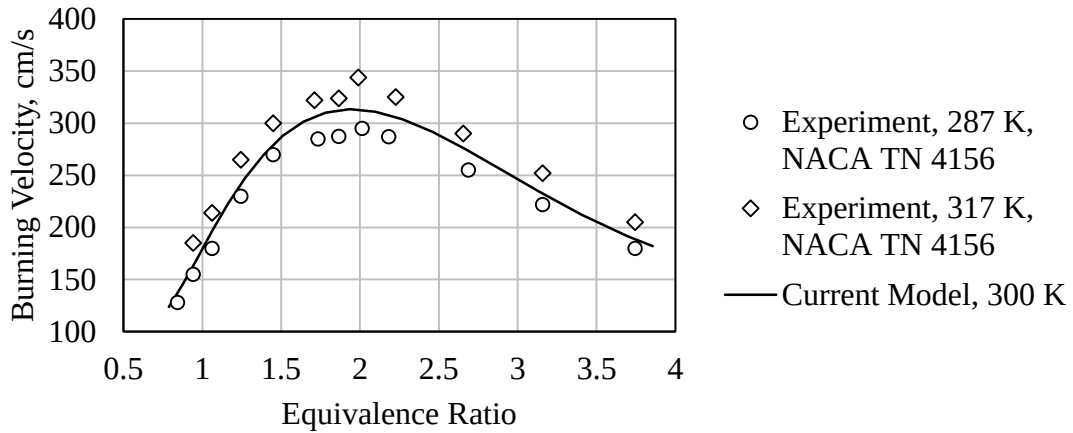


Figure A4.4 Laminar flame speed model for hydrogen air at a reference condition of 1 atm and 300K with experimental data from (157)

the residuals and the coefficient of determination suggested that, while not perfect, the model accurately captured the data trends for this limited range in temperature.

Additional information would be needed to capture the changes in the flame speed due to initial temperature variation (such as placing an exponent on the temperature term).

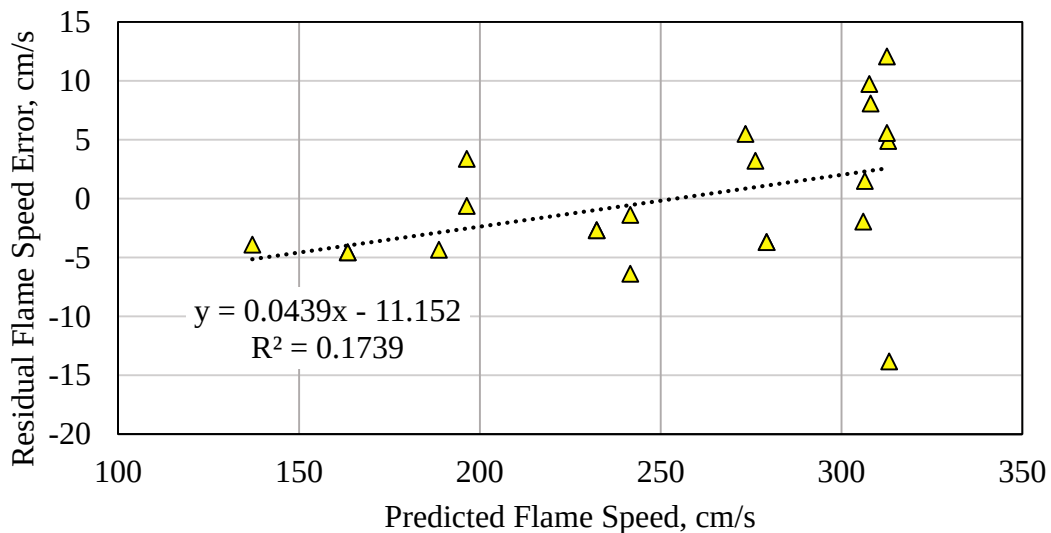


Figure A4.5 Residual errors for hydrogen-air flame speed model at reference condition of 300K

Table A4.2 Summary of fit for the hydrogen-air flame speed model

Quantity	Value
R^2	0.989
R^2_{adjusted}	0.984
Root Mean Squared Error	6.053
Mean of Response	253.7
Observations	21

2.3. Quenching Diameter Estimates

In the design of combustion systems for premixed fuel-oxidizer mixtures, it is desirable to feed the mixture into the combustion area through a channel, slot, or tube that is small enough that the flame cannot progress back up the tube when the mixture flow is turned off. The maximum diameter or distance between two plates that successfully quench the combustion as it reaches the exit plane of the mixture flow is called the quenching distance. Turns (108) showed, with a simplified analysis, that the quenching distance is a function of the cold flowing gas mixture and may be described as

$$d_Q = \frac{2\alpha\sqrt{b}}{S_L} \quad (\text{A4.11})$$

where d_Q is the quenching distance, α is the thermal diffusivity of the mixture, b is a constant specific to the mixture greater than 2, and S_L is the laminar flame speed of the gas. The laminar flame speed can be found either by referring to empirical data, utilizing curve fits to that data, or by employing chemical kinetic models that have been verified against that data, like the effort of Kopp et al.(158,159). A simple model was sought that could be programmed as part of other data reduction routines and captured the variation with temperature and pressure; commending the use of Equation A4.11. Thermal diffusivity was calculated from gas property models (using the *get_gas_props* Matlab

function described in Appendix V of this document), but there was not a table of b values. This issue was side-stepped by using a reference data point such that

$$d_Q = \left(\frac{2\alpha\sqrt{b}}{S_L} \right)_{ref} \cdot \frac{\left(\frac{2\alpha\sqrt{b}}{S_L} \right)}{\left(\frac{2\alpha\sqrt{b}}{S_L} \right)_{ref}} \quad (\text{A4.12})$$

Assuming that b was a constant that does not change with temperature and pressure, the equation was simplified to

$$d_Q = \left(\frac{2\alpha\sqrt{b}}{S_L} \right)_{ref} \cdot \frac{\left(\frac{\alpha}{S_L} \right)}{\left(\frac{\alpha}{S_L} \right)_{ref}} \quad (\text{A4.13})$$

Substituting the relation of Equation A4.13 for the first term, generated:

$$d_Q = d_{Q_{ref}} \cdot \frac{\left(\frac{\alpha}{S_L} \right)}{\left(\frac{\alpha}{S_L} \right)_{ref}} \quad (\text{A4.14})$$

which allowed a simple algebraic formulation for the quenching distance based on empirically modeled thermal diffusivity and laminar flame speed.

2.4. Ethylene-Air Quenching Distances

A comparative plot of experimental data and ethylene air quenching distances from Equation A4.11 was plotted in Figure A4.6 using the reference datum from Turns (108) and additional data from Gutkowski (155). The laminar flame speed relationship was calculated using Equation A4.9. Thermal diffusivity is a derived quantity that was calculated as:

$$\alpha = \frac{k}{\rho c_p} \quad (\text{A4.15})$$

where α is the thermal diffusivity, k is the thermal conductivity, ρ is the density, and c_p is the constant-pressure specific heat. Thermal diffusivity used to generate Figure A4.6 was calculated using Equation A4.15, which required models for thermal conductivity, density, and specific heat as a function of temperature and pressure. Thermal conductivity for ethylene and air was calculated separately for each gas using the Sutherland model as described in White (123). The constant-pressure specific heat was calculated using a least squares linear fit to the data provided by (160) on the NIST webbook website (161) for ethylene and a curve fit provided in (162, pp. 91-93). The thermal conductivity and specific heats of the mixture were then mass averaged from the separate constituents. Density was calculated using the Beattie-Bridgeman real-gas equation of state as described by Kuo (38, p. 630) and programmed into the *get_gas_props* subroutine found in Section 2.1 of Appendix V. The mass averaging of mixture properties was well implemented in the function *mix_properties* found in Section 2.2 of Appendix V, and

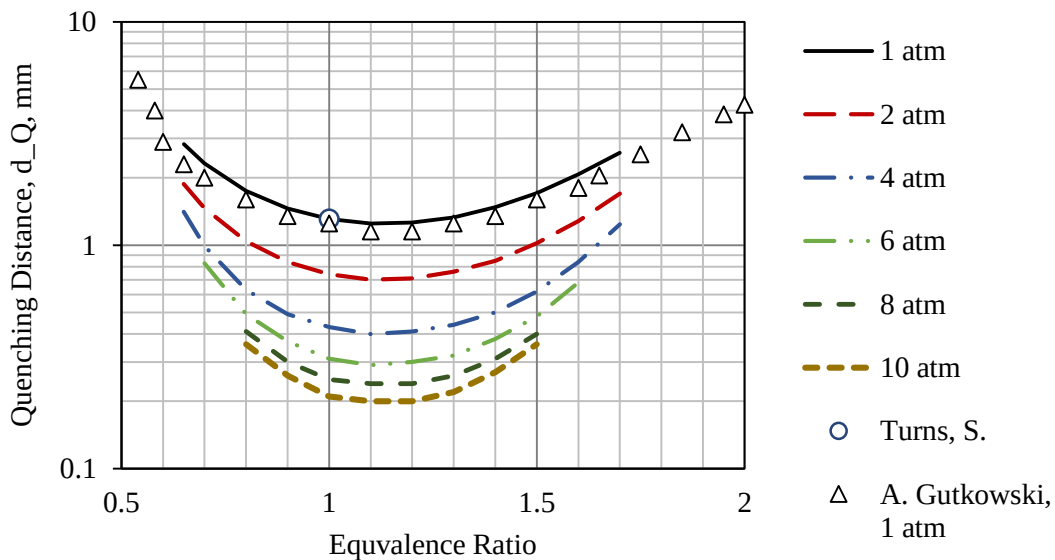


Figure A4.6 Modeled ethylene air flame quenching distance model presented with published experimental data (108,155)

could be improved for future work by using some of the mixing methods described in Kuo (38, pp. 623-692) or by using the NIST subroutine.

This model matched the datum found in Turns (108) exactly because that datum was used as the reference point. The data set from Gutkowski (155) does not lie on the model line because his apparatus had a flame front propagating into a narrow converging channel that stretched the laminar flame. The stretched flame increased the laminar flame speed and decreased the quenching distance slightly. This was different from the previous studies that used counter flow or prismatic conduit (i.e. tube) flow in experimental studies where the laminar flames were either not quenched, or planar when they arrive at the quenching location. So although there was a bias offset between the current model and the data of Gutkowski, it was only a bias offset due to differences in experimental setup and not a failure to capture the underlying physics. Furthermore, using the tube-flow quenching distance as the model reference data point was important because it provided a reference condition that matched those used for the burner stability charts of Grumer et al. (30).

The model of Equation A4.11 did not directly account for variations in equivalence ratio and pressure. Instead, it used the models for laminar flame speed and thermal conductivity to accomplish this. The assumption was that variations in temperature and pressure were captured by the thermal conductivity, and that the laminar flame speed model fell within the range of predictor data. Without experimental data to verify that ethylene flames do indeed follow this trend, extrapolations beyond the modeled reference point should be used with caution and reserve.

2.5. Hydrogen-Air Flame Speed and Quenching Distances

Hydrogen-air mixtures provided a cautionary tale of ensuring the quenching relationship of Equation A4.14 correctly matched the experimental quenching data.

Figure A4.7 shows Equation A4.14 plotted against data from (118).

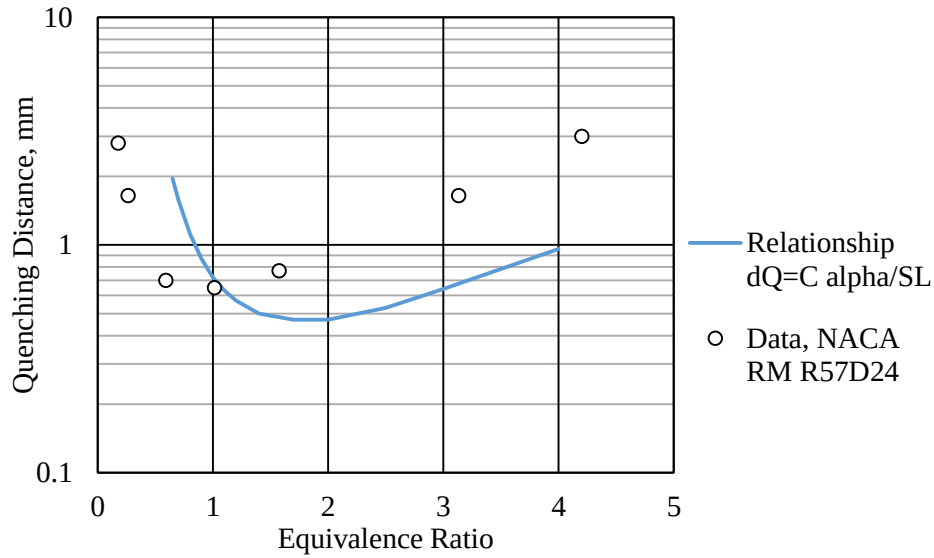


Figure A4.7 A comparison of the failure of the thermal conductivity model to predict hydrogen air quenching distances based on reference conditions

This represents an unusable model for predicting the thermal quenching of hydrogen air mixtures. Instead, a least squares linear regression was performed using the experimental data generated by Lewis and von Elbe (118) and Yang et al. (156). The JMP statistical software package (150) was used to generate a linear fit model using the least squares method:

$$\begin{aligned} \ln(d_{Q_{H_2 \text{ air}}}) = & 2.826173 - 0.342564\dot{V}_f + 0.0127657\dot{V}_f^2 \\ & - 0.000205\dot{V}_f^3 + 1.2987 \cdot 10^{-6}\dot{V}_f^4 \\ & - 2.178311 \log_{10}(P) \end{aligned} \quad (\text{A4.16})$$

This model used transformations for all variables to achieve linearity. The laminar flame speed was transformed with the natural logarithm, the equivalence ratio was transformed to mixture percent fuel by volume using Equation A4.7, and the pressure was transformed using the base 10 logarithm. Additionally, a weighting system was implemented so that the data points associated with small quenching distances and rich mixtures influenced the model more heavily. The weighting of each data point is mathematically represented as:

$$w = \frac{1}{d_Q \dot{V}_f} \quad (\text{A4.17})$$

Data points on the lean side of the curve were thrown out. Since the intended use of this data is for RDE research, and the intended RDE design favors equivalence ratios between 0.7 and 1.5, the removal of these data points is acceptable. In an effort to capture the trends at equivalence ratios near 1, the data points above an equivalence ratio of 2.5 were removed as outliers. Since the range of experimental data used to create Model 2 spanned the range from 0.2 to 2.5 atm, and equivalence ratios from 0.5 to 2.5, extrapolation beyond this range should be done with caution and the understanding that things may change suddenly.

The model was plotted over the source data in Figure A4.8. The model's deviation from the actual quenching distance at equivalence ratios greater than 2.5 was easily noted. Since the model predicted a larger gap than was experimentally verified for this region, the model is not conservative. For the region between equivalence ratios of 0.5 and 2 the model tended to predict quenching distances smaller than the experimentally measured values, presenting a conservative approach. The summary of fit

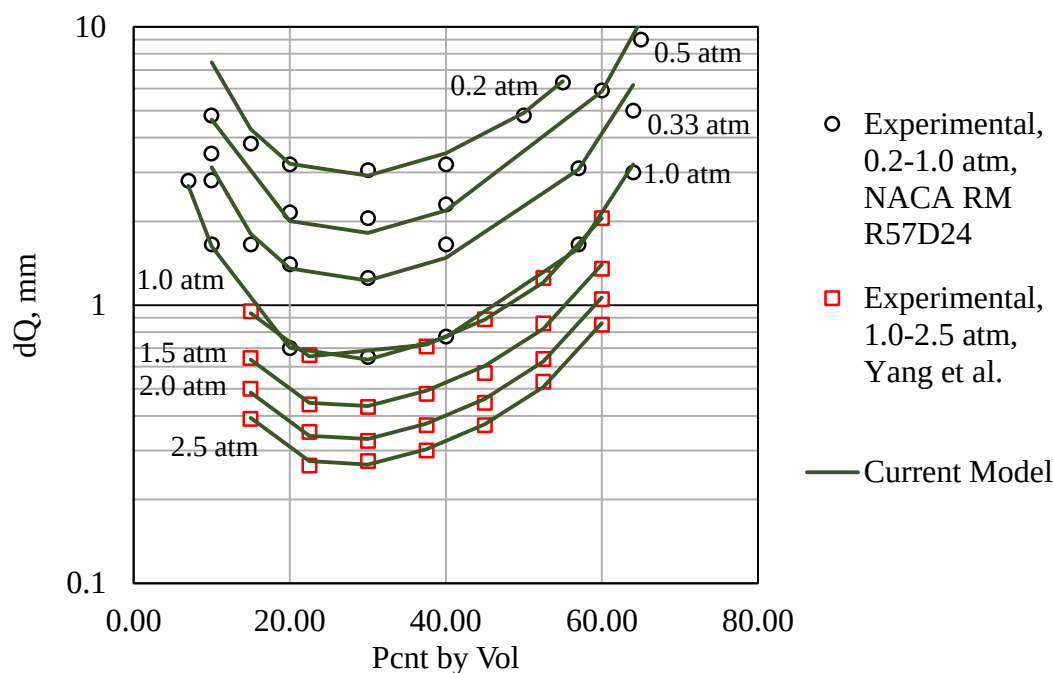


Figure A4.8 Quenching distance experimental data and linear regression model for a hydrogen-air mixture, data from Lewis and Von Elbe (118) and Yang et al. (156)

is shown in Table A4.3. The R^2 value of 0.98 indicated that the model captured the trend in the data almost perfectly. The root mean squared error indicated that the model predicted the experimental data with a standard deviation of 0.029 mm. The parameter estimates summary in Table A4.4 exhibited “t values” for all the terms in the model that were very low, and indicated that each term was significant enough that it should be included in the model.

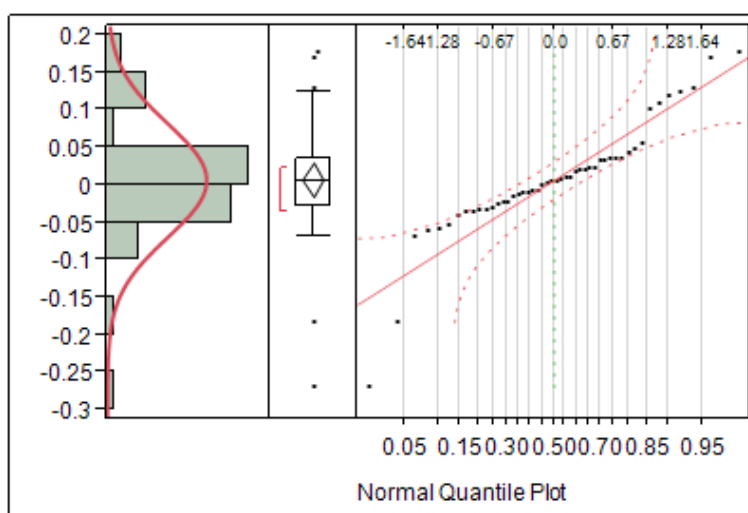
Table A4.3 Summary of fit for the ethylene-air flame speed model

Quantity	Value
R^2	0.980
R^2_{adjusted}	0.978
Root Mean Squared Error	0.0288
Mean of Response	0.838
Sum of weights	2.417

Table A4.4 Parameter estimates for the hydrogen-air quenching distance model

Term	Estimate	Std Error	t Ratio	Prob > t
Intercept	2.826	0.151543	17.41	< 0.0001
$\dot{V}_f$	-0.31739	0.024005	-13.22	< 0.0001
$\dot{V}_f^2$	0.011698	0.001278	9.15	< 0.0001
$\dot{V}_f^3$	$1.86 \cdot 10^{-4}$	$2.757 \cdot 10^{-5}$	-6.76	< 0.0001
$\dot{V}_f^4$	$1.179 \cdot 10^{-6}$	$2.056 \cdot 10^{-7}$	5.74	< 0.0001
$\log_{10} P$	-2.143044	0.032692	-65.55	< 0.0001
$(\log_{10} P)^2$	-0.24292	0.089616	-2.71	< 0.0098

The residual errors represented the difference between the experimental data and the model. Figure A4.9 shows these errors in a normal quantile plot. The deviation of the residual errors from the diagonal line indicated that the data did not come from a normal distribution. The distribution implied that there were non-linear effects driving the data away from a normal distribution of errors. This was expected due to the weighting provided to each of the data points. By weighting the data, some errors were inherently driven larger as others were reduced. A Shapiro-Wilkes W test was performed to see if the residuals followed a normal distribution. As shown in Figure A4.10, the probability

**Figure A4.9 Normal quantile plot for hydrogen-air quenching distance model**

Goodness-of-Fit Test	
Shapiro-Wilk W Test	
W	Prob<W
0.896905	0.0005*
Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.	

Figure A4.10 Shapiro-Wilk W test for normality of the hydrogen-air quenching distance residuals generated by the JMP (150) software package

value (p-value) was smaller than the 5 percent confidence value, and indicated that the data (the residuals, in this instance) did not come from a normal distribution. When the residuals were plotted against the predicted values, as shown in Figure A4.11, the errors were seen to grow with the predicted values, which is desirable to maintain a good fit at the higher pressure data points. These views all indicate that the model is a good fit for higher pressures and equivalence ratios between 0.5 and 2 and pressures from 0.2 atm to 2.5 atm. When the model is used outside of these ranges, the errors may be much larger, so caution should be used when employing this model for those conditions.

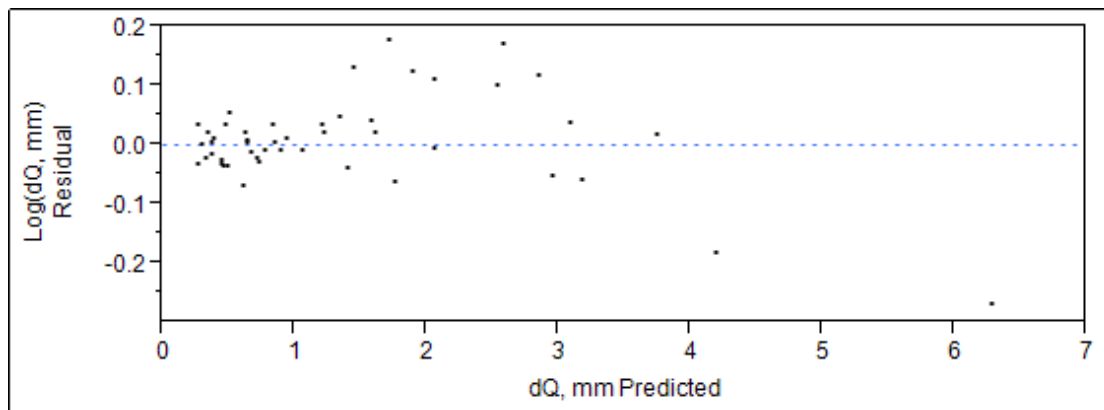


Figure A4.11 Plot of the predicted natural log of quenching distance with the actual quenching distance for hydrogen air

2.6. Ethane-Air Quenching Distance

A model for ethane-air quenching distances was made using the least squares linear regression method. Only 8 data points published in the text by Lewis and von Elbe (118) were found to build the model shown in Equation A4.18.

$$d_{Q_{C_2H_6}} = (2.1316 - 0.183) - 3.5677\dot{V}_f + 1.6289\dot{V}_f^2 + 0.1818P^{-0.901} \quad (A4.18)$$

The model was constructed in two parts. First, a linear regression for the data at 1 atm captured the quenching distance trend with respect to equivalence ratio. This model had an intercept of 2.1316. Second, a linear regression was performed using the 3 points at an equivalence ratio of 1.15 to obtain the pressure trend. The intercept for the pressure curve was -0.183. These two equations were combined to obtain the final form of Equation A4.18 and are plotted with the data in Figure A4.12. The intercepts were left

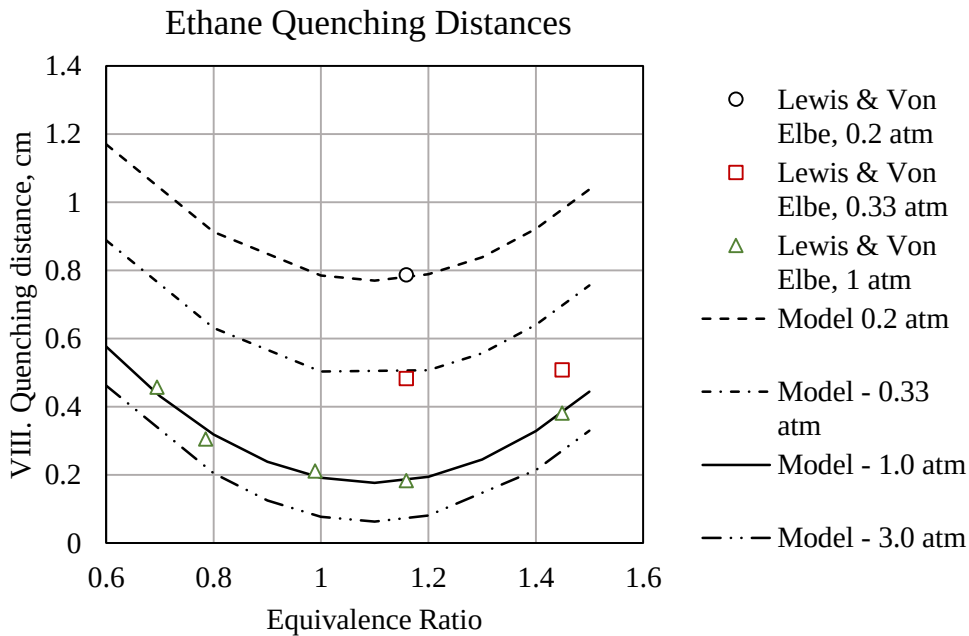


Figure A4.12 Experimental data from (118) and model for ethane-air quenching distances

uncombined in parentheses to highlight that the model combined two separate models. The model range spanned 0.2 atm to 1.0 atm and equivalence ratios from 0.6 to 1.5, however, that range was not all inclusive. Without a data set spanning more equivalence ratios at the low-pressures, it is impossible to predict how this model will perform in the rich or lean low-pressure conditions. The summary of fit, shown in Table A4.5, reports a coefficient of determination of 0.865 which calls into question the ability of this model to accurately capture the variation in quenching distance as a function of pressure and equivalence ratio. Additionally, predicting response of the model to elevated pressures is questionable. Subsequently, use of this model should be a last resort. Model improvements should be made by seeking more data at both reduced and elevated pressures.

Table A4.5 Summary of fit for the ethane-air quenching distance model

Quantity	Value
R^2	0.865
R^2_{adjusted}	0.595
Root Mean Squared Error	0.0270
Mean of Response	0.437
Observations	7

Appendix V Selected Computer Algorithms

This appendix contains the key algorithms that enabled the design and analysis of the RDE feed system. One note should be made regarding the subroutines used for the calculation of gas properties: the work of a PhD student is no substitute for rigorous checking and testing. The algorithms presented here were sufficient for this research, but were not fully tested or verified. For accurate fluid properties at specified temperatures and pressures, future work is recommended to fund and utilize the NIST chemical properties DLL. (see the NIST webbook for more information: webbook.nist.gov).

1. Matlab Script *LengthEquation.m*

The Matlab script *LengthEquation* was used to identify the maximum quenching length required to support a detonation cycle of predetermined frequency. The code required the user to input a predetermined frequency (in Hz), plenum Mach number, speed of sound (in m/s), and refill to cycle time ratio.

```
% Non-Dimensionalized Slot length calculations
% Programmer: Ionio Q. Andrus, Maj, USAF
% As part of the PhD program research requirements at the
% Air Force Institute of Technology
5 % April 2016
%
% Purpose: This script is intended to be used when calculating the
% estimated length of channel in which a detonation flashback into a
% premixed feed system must be halted and reversed in order to support a
10 % continued detonation cycle. To do this, the quenching distance and time
% relation is coded, and each variable is allowed to vary over a range of
% values. The line of each variance is plotted, after which the design
% point is plotted as well. All inputs are hard coded up front, the output
% is a plot of slot length ranging from the non-dimensional (x-values) 0
15 % to 2, and the slot length as calculated with the equation
% length =  $(1 - \tau_R^2) * M_{pl} * a / (f * (1 + M))$ 
% where length is the length required to reverse the flashback,  $\tau_R$  is
```

```

% the non-dimensional ratio of the fresh reactant flow to the sum of
% flashback and blowout times, a is the speed of sound in the gases, and M
20 % is the Mach number of the bulk flow within the feed slot.

% Given and assumptions
x = linspace(0,2); % Non-dimensional range of variables
l=zeros(4,100); % Empty array containing four characteristic lines
25 M=0.3;          % Assumed Mach flow in the feed plenum (low is cons.
a=340;           % Assumed speed of sound within the cool reactants
taur=0.75;       % Ratio of fresh reactant flow to cycle time
f=1800;          % Operating frequency

30 % Generate plot lines
l(1,:)=(1-taur^2)*(x*M)*a./(f*(1+(x*M))); % vary Mach
l(2,:)=(1-(x*taur).^2)*M*a./(f*(1+M));   % vary tau R
l(3,:)=(1-taur^2)*M*(x*a)/(f*(1+M));     % vary a
l(4,:)=(1-taur^2)*M*a./((x.*f)*(1+M));   % vary frequency

35
set(groot,'DefaultAxesColorOrder',[0 0 0],...
'DefaultAxesLineStyleOrder','-|---|:-|.')
% plot the lines on a semi-log plot and label appropriately
semilogy(x,l*100)
40 set(gca,'FontName','Times New Roman','FontSize',12);
xlabel('x','FontName','Times New Roman','FontSize',12)
ylabel('length, cm','FontName','Times New Roman','FontSize',12)
legend({sprintf('x = M/%g',M) sprintf('x = \tau_R/%g',taur) ...
sprintf('x = a/%g',a) sprintf('x = f/%g',f) },...
45 'FontName','Times New Roman','FontSize',12)

% put the design point given and assumed values on the plot
text(0.2, l(4, 4)*100, ...
'\it l = \rm {(1-\tau_R^2)M_{pl}a)}/{\it f\rm (1+M_{pl})}',...
50 'FontName','Times New Roman','FontSize',12)
text(0.2, l(4, 7)*100, sprintf('M_{pl} = %g',M),...
'FontName','Times New Roman','FontSize',12);
text(0.2, l(4,12)*100, sprintf('\tau_R = %g',taur),...
'FontName','Times New Roman','FontSize',12);
55 text(0.2, l(4,18)*100, sprintf('a = %g m/s',a),...
'FontName','Times New Roman','FontSize',12);
text(0.2, l(4,30)*100, sprintf('\it f = \rm %g Hz',f),...
'FontName','Times New Roman','FontSize',12);

60 % print the design point length on the plot
length = (1-taur^2)*M*a./(f*(1+M));
hold on;
plot(1,length*100,'ok');
text(0.2,l(4,50)*100, ...
65 sprintf('\downarrow \it l = \rm %g cm',length*100),...
'FontName','Times New Roman','FontSize',12);

hold off;

```

2. Matlab Script Design VelGradCalc.m

The VelGradCalc function estimated the boundary layer velocity gradient for a range of mass flow rates and feed slot heights. Other slot parameters, including feed pressure, were taken as inputs. Feed pressure was constant and no calculations were made to relate the feed pressure to the mass flow rate. Future work should connect the mass flow rate and feed pressure through standard viscous and compressible flow relations to achieve an estimate of one based on the input of the other.

```
% Height and Velocity Gradient calculation for premixed ethylene-air flame
% Programmer: Ionio Q. Andrus, Maj, USAF
% As part of the PhD program research requirements at the
% Air Force Institute of Technology
5 % April 2016
%
% Purpose: This is a design iteration effort with some given/assumed inputs
% that will help to calculate an adjusted velocity gradient for a premixed
% feed system. The adjusted velocity gradient will be compared with the
10 % flame stability diagrams of Grumer et al. If the adjusted gradient is
% above the flashback limit, the design is assumed marginally safe. If it
% resides above the blowout limit, it is assumed safe. Generally it would
% be desirable to increase the feed slot height to the largest value that
% results in a gradient that falls above the blowout line.
15 % OTHER UNIQUE SUBROUTINES CALLED:
%   get_gas_props - returns physical properties for gases at given T, P
%   mix_properties - calculates the physical properties of a binary
%                   mixture of gases
%   StabVelGrad - calculates the velocity gradient used in flame
20 %                   stability diagrams assuming steady-state flow and using
%                   the Blasius' relation for turbulent flow
%   get_flame_props - calculates flame speed and quenching distance for a
%                   fuel-air mixture specified in the inputs
% OUTPUT:
25 %   This produces a contour plot showing the calculated velocity gradient,
%   as the slot height and mass flow rate are varied
% Programmer: Ionio Q. Andrus, Maj, USAF
% As part of the research requirements at the Air Force Institute of
% Technology PhD program
30
clear all;
set(groot,'DefaultAxesColorOrder',...
    [[0 0 0]; [1 .2 .2]; [.2 .8 .2]; [.3 .4 1]; [.2 .2 .2] ],...
    'DefaultAxesLineStyleOrder','-|--:|-.'')
35
% Given:
```



```

mdot = [0.1 0.2 0.4 0.8 1.6]; %kg/s total mix mass flow rate through RDE
lngth = 0.012; % m Design length for quenching based on timeline analysis
hght = 0.00039* linspace(0.2,8); % m - design point from PDE data
40 nSlt = 5; %no unit - number or concentric feed slots
D = 0.15; % m - nominal diameter of the concentric feed slots

% Assumptions:
epsilon = 16*0.000001*0.0254; % m - roughness of machined steel... smooth
45 temp = 300; % deg K - Temperature mixture
pFeed = 6.8*101325; % Pa - Feed pressure
phi = 1.05; %no unit - Equivalence ratio @ flashback curve local max
fuelTyp = 'Ethylene'; % - Name of fuel - phys. properties in subroutine
oxdzTyp = 'Air'; % - Name of oxidizer - phys. prop in subroutine
50 pExit = 2; % atm - A Guess

% Retrieve the properties of the fuel and oxidizer at the given conditions

55 % initialize an array to hold the adjusted velocity graidents
gc_adj = zeros(length(mdot),length(hght));

% loop through each of the mass flow rates and calculate the adjusted
% velocity gradient for a range of slot heights
60 for j = 1:length(mdot)

    % get the flow properties
    fuel = get_gas_props(fuelTyp,temp,pFeed);
    oxdz = get_gas_props(oxdzTyp,temp,pFeed);

65    oxdz.mdot = mdot(j)/(1.0+(phi*fuel.FAR_stoich) );
    fuel.mdot = mdot(j)-oxdz.mdot;

    mix = mix_properties(fuel, oxdz);

70    % loop through each of the slot heights, and calculate the adjusted
    % velocity gradient
    for i=1:length(hght)
        arExt = pi*D*nSlt*hght(i); % m^2
75        Re = mdot(j)*(2*hght(i))/(mix.mu*arExt); % Reynolds number in feed slot

        g_calc = StabvelGrad(mix.mdot, mix.mu, epsilon, ...
                               hght(i), pi*D*nSlt, mix.rho);

80        [SL,dQ,SL_ref,dQ_ref,h_dQ,pcntVol]= ...
            get_flame_props(mix,fuel,oxdz,hght(i));

        mix.V = mix.mdot*mix.R*mix.T/(arExt*mix.P); % m/s
        gc_adj(j,i) = g_calc*(SL_ref*0.01/(mix.a-mix.V))*(dQ/dQ_ref);
85        %fprintf(' %g: %g, %g %g , ' , mix.V, h_dQ, SL, SL_ref)
    end

fprintf('\n')

```

```

end
90
% plot the data
figure( 'Position',[400 400 650 300] );
loglog(hght*1000,gc_adj)
set(gca,'FontName','Times New Roman','FontSize',12);
95
xlabel('height, mm');
ylabel('adjusted velocity gradient, 1/s');
grid on;
xlim([.0001 hght(end)*3]*1000);
ylim([10^2 10^10])
100
% label the lines
for j=1:length(mdot)
    text(hght(end)*990,gc_adj(j,end)*1.1,...
        sprintf('\leftarrow %g kg/s',mdot(j)), ...
105        'FontName','Times New Roman','FontSize',12);
end

hold on;
text(hght(end*.6)*990,gc_adj(j-1,10)*100,sprintf('# slots = %g',nsl),...
110    'FontName','Times New Roman','FontSize',12)
text(hght(end*.6)*990,gc_adj(j-1,10)*10,sprintf('P_f_e_e_d = %g atm', ...
    pFeed/101325), 'FontName','Times New Roman','FontSize',12 )
text(hght(end*.6)*990,gc_adj(j-1,10)*1.0,sprintf('\phi = %g',phi),...
    'FontName','Times New Roman','FontSize',12)
115
%text(hght(1)*1000,60E6,sprintf('\leftarrow Hydrogen Blowoff Gradient, ...
%    '\phi = 1.3 ') , 'FontName','Times New Roman','FontSize',12)
%text(hght(1)*1100,50E4,sprintf(' Ethylene Blowoff, \phi = 1.3 ') ,...
%    'FontName','Times New Roman','FontSize',12)
text(hght(end)*800,50E4,sprintf(' Ethylene Blowoff ') , 'FontName', ...
120    'Times New Roman','FontSize',12)
% plot the blowoff line for laminar flow that was published in Grumer etal
loglog( [hght(1)*1000 hght(end)*2000], [20E4 20E4], ':k', 'Linewidth',2)
loglog([dQ dQ]*1000, [10^2 10^8], ':k')
hold off;
125
fprintf('dQ/dQ_ref = %g \n',dQ/dQ_ref)
fprintf('dQ = %g \n',dQ)

set(groot,'DefaultAxesColorOrder','remove',...
    'DefaultAxesLineStyleOrder','remove')

```

2.1. Matlab Function get_gas_props.m

The function get_gas_props returns the properties of a specified gas at a user selected temperature and pressure. Underlying models and data came from various reference sources listed here.

Andrews and Biblarz (163) were referenced when other sources could not be found to calculate the viscosity for helium, thermal conductivity for propane, ethane and helium, and the specific heat at constant pressure for at least partial temperature ranges of carbon dioxide, hydrogen, argon, nitric oxide, and nitrous oxide.

Kuo (38, pp. 681-682) referenced Svelha (164) for the Leonard-Jones potential data for air, oxygen, carbon dioxide, hydrogen, nitrogen, argon, ethylene, propane, ethane, carbon monoxide, methane, water vapor, nitric oxide, nitrous oxide, and helium. Ghiaasiaan (165) was also referenced for the Leonard-Jones potential, but did not provide any unique data nor provide the b_0 coefficients.

White (123, pp. 27-31, 577) was referenced for Sutherland model (166) formulae and data (167,168) for both kinematic viscosity and thermal conductivity of air, oxygen, carbon dioxide, hydrogen, nitrogen, and argon. Coefficients for the viscosity of ethylene in the Sutherland Model were reported by Breitenbach (169) as related by Jeans (170). Biblarz et al. (163) provided the kinematic viscosity and thermal conductivity curve fits for helium, propane, and ethane. Holland et al. (171) reported the data for the viscosity and thermal conductivity of ethylene.

Çengal and Boles (39, p. 898) were referenced for critical temperatures, pressures, and densities for air, carbon monoxide, methane, water vapor, nitric oxide, nitrous oxide, and helium. The data was sourced from (172,173).

Atkins and Jones (174) was referenced for was referenced for the universal gas constant, R_u , and molecular weights.

Lemmon et al. (175) was referenced for the mole fractions of oxygen, nitrogen, argon, and carbon dioxide in air.

The NIST Chemistry Webbook (161) was referenced for polynomial curve fits for specific heat, c_p . The NIST does not perform experiments, instead they reference published data. Chase (176) reported the specific heat data for oxygen, carbon dioxide, hydrogen, nitrogen, argon, carbon monoxide, and helium. Curve fits available from Andrews and Biblarz (163) were also used for portions of the carbon dioxide, hydrogen, argon, carbon monoxide, nitric oxide, and nitrous oxide. The Thermodynamics Research Center at Texas A&M (160) provided a specific heat model for ethylene, Chao (177) provided curve fit data for propane, and Gurvich et al. (178) for ethane.

```

function [ fluid ] = get_gas_props( type, T, P)%, p, t
%get_gas_properties returns a structure with the key real gas properties
% of a fluid of specified type at the given temperature and pressure.
% *** Assumes SI units
5 % Outputs: specific heat (Cp) in J/kgK, density (rho) in kg/m^3 , Molecular
% weight(MW) in g/mol, Gas Constant (R) in J/kgK, conductivity (k),
% viscosity (mu), speed of sound (a), reduced temperature, reduced
% pressure, reduced density, critical temperature, critical pressure,
% critical density, ratio of specific heats (gamma)
10 % Inputs:
% type - Type of fluid - (acceptable type labels are listed below)
% T - Temperature (in Kelvin)
% P - Pressure (in Pascal)
% Required Functions
15 % BB_EqnOfState(T, P, type) - returns the real gas density (rho) and
% compressibility factor (Z) for select gases
% BWR_EqOState(T,P,Substance)
% Fully supported Fluids (use BB_EqnOfState):
% 'air', 'Air'
20 % 'O2', 'Oxygen', 'oxygen'
% 'CO2', 'Carbon Dioxide', 'carbon dioxide'
% 'H2', 'Hydrogen', 'hydrogen'
% 'Ar', 'Argon', 'argon'
% 'N2', 'Nitrogen', 'nitrogen'
25 % 'C2H4', 'Ethylene', 'ethylene', 'Ethene', 'ethene'
% 'C3H8', 'Propane', 'propane'
% 'Ethane', 'C2H6', 'ethane'
% 'CO', 'Carbon Monoxide'
% Not fully supported (and will give an error because of where I've placed
30 % the call to Beattie-Bridgman routine)
% 'JP8'

```

```

%
% Output: fluid structure containing the following:
%   fluid.Type
35 %   fluid.T     fluid Temperature, K
%   fluid.P     fluid Pressure, Pa
%   fluid.MW    fluid molecular weight, atomic mass units
%   fluid.R     fluid gas constant, J/kgK
%   fluid.constituents cell array containing [name, molar fraction,
40 %   mass fraction]
%   fluid.mu    fluid dynamic viscosity, Ns/m^2
%   fluid.k     fluid thermal conductivity, W/mK
%   fluid.Tcrit fluid critical temperature (compressibility), K
%   fluid.Pcrit fluid critical pressure (compressibility), Pa
45 %   fluid.rhoCrit fluid critical density (compressibility), kg/m^3
%   fluid.Cp    fluid specific heat at constant pressure, J/kgK
%   fluid.gamma fluid ratio of specific heats
%   fluid.LJ    fluid leonard-jones potential
%   fluid.rho_ideal fluid density from ideal gas law, kg/m^3
50 %   fluid.rho  fluid real gas law density, kg/m^3
%   fluid.Z     compressibility factor
%   fluid.alpha fluid thermal diffusivity (calculated as k/(rho*Cp))
%   fluid.a     fluid speed of sound, m/s
%   fluid.P     fluid pressure, Pa (static - no assumed velocity)
55 %   fluid.T     fluid temperature, K
%   fluid.Pred  fluid reduced pressure, Pa
%   fluid.Tred  fluid reduced temperature, K
%   fluid.rhored fluid reduced density
%
60 % Programmed by Ionio Andrus in support of his PhD dissertation, Jun 2015
% Air Force Institute of Technology, Wright-Patterson AFB, Dayton, OH
%
% Gases that need additional help, or desired to be input:
% Needs work:
65 %   C3H8: mu & k (viscosity, thermal conductivity) equations
%   C2H6: mu & Cp (viscosity, specific heat) equations
%
% Add: 'JP8', , CH4, H2O, NO, N2O, C4H10, C7H16
%
70 % Bibliography
%{

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   2005, Table A.19, page 681-682, and the Chapman and Enskog's Method
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3. White, Frank M. "Viscous Fluid Flow, Third Edition", McGraw Hill, NY,
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```

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    Nitrogen, Argon, and Oxygen from 60 to 2000K at pressures to 2000 MPa",
    J Phys Chem Ref Data, Vol 29, No3, 2000, pp331-385
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    JEANS21 - Jeans, James Hopwood Sir, "The dynamical Theory of Gases",
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    TURNS99 - Turns, Stephen R. "An Introduction to Combustion: Concepts and
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    2011 Cambridge University Press, Online Book
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105 http://ebooks.cambridge.org/ebook.jsf?bid=CB09780511800603 Appendix K

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    CHASE98 - Chase, M.W. Jr; , NIST-JANAF Thermochemical Tables, Fourth
    Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
110
    %}

    fluid.type = {type};
    R_universal = 8314.47; %J/kgK Ref: ATKINS08
115
    switch type
    %~~~~~
        case {'air','Air'}
            fluid.type = 'air';
120 % fluid.gamma = 1.40; % specific heat ratio
            fluid.MW = 28.85; % Molecular weight (mass units)
            fluid.R = R_universal/fluid.MW; % J/kgK REF: ATKINS08
            fluid.constituents = {'O2', 'N2', 'Ar', 'CO2'; ...
125 0.2092, 0.7812, 0.0093, 0.0032; ... Mol Fractions, REF: LEMMON00
            ...%Mass Fractions
            0.2092*31.9988, 0.7812*28.0134, 0.0093*39.948 , 0.0032*44.095 };

            % Calculate viscosity with the Sutherland Model
            % Eq. 1-36, Ref 3.
130 T_0 = 273; %K REF: 3 Appendix
            S = 111; %K
            mu_0 = 1.716E-5; %Ns/m^2
            fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);

135 % Calculate thermal conductivity with the Sutherland Model -

```

```

% Eq. 1-44b, REF: 3
S = 194; %K
T_0 = 273; %K
k_0 = 0.0241; %W/mK
140 fluid.k = k_0*(T/T_0)^1.5*(T_0+S)/(T + S);

fluid.Tcrit = 132.5; %K REF: 4, Table A-1
fluid.Pcrit = 3.77E6; %Pa
fluid.rhoCrit = 328.1 ;%kg/m^3
145

%{
% THIS FIRST CALCULATION IS COMMENTED OUT - ERROR SOMEWHERE...
%Calculate specific heat ratios
150 Coef = [ 1003.2927 -54.34326 756.133134 -4804.90458 ...
          14615.686 -18754.7509 8784.313 0.0; ... 100-600
          -11525.8566 99425.819 -327302.61 571826.25 557886.04...
          288232.48 -61629.6298 0.0; ... 600-1000K
          827.955 382.29047 673.852611 -252.286 149.83567...
155          -38.7645 3.8413 0.0; ... 1000-2400K
          -1028.9 3730.37364 -2482.7987 838.6509 ...
          -14204.5456 -9.61538468 0.0 0.0]; % 2400 - 3600
if T >= 100 && T < 500
160 A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
elseif T >= 500 && T < 2000
A = Coef(2,1); B = Coef(2,2); C = Coef(2,3); D = Coef(2,4);
E = Coef(2,5); F = Coef(2,6); G = Coef(2,7); H = Coef(2,8);
elseif T >= 2000 && T < 6000
165 A = Coef(3,1); B = Coef(3,2); C = Coef(3,3); D = Coef(3,4);
E = Coef(3,5); F = Coef(3,6); G = Coef(3,7); H = Coef(3,8);
else
error('Gas input temp. in get_gas_props is out of range')
end
170 fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
+ E*(T*0.001)^4 + F*(T*0.001)^5 + G*(T*0.001)^6)*1000/fluid.MW;
% fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
+ D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
% fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
175 + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
%}

% Cp from Un_FAIR in Andrus' Master's Thesis...
if (T >= 2200.0 && T < 3400)
180 fluid.Cp = 9.61538464E-15*T^5 - 1.42045455E-10*T^4 ...
+ 8.38650933E-07*T^3 - 2.48279866E-03*T^2 ...
+ 3.73037360E+00*T - 1.02890035E+03 ;

elseif (T >= 1000.0)
185 fluid.Cp = 3.84130243E-18*T^6 - 3.87645198E-14*T^5 ...
+ 1.49983572E-10*T^4 - 2.52286136E-07*T^3 ...
+ 6.73853421E-05*T^2 + 3.82290380E-01*T ...

```

```

        + 8.27955488E+02;

190     elseif (T >= 600.0)
        fluid.Cp =- 6.16296284E-14*T^6 + 2.88232473E-10*T^5 ...
            - 5.57886027E-07*T^4 + 5.71826233E-04*T^3 ...
            - 3.27302607E-01*T^2 + 9.94258161E+01*T ...
            - 1.15258562E+04;

195     else
        fluid.Cp = 8.78431367E-15*T^6 - 1.87547510E-11*T^5 ...
            + 1.46156861E-08*T^4 - 4.80490455E-06*T^3 ...
            + 7.56133102E-04*T^2 - 5.43432552E-02*T ...
200     + 1.00329273E+03;

    end

    fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

205    % Provide the Leonard-Jones Potential constants,
    % REF: 2 Table A.19, page 681-682, and the Chapman and Enskog's
    % Method found as equation A-204, p679
    % and REF: GHIAASIAAN11
    %Substance[ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
210    fluid.LJ = [ 64.50    3.711  78.6    fluid.MW ];

    %~~~~~

    case {'O2','Oxygen','oxygen'} % 'O2'
        fluid.type = 'Oxygen';
215        fluid.MW = 31.9988;
        fluid.R = R_universal/fluid.MW; %259.8; %J/kgK

        fluid.TCrit = 154.581; %K
        fluid.PCrit = 5043000; %Pa
220        fluid.rhoCrit = 436.1; %kg/m^3

        fluid.constituents = {'O2'; ...
            1.00; ... Mol Fractions,
            1.00*fluid.MW }; %Mass Fractions

225

        % Calculate viscosity with the Sutherland Model
        % Eq. 1-36 , REF 3.
        T_0 = 273; %K
        S = 139; %K
230        mu_0 = 1.919E-5; %Ns/m^2
        fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);
        %fluid.mu = 18.46*10^-6; % N-s/m^2 Viscosity

        % Calculate thermal conductivity with the Sutherland Model -
235        % Eq. 1-44b REF: 3
        S = 240; %K
        T_0 = 273; %K
        k_0 = 0.0244; %W/mK
        fluid.k = k_0*(T/T_0)^1.5*(T_0+S)/(T + S);

```



```

240      % Calculate constant-pressure specific heat, Enthalpy, Entropy
      % REF webbook.nist.gov - O2 Coefficients and Formulae
      % Chase, M.W. Jr.;, NIST-JANAF Thermochemical Tables, Fourth
      % Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
245     Coef = [31.32234 -20.23531 57.86644 -36.50624 -0.007374 -8.903471 ...
              246.7945 0.0; ...
              30.03235 8.772972 -3.988133 0.788313 -0.741599 -11.32468...
              236.1663 0.0; ...
              20.91111 10.72071 -2.020498 0.146449 9.245722 5.337651 ...
250              237.6185 0.0 ];

      if T >= 100 && T < 700
          A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
          E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
      elseif T >= 700 && T < 2000
255          A = Coef(2,1); B = Coef(2,2); C = Coef(2,3); D = Coef(2,4);
          E = Coef(2,5); F = Coef(2,6); G = Coef(2,7); H = Coef(2,8);
      elseif T >= 2000 && T < 6000
          A = Coef(3,1); B = Coef(3,2); C = Coef(3,3); D = Coef(3,4);
          E = Coef(3,5); F = Coef(3,6); G = Coef(3,7); H = Coef(3,8);
260      else
          error('Gas input temperature in get_gas_props is out of range')
      end

      fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
              + E/(T*0.001)^2)*1000/fluid.MW;
265      fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
              + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
      fluid.So = A*log(T*0.001) + B*T*0.001 + C*(T*0.001)^2/2 ...
              + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;

270      %Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 O2
      % [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
      fluid.LJ = [ 52.60 3.467 106.7 fluid.MW ];
      % note - b_0 data given.... in REF 2

275      fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);
      %~~~~~

      case {'CO2', 'Carbon Dioxide', 'carbon dioxide'} % 'CO2'
          fluid.type = 'Carbon Dioxide';
          fluid.MW = 44.0095;
280          fluid.R = R_universal/fluid.MW;% 188.9; %J/kgK
          fluid.Tcrit = 304.1282; %K
          fluid.Pcrit = 7377300; %Pa
          fluid.rhoCrit = 467.6; %kg/m^3

285          fluid.constituents = {'CO2'; ...
              1.00; ... Mol Fractions,
              1.00*fluid.MW }; %Mass Fractions

      % Calculate viscosity with the Sutherland Model
290      % - Eq. 1-36 REF. 3
      T_0 = 273; %K

```

```

S = 222; %K
mu_0 = 1.370E-5; %Ns/m^2
fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);
295 %fluid.mu = 18.46*10^-6; % N-s/m^2 Viscosity

% Calculate thermal conductivity with the Sutherland Model -
% Eq. 1-44b REF 3
S = 1800; %K
300 T_0 = 273; %K
k_0 = 0.0146; %W/mK
fluid.k = k_0*(T/T_0)^1.5*(T_0+S)/(T + S);

305 % Calculate Cp using curve fits found in
% REF webbook.nist.gov - CO2 Coefficients and Formulae
% Chase, M.W. Jr.;, NIST-JANAF Thermochemical Tables, Fourth
% Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
% And REF 1 where noted
310 Coef = [24.99735 55.18696 -33.69137 7.948387 -0.136638 -403.6075...
228.2431 -393.5224; ...
58.16639 2.720074 -0.492289 0.038844 -6.447293 -425.9186...
263.6125 -393.5224 ];

if T >= 298 && T < 1200
315 A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
fluid.Cp =(A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
+ E/(T*0.001)^2)*1000/fluid.MW;
fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
320 + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
+ D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
elseif T >= 1200 && T < 6000
325 A = Coef(2,1); B = Coef(2,2); C = Coef(2,3); D = Coef(2,4);
E = Coef(2,5); F = Coef(2,6); G = Coef(2,7); H = Coef(2,8);
fluid.Cp =(A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
+ E/(T*0.001)^2)*1000/fluid.MW;
fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
+ D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
330 fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
+ D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
elseif T>=200 && T<=1365 %REF 1; pp A-9,Carbon Dioxide,Real Gas,
fluid.Cp = 678.012 - 0.390396*T + 6.23594E-03*T^2 ...
- 1.3596256E-05*T^3 ...
335 + 1.3942973E-08*T^4 - 7.036E-12*T^5 + 1.40115E-15*T^6; %
else
error('CO2 input temp. in get_gas_props is out of range')
end
340 fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

% Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 CO2
% [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
fluid.LJ = [ 77.25 3.941 195.2 fluid.MW ];

```

```

345         % note - b_0 data given.... in REF 2
%~~~~~
case {'H2', 'Hydrogen', 'hydrogen'} %{' '} |
    fluid.type = 'Hydrogen';
    fluid.FAR_stoich = 0.029138;
350 %     fluid.gamma = 1.41;
%     fluid.mu = 87.46*10^-7; %Ns/m^2
    fluid.MW = 2.01588; %kg/kmol
    fluid.R = R_universal/fluid.MW; %4124; % J/(kg K)

355     % Critical properties REF: webbook.nist.gov
    fluid.TCrit = 33.145; %K
    fluid.PCrit = 1296400; %Pa
    fluid.rhoCrit = 31.263 ;%kg/m^3
    fluid.constituents = {'H2'; ...
360         1.000; ...
        1.000*fluid.MW }; %Mass Fractions

    % Calculate viscosity with the Sutherland Model
    % Eq. 1-36 REF. 3
365     T_0 = 273; %K
    S = 97; %K
    mu_0 = 8.411E-6; %Ns/m^2
    fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);

370     % Calculate thermal conductivity with the Sutherland Model -
    % Eq. 1-44b "Viscous Fluid Flow," White, Frank M.
    S = 120; %K
    T_0 = 273; %K
    k_0 = 0.168; %W/mK
375     fluid.k = k_0*(T/T_0)^1.5*(T_0+S)/(T + S);

    % Calculate Cp using curve fits found in
    % REF webbook.nist.gov - H2 Coefficients and Formulae
    % Chase, M.W. Jr.;, NIST-JANAF Thermochemical Tables, Fourth
380     % Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
    % And REF 1 where noted
    Coef = [33.066178 -11.363417 11.432816 -2.772874 -0.158558 ...
            -9.980797 172.707974 0.0; ...
            18.563083 12.257357 -2.859786 0.268238 1.977990 ...
385            -1.147438 156.288133 0.0; ...
            43.413560 -4.293079 1.272428 -0.096876 -20.533862 ...
            -38.515158 162.081354 0.0];

    if T>=100 && T<=365 % REF: 1. pp A-28, Hydrogen - Real Gas
        fluid.Cp = 6436.5105+63.161307*T-0.1685728*T^2 ...
390            +1.5229265E-4*T^3;
    elseif T >= 298 && T< 1000 % REF:
        A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
        E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
        fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
395            + E/(T*0.001)^2)*1000/fluid.MW;

```

```

        fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
                + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
        fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
                + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
400     elseif T >= 1000 && T< 2500
        A = Coef(2,1); B = Coef(2,2); C = Coef(2,3); D = Coef(2,4);
        E = Coef(2,5); F = Coef(2,6); G = Coef(2,7); H = Coef(2,8);
        fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
                + E/(T*0.001)^2)*1000/fluid.MW;
405     fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
                + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
        fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
                + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
        elseif T >= 2500 && T< 6000
410     A = Coef(3,1); B = Coef(3,2); C = Coef(3,3); D = Coef(3,4);
        E = Coef(3,5); F = Coef(3,6); G = Coef(3,7); H = Coef(3,8);
        fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
                + E/(T*0.001)^2)*1000/fluid.MW;
        fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
415     + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
        fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
                + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
        else
            error(...
420     'Gas input temperature in get_gas_props is out of range')
        end
%     fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
%     + E/(T*0.001)^2)*1000/fluid.MW;
% fluid.Cp = (
425     fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

% Provide the Leonard-Jones Potential constants,
% REF: 2 Table A.19, page 681-682, and the Chapman and Enskog's
% Method found as equation A-204, p679
430 %Substance [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ = [ 28.51    2.827    59.7    fluid.MW];

%~~~~~

case {'N2', 'Nitrogen', 'nitrogen'} %{' '} |
435     fluid.type = 'Nitrogen';
        fluid.gamma = 1.40;
        %fluid.mu = 17.9*10^-7; %Ns/m^2
        fluid.MW = 28.0134; %kg/kmol
        fluid.R = R_universal/fluid.MW; %296.8; % J/(kg K)
440
        % Critical properties REF: webbook.nist.gov
        fluid.Tcrit = 126.192; %K
        fluid.Pcrit = 3395800; %Pa Source: NIST WEBBOOK
        fluid.rhoCrit = 313.300 ;%kg/m^3
445     fluid.constituents = {'N2'; ...
        1.000; ... Mol Fractions,
        1.000*fluid.MW }; %Mass Fractions

```

```

% Calculate viscosity with the Sutherland Model
450 % - Eq. 1-36 REF. 3
    T_0 = 273; %K
    S = 107; %K
    mu_0 = 1.6630E-5; %Ns/m^2
    fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);
455 %fluid.mu = 18.46*10^-6; % N-s/m^2 Viscosity

% Calculate thermal conductivity with the Sutherland Model -
% Eq. 1-44b "Viscous Fluid Flow," White, Frank M.
    S = 150; %K
460 T_0 = 273; %K
    k_0 = 0.0242; %W/mK
    fluid.k = k_0*(T/T_0)^1.5*(T_0+S)/(T + S);

% Calculate Cp using curve fits found in
465 % REF webbook.nist.gov - N2 Coefficients and Formulae
% Chase, M.W. Jr.;, NIST-JANAF Thermochemical Tables, Fourth
% Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
Coef = [29.98641 1.853978 -9.647459 16.63537 0.000117 -8.671914 ...
        226.4168 0.0; ...100-500
        19.50583 19.88705 -8.598535 1.369784 0.527601 -4.935202 ...
        212.3900 0.0; ...500-2000
        35.51872 1.128728 -0.1906103 0.014662 -4.553760 -18.97091...
        224.9810 0.0];

% NEED TO CHECK THIS SECTION (COEFFICIENTS... gamma doesn't look right...
475 if T >= 100 && T < 500
    A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
    E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
elseif T >= 500 && T < 2000
    A = Coef(2,1); B = Coef(2,2); C = Coef(2,3); D = Coef(2,4);
480 E = Coef(2,5); F = Coef(2,6); G = Coef(2,7); H = Coef(2,8);
elseif T >= 2000 && T < 6000
    A = Coef(3,1); B = Coef(3,2); C = Coef(3,3); D = Coef(3,4);
    E = Coef(3,5); F = Coef(3,6); G = Coef(3,7); H = Coef(3,8);
else
485 error('Gas input temperature in get_gas_props is out of range')
end

fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
           + E/(T*0.001)^2)*1000/fluid.MW;
fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
           + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
490 fluid.So = A*log(T*0.001) + B*T*0.001 + C*(T*0.001)^2/2 ...
           + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;

fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);
495 % Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 N2
% [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
fluid.LJ = [ 69.14 3.798 71.4 fluid.MW ];
% note - b_0 data given.... in REF 2

```

```

500 %~~~~~
    case {'Ar', 'Argon', 'argon'} %{' '} |
        fluid.type = 'Argon';
        fluid.gamma = 1.66;
        % fluid.mu = 22.7*10^-7; %Ns/m^2
505 fluid.MW = 39.948; %kg/kmol
        fluid.R = R_universal/fluid.MW; %208.1; % J/(kg K)

        % Critical properties REF: webbook.nist.gov
        fluid.TCrit = 150.687; %K
510 fluid.PCrit = 4863000; %Pa Source: NIST WEBBOOK
        fluid.rhoCrit = 535.599; %kg/m^3
        fluid.constituents = {'Ar'; ...
            1.000; ... Mol Fractions,
            1.000*fluid.MW }; %Mass Fractions

515 % Calculate viscosity with the Sutherland Model
        % - Eq. 1-36 REF. 3
        T_0 = 273; %K
        S = 144; %K
520 mu_0 = 2.125E-5; %Ns/m^2
        fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);
        %fluid.mu = 18.46*10^-6; % N-s/m^2 Viscosity

        % Calculate thermal conductivity with the Sutherland Model -
525 % Eq. 1-44b "Viscous Fluid Flow," White, Frank M.
        S = 1080; %K
        T_0 = 250; %K
        k_0 = 0.015; %W/mK
        fluid.k = k_0*(T/T_0)^1.5*(T_0+S)/(T + S);

530 % Calculate Cp using curve fits found in
        % REF webbook.nist.gov - Coefficients and Formulae
        % Chase, M.W. Jr.;, NIST-JANAF Thermochemical Tables, Fourth
        % Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
535 Coef = [20.78600 2.825911e-7 -1.464191e-7 1.092161e-8 ...
            -3.661371e-8 -6.197350 179.999 0.0;
            0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ];
        if T >= 298 && T < 6000
            A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
540 E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
            fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
                + E/(T*0.001)^2)*1000/fluid.MW;
            fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
                + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
545 fluid.So = A*log(T*0.001) + B*T*0.001 + C*(T*0.001)^2/2 ...
                + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
        elseif T < 300
            fluid.Cp = 520.34; % J/kg K from NPS report
        else
550 error('Gas input temperature in get_gas_props is out of range')
        end

```

```

        fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

555     % Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 Ar
        % [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
        fluid.LJ = [ 56.08 3.542 93.3 fluid.MW ];
        % note - b_0 data given.... in REF 2

560 %~~~~~
        case {'C2H4','Ethylene','ethylene','Ethene','ethene'} %
            fluid.type = 'Ethylene';
            fluid.FAR_stoich = 0.068109 ;
            fluid.MW = 28.054;
565     fluid.R = R_universal/fluid.MW; %296; %J/kgK

            % Critical properties REF: webbook.nist.gov
            fluid.TCrit = 282.3; %K
            fluid.PCrit = 5041800; %Pa Source: NIST WEBBOOK
570     fluid.rhoCrit = 214.2; %kg/m^3
            fluid.constituents = {'C2H4'; ...
                1.00; ... Mol Fractions,
                1.00*fluid.MW }; %Mass Fractions

575     % Calculate viscosity with the Sutherland Model
        % Eq. 1-36 REF. 3
        T_0 = 250; %K
        S = 225.9; %K REF: JEANS21
        mu_0 = 9.613E-5; %Ns/m^2 REF: JEANS21
580     fluid.mu = mu_0*(T/T_0)^1.5*(T_0+S)/(T + S);
        %fluid.mu = 18.46*10^-6; % N-s/m^2 Viscosity

        % Calculate viscosity with the Sutherland Model
        % Eq. 1-36 REF 3
585     S = 1080; %K
        T_0 = 250; %K
        k_0 = 0.015; %W/mK
        fluid.k = k_0*(T/T_0)^2.0*(T_0+S)/(T + S);
        %WARNING: Note the modified formula - due to a curve fit of data
590     %from the NIST webbook to match the sutherland form...

        % Calculate Cp using curve fits found in
        % REF webbook.nist.gov - C2H4 data, independent curve fit by Andrus
        % Curve fits on site, break up the data into different temperature
595     % ranges, and provide for other calculations - may go back and
        % implement at some point, but not today. Original data from
        % "Selected Values of Properties of Chemical Compounds," 1997,
        % Thermodynamics Research Center, 1997, Texas A&M University,
        % College Station Texas
600     if T>=150 && T <=3000;
        x = T*0.001;
        fluid.Cp = (6.0378*x^6 - 59.886*x^5 + 228.82*x^4 ...
            - 415.35*x^3 + 336.28*x^2 -34.162*x + 33.145) ...

```

```

        *1000/fluid.MW;
605     % fluid.DH = 6.0378*x^7/7 - 59.886*x^6/6 + 228.82*x^5/5 ...
        % - 415.35*x^4/4 + 336.28*x^3/3 -34.162*x^2/2 + 33.145*x;
        % fluid.So =
else
    error(['Temperature is out of range' ...
610         ' for Ethylene in subroutine get_gas_props'])
end

    fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);
    % Provide the Leonard-Jones Potential constants,
615    % REF: 2 Table A.19, page 681-682, and the Chapman and Enskog's
    % Method found as equation A-204, p679
    %Substance[ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ= [ 91.06    4.163    224.7    28.06 ]; % Ethylene

620    %~~~~~
    case {'C3H8', 'Propane', 'propane'} %{} |
        fluid.type = 'Propane';
        fluid.FAR_stoich = 0.064242 ; % Assumes Air is the oxidizer
625    % fluid.gamma = 1.127;
        fluid.mu = 8.2*10^-6;% N*s/m^2 (=Pa*s) ref webbook.nist.gov 2/25/13
        fluid.MW = 44.096;
        fluid.R = R_universal/fluid.MW; %J/kgK

630    % Critical properties REF: webbook.nist.gov
        fluid.Tcrit = 369.825; %K
        fluid.Pcrit = 4247660; %Pa
        fluid.rhoCrit = 220; %kg/m^3

635    fluid.constituents = {'C3H8'; ...
        1.00; ... Mol Fractions,
        1.00*fluid.MW }; %Mass Fractions

    % Calculate Cp using curve fits found in
640    % REF webbook.nist.gov - C3H8 data, independent curve fit by Andrus
    % Curve fits on site, break up the data into different temperature
    % ranges, and provide for other calculations - may go back and
    % implement at some point, but not today. Original data from
    % Chao, J. "Ideal Gas Thermodynamic Properties of Ethane and
645    % Propane" 1973, J. Phys. Chem. Ref. Data, 2, 427-438
    if T>50 && T<=1500;
        x = T*0.001;
        fluid.Cp = (-93.314*x^5 + 433.76*x^4 - 735.88*x^3 ...
            + 483.26*x^2 + 55.907*x + 30.848)*1000/fluid.MW;
650    % fluid.DH = -93.314*x^6/6 + 433.76*x^5/5 - 735.88*x^4/4 ...
        % + 483.26*x^3/3 + 55.907*x^2/2 + 30.848*x;
    elseif T>1500 && T<=3001;
        x = 1500*0.001;
        fluid.Cp = (-93.314*x^5 + 433.76*x^4 - 735.88*x^3 ...
655        + 483.26*x^2 + 55.907*x + 30.848)*1000/fluid.MW;

```



```

        warning('Temperature input for PROPANE is out of range of model')
    else
        error(['Temperature out of range for PROPANE' ...
            ' in get_gas_props subroutine']);
660    end

    if T>=200 && T<=500 % Formula from REF 1, valid from 200-500K
        fluid.k = -1.07682209E-02 + 8.38590352E-05*T ...
            + 4.22059864E-08*T^2;
665    elseif T>500
        fluid.k = -1.07682209E-02 + 8.38590352E-05*500 ...
            + 4.22059864E-08*T^500;
        warning(['Thermal conductivity of PROPANE is calculated' ...
            ' using a model that is not valid for the input temperature'])
670    else
        error(['Temperature for calculating PROPANES thermal ' ...
            'conductivity is out of range'])
    end

675    fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

    % Provide the Leonard-Jones Potential constants,
    % REF: 2 Table A.19, page 681-682, and the Chapman and Enskog's
    % Method found as equation A-204, p679
680    %Substance[ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ = [ 169.2    5.118    237.1    44.097]; %nPropane

    %~~~~~
685    %~~~~~
    case {'Ethane', 'C2H6', 'ethane'} %
        fluid.type = 'Ethane';
        fluid.FAR_stoich = 0.062581 ; % Assumes Air is oxidizer
        %fluid.gamma = 1.187;
690    fluid.mu = 9.6*10^-6;% N*s/m^2 (=Pa*s) ref webbook.nist.gov 2/25/13

        fluid.MW = 30.069;
        fluid.R = R_universal/fluid.MW; % 276.5; %J/kgK

695    % Critical properties REF: webbook.nist.gov
        fluid.TCrit = 305.33; %K
        fluid.PCrit = 4871800; %Pa
        fluid.rhoCrit = 207; %kg/m^3

700    fluid.constituents = {'C2H6'; ...
        1.00; ... Mol Fractions
        1.00*fluid.MW }; %Mass Fractions

    % Calculate thermal conductivity using polynomial curve fit for
    % Ethane taken from REF 1
705    if T>=100 && T <=1000;
        fluid.k = -3.83815197e-2 +5.47282126e-4*T-2.80760648e-6*T^2 ...

```

```

+8.74854603e-9*T^3 - 1.369896e-11*T^4 + 1.05765043e-14*T^5 ...
-3.16347435e-18*T^6; % From NPS report
710 elseif T>1000
% Rather than spit out an error, just give the last good data point...
warning(['Temperature input for thermal conductivity of ' ...
'ETHANE is %f K, out of range of model.'], T)
T_temp = T;
715 T = 1000;
fluid.k = -3.83815197e-2 +5.47282126e-4*T-2.80760648e-6*T^2 ...
+8.74854603e-9*T^3 - 1.369896e-11*T^4 + 1.05765043e-14*T^5 ...
-3.16347435e-18*T^6; % From NPS report...
T = T_temp;
720 end

% REF webbook.nist.gov - C2H6 data, independent curve fit by Andrus
% Curve fits on site, break up the data into different temperature
% ranges, and provide for other calculations - may go back and
725 % implement at some point, but not today. Original data from
% Gurvich, L.V.; Veyts, I.V.; Alcock, C.B., "Thermodynamic
% Properties of Individual Substances, 4th Ed.; Vols. 1 and 2"
% Hemisphere, New York, 1989
if T>=150 && T <=3000;
730 x = T*0.001;
fluid.Cp = (4.1933*x^6 - 42.977*x^5 + 170.48*x^4 ...
- 319.86*x^3 + 251.28*x^2 + 30.773*x + 29.265)*1000/fluid.MW;
% fluid.DH = 4.1933*x^7/7 - 42.977*x^6/6 + 170.48*x^5/5 ...
% - 319.86*x^4/4 + 251.28*x^3/3 + 30.773*x^2/2 + 29.265*x;
735 % fluid.So =
else
error(['Temperature is out of range for Ethylene in ' ...
'subroutine get_gas_props'])
end
740 fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

% Provide the Leonard-Jones Potential constants,
% REF: 2 Table A.19, page 681-682, and the Chapman and Enskog's
% Method found as equation A-204, p679
745 %Substance [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
fluid.LJ = [ 110.7 4.443 215.7 30.07 ]; % Ethane

%~~~~~
% Incomplete Gas properties follow...
750 case {'JP8'}
fluid.type = 'Flash Vaporized JP8';
warning('JP8 is not complete, function "get_gas_props" ');
% fluid.mu = 8.2*10^-6;% N*s/m^2 (=Pa*s) ref webbook.nist.gov 2/25/13
fluid.MW = 44.096;
755 fluid.R = R_universal/fluid.MW; %189; %J/kgK
fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

case{'CO', 'Carbon Monoxide', 'carbon monoxide'}
fluid.type = 'Carbon Monoxide';

```

```

760     warning(['CO - Carbon Monoxide - is not complete, ' ...
              'function "get_gas_props" ']);
% Still need viscosity and thermal conductivity equations
fluid.MW = 1*12.0107+1*15.9994; %m.u.
fluid.R = R_universal/fluid.MW; % %J/kgK

765     fluid.TCrit = 133.; %K    REF: 4, Table A-1
fluid.PCrit = 3.50E6; %Pa
fluid.rhoCrit = fluid.MW/.0930; %kg/m^3

770     fluid.constituents = {'CO'; ...
        1.00; ... Mol Fractions,
        1.00*fluid.MW }; %Mass Fractions
% Calculate Cp using curve fits found in
% REF webbook.nist.gov - CO Coefficients and Formulae
775     % Chase, M.W. Jr.;, NIST-JANAF Thermochemical Tables, Fourth
% Edition, J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951
Coef = [25.56759      6.09613 4.054656      -2.671301      0.131021
...
        -118.0089 227.3665      -110.5271; ...298-1300
780        35.1507      1.300095      -0.205921      0.01355 -3.28278
...
        -127.8375 231.712 -110.5271 ]; %1300-6000
    if T >= 298 && T < 1300
%NEED TO CHECK THIS SECTION (COEFFICIENTS... gamma doesn't look right...
785        A = Coef(1,1); B = Coef(1,2); C = Coef(1,3); D = Coef(1,4);
        E = Coef(1,5); F = Coef(1,6); G = Coef(1,7); H = Coef(1,8);
    elseif T >= 1300 && T < 6000
        A = Coef(2,1); B = Coef(2,2); C = Coef(2,3); D = Coef(2,4);
        E = Coef(2,5); F = Coef(2,6); G = Coef(2,7); H = Coef(2,8);
790    else
        error('Gas input temperature in get_gas_props is out of range')
    end
    fluid.Cp = (A + B*T*0.001 + C*(T*0.001)^2 + D*(T*0.001)^3 ...
        + E/(T*0.001)^2)*1000/fluid.MW;
795    fluid.DH = A*T*0.001 + B*(T*0.001)^2/2 + C*(T*0.001)^3/3 ...
        + D*(T*0.001)^4/4 - E/(T*0.001) + F - H;
    fluid.So = A*log(T*0.001)+ B*T*0.001 + C*(T*0.001)^2/2 ...
        + D*(T*0.001)^3/3 - E/(T*0.002)^2 + G;
% Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 CO
800    % [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ = [ 63.41      3.690 91.7      fluid.MW ];
% note - b_0 data given.... in REF 2

case{'H2O','water','water','water vapor'}
805    fluid.type = 'water Vapor';
    warning('water Vapor is not complete, function "get_gas_props" ');
    fluid.MW = 2*1.00794+1*15.9994; %m.u.
    fluid.R = R_universal/fluid.MW; % %J/kgK
    fluid.TCrit = 647.3; %K    REF: 4, Table A-1
810    fluid.PCrit = 22.09E6; %Pa
    fluid.rhoCrit = fluid.MW/.0568; %kg/m^3

```

```

        fluid.constituents = {'H2O'; ...
            1.00; ... Mol Fractions,
            1.00*fluid.MW }; %Mass Fractions
815 % Set Lennard-Jones Potential Constants REF: 2
    % [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ = [ 23.25 2.641 809.1 fluid.MW ];
    % note - b_0 data given.... in REF 2
case{'CH4'}
820 fluid.type = 'Methane';
    warning(['CH4 - Methane - is not complete, function'...
        ' "get_gas_props" ']);
    fluid.MW = 1*12.0107+4*1.00794; %m.u.
    fluid.R = R_universal/fluid.MW; % %J/kgK
825 fluid.Tcrit = 191.1; %K REF: 4, Table A-1
    fluid.Pcrit = 4.64E6; %Pa
    fluid.rhoCrit = fluid.MW/.0924; %kg/m^3
    fluid.constituents = {'CH4'; ...
        1.00; ... Mol Fractions,
830 1.00*fluid.MW }; %Mass Fractions
    % Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 CO
    % [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ = [ 66.98 3.758 148.6 fluid.MW ];
    % note - b_0 data given.... in REF 2
835 case{'NO'}
    fluid.type = 'Nitric Oxide';
    warning(['NO - Nitric Oxide - is not complete, function '...
        '"get_gas_props" ']);
    fluid.MW = 1*14.0067+1*15.9994; %m.u.
840 fluid.R = R_universal/fluid.MW; % %J/kgK
    fluid.constituents = {'NO'; ...
        1.00; ... Mol Fractions,
        1.00*fluid.MW }; %Mass Fractions
    % Calculate specific heat using REF 1
845 if T>=200 && T <=1365;
        %x = T;
        fluid.Cp = 806.451 + 0.506398*T - 2.0853977E-04*T^2 ...
            + 2.8257004E-08*T^3;
    else
850 warning('NO Cp calculation is out of bounds for model');
    end
    fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

    % Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 CO
855 % [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
    fluid.LJ = [ 53.74 3.492 116.7 fluid.MW ];
    % note - no b_0 data given.... in REF 2
case{'N2O'}
    fluid.type = 'Nitrous Oxide';
860 warning(['N2O - Nitrous Oxide - is not complete, function '...
        'get_gas_props']);
    fluid.MW = 2*14.0067+1*15.9994; %m.u.
    fluid.R = R_universal/fluid.MW; % %J/kgK

```

```

fluid.constituents = {'N2O'; ...
865     1.00; ... Mol Fractions,
        1.00*fluid.MW }; %Mass Fractions

% Calculate specific heat using REF 1
if T>=200 && T <=1365;
870     %x = T;
        fluid.Cp = 419.153 + 2.2147124*T - 2.922847E-03*T^2 + ...
            2.51402093E-06*T^3 - 1.21894601E-09*T^4 + 2.4536593E-13*T^5;
else
    warning('N2O Cp calculation is out of bounds for model');
875 end
fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);

% Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 CO
% [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
880 fluid.LJ = [ 70.80 3.828 232.4 fluid.MW ];
% note - b_0 data given.... in REF 2

case{'He','Helium','helium'}
    fluid.type = 'Helium';
885    warning('He - Helium - is not complete, function "get_gas_props"');
    fluid.MW = 4.002602; %m.u.
    fluid.R = R_universal/fluid.MW; % J/kgK
    fluid.constituents = {'He'; ...
        1.00; ... Mol Fractions,
890        1.00*fluid.MW }; %Mass Fractions

    fluid.Tcrit = 5.1953; %K REF: 4, Table A-1
    fluid.Pcrit = 0.22746E6; %Pa
    fluid.rhoCrit = 69.641 ;%kg/m^3
895

% Calculate specific heat using REF 1
if T>=298 && T <=6000;
    %x = T;
    T1k = T/1000; %Seems to be giving results off by factor of 10
900    fluid.Cp = (20.78603 + 4.850638E-10*T1k ...
        -1.582916E-10*T1k^2 + ...
        1.525102E-11*T1k^3 + 3.196347E-11/T1k^2)...
        *1000.0/fluid.MW ;% J/(kgK);
else
    warning('He Cp calculation is out of bounds for model');
905 end
fluid.gamma = fluid.Cp/(fluid.Cp-fluid.R);
% REFS: Cox, J. D., Wagman, D. D., Medvedev, V. A., CODATA Key
% Values for Thermodynamics, Hemisphere Publishing, New York, 1984,
% 1
910 % Chase, M.W., Jr., NIST-JANAF Thermochemical Tables, Fourth Edition,
% J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951.

fluid.k = 1.028793E-02 + 8.51625139E-04*T - 3.14258034E-06*T^2 ...
915 + 1.02188556E-08*T^3 - 1.3477236E-11*T^4;% from REF 1

```

```

fluid.mu =( 0.39414 + 0.17213335*T - 1.38733E-03*T^2 ...
+ 8.020045E-06*T^3 - 2.4278655E-08*T^4 ...
+ 3.641644E-11*T^5 - 2.14117E-14*T^6)*1E-6;% from REF 1

920 % Set Lennard-Jones Potential Constants REF: GHIAASIAAN11 CO
% [ b_0,cm^3/gmol \sigma,Angstrom, \epsilon/k_B, K MW,mu]
fluid.LJ = [ 70.80 3.542 93.3 fluid.MW ];
% note - b_0 data given.... in REF 2 - 70.80 is wrong for helium

925 end

% Additional Cp Formulae may be found in
% - REF 1,
% - Turns, "An Introduction to Combustion", 2000, McGraw Hill, 2nd Ed, pp
930 % 645-652 (tables A.13, B.2, and B.3)
% - Cengel & Boles "Thermodynamics, an Engineering Approach", 1998,
% McGraw Hill, 3rd Ed., pp 901 and 951
% - REF 2, pp 641, Eq A-8 and Table A.8

935 % Use perfect gas laws to get thermal diffusivity see REF 4.
fluid.rho_ideal = P/(fluid.R*T); % kg/m^3 Ideal gas law density
% [kg/m^3 ND] Density and Compressibility
[fluid.rho, fluid.Z] = BB_EqnOfState(T, P, type);

940 if fluid.rho == -1
fluid.rho = fluid.rho_ideal;
end

945 fluid.alpha = fluid.k/(fluid.rho*fluid.Cp); % W/mK Thermal Diffusivity
fluid.a = sqrt(fluid.gamma*fluid.R*T); % m/s Speed of Sound

fluid.P = P;
fluid.T = T;
950 fluid.Pred = P/fluid.PCrit;
fluid.Tred = T/fluid.TCrit;
fluid.rhored = fluid.rho/fluid.rhocrit;
end

```

2.1.1. Matlab Function BB_EqnOfState.m

The function BB_EqnOfState calculates the density, and compressibility factor for various gaseous compounds. The formulae and constants were collected from Çengel and Boles (39), Kuo (38), and Wisniak (179).

```

function [ density, Z ] = BB_EqnOfState( T, P, Gas )

% Beattie Bridgemen Equation of State As described in Kuo, and Wisniak
% (data from Wisniak)
% INPUTS:
5 %      T - Temperatue in Kelvin
%      P - Pressure in Pascal
%      Substance - Type of substance (see list of available gases
%      below)
% OUTPUT:
10 %      density - Density of the gas in kg/m^3
%      Z - Compressibility factor (no dimensions)
% Programming:
%      By Ionio Andrus in support of efforts to model gas properties in
%      pursuid of a PHD Thesis at the Air Force Institute of Technology,
15 %      wright Patterson AFB, Spring 2015
%
% Note: this routine has not been thouroughly error checked use at your own
% risk!
%
20 % Allowable substance inputs:
%      'He', or 'Helium'
%      'Ne', or 'Neon'
%      'Ar', or 'Argon'
%      'H2','hydrogen', or 'Hydrogen'
25 %      'N2','nitrogen', or 'Nitrogen'
%      'O2','oxygen', or 'Oxygen'
%      'Air', or 'air'
%      'CO2','carbon-dioxide', or 'Carbon Dioxide'
%      'C2H4','ethylene','Ethylene','Ethene', or 'ethene'
30 %      'NH3', or 'ammonia'
%      'CO', or 'carbon monoxide'
%      'CH4', or 'Methane'
%      'C2H6', or 'Ethane','ethane'
%      'C3H8', or 'propane', 'Propane'
35 %      'n-C4H10', or 'n-Butane','n-butane'
%      'n-C7H16', or 'n-Heptane','n-heptane'
%
% % Unique to BB_EqnOfState when compared with BWR_EqOState function are:
% He, Ne, Ar, H2, N2, O2, Air, CO2, NH3, and CO,
40 % Repeated are: 'CH4, C2H4, C2H6, C3H8, C4H10, C7H16
%
%
% Ref: - Wisniak, Jaime, "Real Gas Computations I-Equations of State",
%      Modular Instruction Series, American Chemical Society [PDF
45 %      Document online]
%      - Kuo, Kenneth, Principles of Combustion 2nd Edition, (c) 2005, John
%      Wiley and Sons, NY
%      - Cengal, Yunus, Boles "Thermodynamics and Engineering
%      Approach"pp940
50 %

switch Gas

```

```

    case{'He','Helium'}
        CoefIndx=1;
55    case{'Ne','Neon'}
        CoefIndx=2;
    case{'Ar','Argon'}
        CoefIndx=3;
    case{'H2','hydrogen','Hydrogen'}
60        CoefIndx=4;
    case{'N2','nitrogen','Nitrogen'}
        CoefIndx=5;
    case{'O2','oxygen','Oxygen'}
        CoefIndx=6;
65    case{'Air','air'}
        CoefIndx=7;
    case{'CO2','carbon-dioxide','Carbon Dioxide'}
        CoefIndx=8;
    case{'C2H4','ethylene','Ethylene','Ethene','ethene'}
70        CoefIndx=9;
    case{'NH3','ammonia'}
        CoefIndx=10;
    case{'CO','carbon monoxide'}
        CoefIndx=11;
75    case{'CH4','Methane'}
        CoefIndx=12;
    case{'C2H6','Ethane','ethane'}
        CoefIndx=13;
    case{'C3H8','propane','Propane'}
80        CoefIndx=14;
    case{'n-C4H10','n-Butane','n-butane'}
        CoefIndx=15;
    case{'n-C7H16','n-Heptane','n-heptane'}
        CoefIndx=16;
85    otherwise
        warning('Call to BB_EqnOfState used incorrect label for gas of interest or
the gas is not included in the function library.');
```

density = -1;

Z = 0;

```

90 end

%% Define Coefficients

Coef = ...
    ... Gas      A0 *      a *      B0 *      b *      C *      MW,mu, Tcrit,K
Pcrit,Pa rhoCrit kg/m^3
95    { 'He',      0.0216, 0.05984, 0.01400,  0.0,      0.0040E4,  4.003, 5.3 ,
0.23E6,  4.003/0.0578 ; ...1
      'Ne',      0.2125, 0.02196, 0.02060,  0.0,      0.101E4 , 20.183, 44.5 ,
2.73E6,  20.183/0.0417; ...2
      'Ar',      1.2907, 0.02328, 0.03931,  0.0,      5.99E4 , 39.948, 151 ,
100 4.86E6, 39.948/0.0749; ...3
      'H2',      0.1975,-0.00506, 0.02096, -0.04359, 0.0504E4, 2.016, 33.3 ,
1.3E6 , 2.016/0.0649 ; ...4
      'N2',      1.3445, 0.02617, 0.05046, -0.00691, 4.20E4 , 28.013, 126.2,
```



```

3.39E6, 28.013/0.0899; ...5
105 'O2', 1.4911, 0.02562, 0.04624, 0.004208, 4.80E4 , 31.999, 154.8,
5.08E6, 31.999/0.0780; ...6
'Air', 1.3012, 0.01931, 0.04611, -0.001101, 4.34E4 , 28.97 , 132.5,
3.77E6, 28.97/0.0883 ; ...7
'CO2', 5.0065, 0.07132, 0.10476, 0.07235, 66.00E4 , 44.01 , 304.2,
110 7.39E6, 44.01/0.0943 ; ...8
'C2H4', 6.152 , 0.04964, 0.12156, 0.03597, 22.68E4 , 28.054, 282.4,
5.12E6, 28.054/0.1242; ...9
'NH3', 2.3930, 0.17031, 0.03415, 0.19112, 476.87E4 , 17.03 , 405.5,
11.28E6, 17.03/0.0724 ; ...10
115 'CO', 1.3445, 0.02617, 0.05046, -0.00691, 4.20E4 , 28.011, 133 ,
3.50E6, 28.011/0.0930; ...11
'CH4', 2.2769, 0.01855, 0.05587, -0.01587, 12.83E4 , 16.043, 191.1,
4.64E6, 16.043/0.0993; ...12
'C2H6', 5.8800, 0.05861, 0.09400, 0.01915, 90.00E4 , 30.070, 305.5,
120 4.48E6, 30.070/0.1480; ...13
'C3H8', 11.920, 0.07321, 0.07321, 0.18100, 120E4 , 44.097, 370 ,
4.26E6, 44.097/0.1998; ...14
'n-C4H10', 17.794, 0.12161, 0.24620, 0.09423, 350E4 , 58.124, 425.2,
3.80E6, 58.124/0.2547; ...15
125 'n-C7H16', 54.520, 0.20066, 0.70816, 0.19179, 400E4 , 100.205, 540.11,
2.736E6, 1.0/0.004314 ...16
};
% * - Pressure in atmospheres, volume in liters/g-mol, temperature in K;
% R = 0.08206 atm liter/g-mol K.
130
%CoefIndx = 13; %Select Air for trouble shooting...
%T = 377; P = 102*101325; % for trouble shooting...

% Define Universal Gas constant in terms of equations used...
135 Ru = 0.08206; %atm liter/g-mol) K

% Pull equation coefficients from the coefficient library
A0 = Coef{CoefIndx,2};
a = Coef{CoefIndx,3};
140 B0 = Coef{CoefIndx,4};
b = Coef{CoefIndx,5};
C0 = Coef{CoefIndx,6};
MW = Coef{CoefIndx,7};
TCrit = Coef{CoefIndx,8};
145 PCrit = Coef{CoefIndx,9};
rCrit = Coef{CoefIndx,10};

% Calculate the reduced pressure and temperature
% T_red = T/TCrit;
150 p_red = P/PCrit;
%Rg = 8314/MW;

%% Iterate to find pressure/ density

v_0 = Ru*T/(P/101325); %liters/g-mole - initial guess with ideal gas properties
v_1 = v_0; %MW ;% (1.0/rCrit)*(Rg*TCrit/PCrit);%m^3/kg

```

```

155 v_2 = v_1; % initialize v_2

    % fprintf('v0: %g v1:%g T_red:%g Pred:%g \n', v_0, v_1, T_red, p_red)

    cnt = 0; err = 1;
160 while err>1E-6 && cnt < 100

        A1 = Ru*T;
        B1 = B0*Ru*T-A0-Ru*C0/T^2;
165 C1 = A0*a - Ru*T*B0*b-B0*Ru*C0/T^2;
        D1 = Ru*B0*b*C0/T^2;

        P1 = A1/v_1 + B1/v_1^2 + C1/v_1^3 + D1/v_1^4;
        % fprintf( 'A1:D4 = %8.3f %8.3f %8.3f %8.3f \n', A1/v_1, B1/v_1^2, C1/v_1^3,
170 D1/v_1^4);

        dpdv = -(A1/v_1^2 + 2*B1/v_1^3 + 3*C1/v_1^4 + 4*D1/v_1^5);

        err = abs((P/101325-P1)/(P/101325)); % /101325
175 v_2 = v_1 + (P/101325-P1)/dpdv; % Newton's method to updated value
        % v_0 = v_1;
        v_1 = v_2;
        cnt = cnt+1;
180 % fprintf('%3d P1/dpdv: %g v1:%g err:%5.3g P1:%g \n', cnt, P1/dpdv, v_1,
        err, P1)

    end

185 Z = v_1/ v_0; % (Actual specific volume)/(ideal specific volume)

    density = (MW/v_1) ;%/(1000.0) (liters/gmol)* ( (m^3/liter)/(kg/g * g/gmol) )

    rho_reduced = density/rCrit;
190 if rho_reduced > 0.8
        warning(' Use of the Beattie-Bridgemen compressibility correction is out of
        bounds: Reduced density is greather than 0.8, equation of state results for this
        calculation are inaccurate!')
        fprintf('density: %8.3g kg/m^3 rho_crit: %8.3g kg/m^3, Z: %8.5f, err:
195 %8.5g', density, rCrit, Z,err);
    end

end

```

2.1.2. Matlab Function BWR_EqOState.m

The function BWR_EqOState performs a Benedict-Webb-Rubin equation of state calculation for selected gaseous compounds, returning the density and compressibility

factor for a desired compound at stated temperature and pressure. Formulae and constants were taken from Bejan (180), Wisniak (179), and Kuo (38).

```

function [ density, Z ] = BWR_EqOState( T, P, Substance )

% Benedict-Webb-Rubin equation of state (Bejan, 1997)
% INPUTS:
%     T - Temperatue in Kelvin
5 %     P - Pressure in Pascal
%     Substance - Type of substance (see list of available gases
%               below)
% OUTPUT:
%     density - Density of the gas in kg/m^3
10 %     Z - Compressibility factor (no dimensions)
% Programming:
%     By Ionio Andrus in support of efforts to model gas properties in
%     pursuid of a PHD Thesis at the Air Force Institute of Technology,
%     wright Patterson AFB, Spring 2015
15 %
% Note: this routine has not been thouroughly error checked use at your own
% risk!
%
% Allowable substance inputs:
20 % 'Methane' , or 'CH4'
% 'Ethylene' , or 'C2H4'
% 'Ethane' , or 'C2H6'
% 'Propylene' , or 'C3H6'
% 'Propane' , or 'C3H8'
25 % 'i-Butane' , or 'C4H10'
% 'i-Butylene', or 'C4H8'
% 'n-Butane' , or 'C4H10'
% 'i-Pentane' , or 'C5H12'
% 'n-Pentane' , or 'C5H12'
30 % 'n-Hexane' , or 'C6H14'
% 'n-Heptane', or 'C7H16'
%
% Unique to BWR when compared with the BB_EqnOfState function are:
% 'n-Hexane', 'n-Pentane', 'i-Pentane', 'i-Butylene', 'i-Butane',
35 % and 'Propylene'
% Repeated are: 'CH4, C2H4, C2H6, C3H8, C4H10, C7H16
%
% REF:- Bejan, A., 1997, Advanced Engineering Thermodynamics, 2nd ed.,
%       John Wiley & Sons, New York, NY
40 % - https://www.thermalfuidscentral.org/encyclopedia/index.php/
%       Properties_of_pure_substances
% - Wisniak, Jaime, "Real Gas Computations I-Equations of State",
%   Modular Instruction Series, American Chemical Society [PDF
%   Document online]
45 % - Kuo, Kenneth, Principles of Combustion 2nd Edition, (c) 2005, John

```

```

%           wiley and Sons, NY

switch Substance
    case {'Methane'   , 'CH4'   }
50         Substance_index = 1;
    case {'Ethylene'  , 'C2H4'  }
        Substance_index = 2;
    case {'Ethane'    , 'C2H6'   }
        Substance_index = 3;
55     case {'Propylene', 'C3H6'  }
        Substance_index = 4;
    case {'Propane'   , 'C3H8'   }
        Substance_index = 5;
    case {'i-Butane'  , 'C4H10'  }
60         Substance_index = 6;
    case {'i-Butylene', 'C4H8'   }
        Substance_index = 7;
    case {'n-Butane'  , 'C4H10'  }
        Substance_index = 8;
65     case {'i-Pentane', 'C5H12' }
        Substance_index = 9;
    case {'n-Pentane' , 'C5H12'  }
        Substance_index = 10;
    case {'n-Hexane'  , 'C6H14'  }
70         Substance_index = 11;
    case {'n-Heptane' , 'C7H16'  }
        Substance_index = 12;
    otherwise
        error(['The requested substance in BWR_EqOState was spelled'...
75              ' incorrectly, or is not in the database'])
end

%% Set Data

Coef = ...
80   ... Gas      A0      A0      B0      C0      a      ...
    ...          b      c      alpha      gamma ...
    ...          MW,mu, Tcrit,K  Pcrit,Pa rhoCrit kg/m^3
    {  'Methane'   , 'CH4'   , 1.85500, 0.0426000, 0.0225700E6, 0.494000, ...
        0.00338004, 0.00254500E6, 0.124359E-3, 0.60000E-2 ,...
        16.043, 191.1,   4.64E6,   16.043/0.0993; ...1
85     'Ethylene'  , 'C2H4'  , 3.33958, 0.0556833, 0.131140E6, 0.259000, ...
        0.0086000, 0.021120E6, 0.178000E-3, 0.923000E-2 ,...
        28.054, 282.4,   5.12E6,   28.054/0.1242; ...2
        'Ethane'   , 'C2H6'  , 4.15556, 0.0627724, 0.179592E6, 0.345160, ...
        0.0111220, 0.0327670E6, 0.243389E-3, 1.18000E-2 ,...
90         30.070, 305.5,   4.48E6,   30.070/0.1480; ...3
        'Propylene', 'C3H6'  , 6.11220, 0.0850647, 0.439182E6, 0.774056, ...
        0.0187059, 0.102611E6, 0.455696E-3, 1.82900E-2 ,...
        42.08, 365.57,   4.6646E6,   223.39; ...4
        ... - source: NIST chemistry webbook for propene
95     'Propane'   , 'C3H8'   , 6.87225, 0.0973130, 0.508256E6, 0.947700, ...
        0.0225000, 0.129000E6, 0.607175E-3, 2.20000E-2 ,...

```

```

44.097, 370 , 4.26E6, 44.097/0.1998; ...5
'i-Butane' , 'C4H10', 10.23264, 0.137544 , 0.849943E6, 1.93763, ...
0.0424352, 0.286010E6, 1.07408E-3, 3.4000E-2 , ...
100 58.124, 273+134.99, 3.648E6, 1.0/0.00452; ...6
'i-Butylene', 'C4H8', 8.95325, 0.116025 , 0.927280E6, 1.69270, ...
0.0348156, 0.274920E6, 0.910889E-3, 2.95945E-2 , ...
56.1063, 419.2, 4.020E6, 56.1063/0.2408; ...7
... - source: NIST chemistry webbook for 1-Butene
105 'n-Butane' , 'C4H10', 10.0847 , 0.124361 , 0.992830E6, 1.88231, ...
0.0399983, 0.316400E6, 1.10132E-3, 3.4000E-2 , ...
58.124, 425.2, 3.797E6, 58.124/0.2547; ...8
'i-Pentane' , 'C5H12', 12.7959 , 0.160053 , 1.74632E6 , 3.75620, ...
0.0668120, 0.695000E6, 1.70000E-3, 4.63000E-2 , ...
110 72.151, 273+187.28, 3.381E6, 1.0/0.004239; ...9
'n-Pentane' , 'C5H12', 12.1794 , 0.156751 , 2.12121E6 , 4.07480, ...
0.0668120, 0.824170E6, 1.81000E-3, 4.75000E-2 , ...
72.151, 273+196.50, 3.369E6, 1.0/0.004214; ...10
'n-Hexane' , 'C6H14', 14.4373 , 0.177813 , 3.31935E6 , 7.11671, ...
115 0.109313, 1.51276E6, 2.80186E-3, 6.66849E-2 , ...
86.178, 273+234.28, 3.012E6, 1.0/0.004295; ...11
'n-Heptane', 'C7H16', 17.5206 , 0.199005 , 4.74574E6 , 10.36475, ...
0.151954, 2.47000E6, 4.35611E-3, 9.00000E-2 , ...
100.205, 540.11, 2.736E6, 1.0/0.004314 ...12
120 };
% Unique are: 'n-Hexane', 'n-Pentane', 'i-Pentane',
% 'i-Butylene', 'i-Butane', and 'Propylene' when compared with BB_Eqn of
% state.
% REPEATED: 'CH4, C2H4, C2H6, C3H8, C4H10, C7H16
125 Ru = 0.08206; % atm liter/g-mol K

% Pull equation coefficients from the coefficient library
A0 = Coef{Substance_index,3};
130 B0 = Coef{Substance_index,4};
C0 = Coef{Substance_index,5};
a = Coef{Substance_index,6};
b = Coef{Substance_index,7};
c = Coef{Substance_index,8};
135 alph= Coef{Substance_index,9};
gamm= Coef{Substance_index,10};
MW = Coef{Substance_index,11};
rCrit = Coef{Substance_index,14};

%% Initialize solver and solve

140 cnt = 0; max_cnt = 250; err=1.0;
v0 = Ru*T/(P/101325); % initialize new_v with perfect gas law...
% B = B0*(1-b/v0);
P0 = Ru*T/v0 + (B0*Ru*T - A0 - C0/T^2)*(1/v0^2) ...
+ (b*Ru*T - a)*(1/v0^3) ...*(v0+B)
145 + a*alph/v0^6 ...
+ c/(v0^3*T^2)*(1+gamm/v0^2)*exp(-gamm/v0^2);
v1 =v0;%Rg*T/(P0);

```

```

C1 = Ru*T;
C2 = (B0*Ru*T - A0 - C0/T^2);
150 C3 = (b*Ru*T - a); %(v1+B)
C4 = a*alph;
C5 = c/T^2;

% Obtain an initial estimate of specific volume
155 P1 = C1/v1 + C2/v1^2 + C3/v1^3 ...*(v1+B)
      + C4/v0^6 ...
      + (C5/v1^3)*(1+gamm/v1^2)*exp(-gamm/v1^2);

dpdv = -(C1/v1^2 + 2*C2/v1^3 + 3*C3/v1^4 ...*(v1+B)
160      + 6*C4/v0^7 ...
      + (C5*exp(-gamm/v1^2)/v1^4)*( ...
      3*(1+gamm/v1^2)+2*gamm*( 1/v1^2 + (1+gamm/v1^2)/v1^2 ) ) );

v1 = v1+(P/101325-P1)/dpdv;
165      fprintf('P0: %9.4g , P1: %9.4g , dpdv: %9.4g \n',P0, P1,dpdv );

% Iterate until specific volume converges
while err >1E-6 && cnt < max_cnt;
170
      C1 = Ru*T;
      C2 = (B0*Ru*T - A0 - C0/T^2);
      C3 = (b*Ru*T - a); %(v1+B)
      C4 = a*alph;
175      C5 = c/T^2;

      P1 = C1/v1 + C2/v1^2 + C3/v1^3 ...*(v1+B)
          + C4/v0^6 ...
          + (C5/v1^3)*(1+gamm/v1^2)*exp(-gamm/v1^2);

180      dpdv = -(C1/v1^2 + 2*C2/v1^3 + 3*C3/v1^4 ...*(v1+B)
          + 6*C4/v0^7 ...
          + (C5*exp(-gamm/v1^2)/v1^4)*( ...
          3*(1+gamm/v1^2)+2*gamm*( 1/v1^2 + (1+gamm/v1^2)/v1^2 ) ) );
185      v2 = v1+(P/101325-P1)/dpdv;
      err = abs((P/101325-P1)/(P/101325));

      v1 = v2;    %;
      cnt = cnt+1;
190      fprintf('Iteration: %3d   Error: %9.4g   vnew: %9.4g\n', cnt, err, v2);
      fprintf('P_BWR: %9.3f   \n',P1 );
end

Z = v1/ v0;
195
density = (Mw/v1) ;% (liters/gmol)* ( (m^3/liter)/(kg/g * g/gmol) )

rho_reduced = density/rCrit;

```

```

200 % Need to update this for the BWR compressibility criteria!
    if rho_reduced > 0.8
        warning([' Use of the Beattie-Bridgemen compressibility correction'...
            'is out of bounds: Reduced density is greater than 0.8, '...
            'equation of state results for this calculation are inaccurate!'])
205 end
    end

```

2.2. Matlab Function mix_properties.m

The mix_properties function was written to allow two separate fluids to be combined. If temperature and pressure are not defined, the fuel and oxidizer must be fluid structures created using fully supported gases from the get_gas_props function. Formulae and data for calculating diffusion rates between gases was taken from Kuo (38), other formulae were taken from either Turns (108), Kuo (38), or Atkins (174) as noted. If no reference was made, the mixing rule was derived from mass averaging the properties.

```

function [ mix ] = mix_properties( fuel, oxdz, T_in, P_in)%, mix )
% mix_properties calculates properties for a gaseous binary mixture -
% presumed to be oxidizer and fuel.
% The input structures for fuel, oxidizer, and mixture are described
5 % below. Mass flow rates should be included for the fuel and oxidizer.
% Output is an updated mixture structure.
%
% INPUTS:
%   fuel.mdot - mass flow rate or mass within the volume kg/s or kg
%   fuel.MW - Molecular weight in mass units (or g/gmol)
10 %   fuel.mu - viscosity, N-s/m^2
%   fuel.FAR_stoich - stoichiometric fuel-to-air ratio, dimensionless
%   fuel.T - temperature, K
%   fuel.gamma - specific heat ratio (Cp/(Cp-R)), dimensionless
15 %
%   oxdz.mdot - mass flow rate or mass within the volume kg/s or kg
%   oxdz.MW - Molecular weight in mass units (or g/gmol)
%   oxdz.mu - viscosity, N-s/m^2
%   oxdz.T - temperature, K
20 %   oxdz.gamma - specific heat ratio (Cp/(Cp-R)), dimensionless
%
% OUTPUT:
%   mix.mdot - mass flow rate or mass within the volume kg/s or kg
%   mix.phi - Equivalence Ratio, dimensionless
25 %   mix.MW
%   mix.R
%   mix.mu

```

```

%      mix.gamma
%      mix.T
30 %      mix.a
%
% Programming:
%      By Ionio Andrus in support of efforts to model gas properties in
%      pursuio of a PHD Thesis at the Air Force Institute of Technology,
35 %      Wright Patterson AFB, Spring 2015
%
% Note: this routine has not been thoroughly error checked use at your own
% risk!
%
40 % Bibliography
%{

KUO05 - Kuo, Kenneth K., "Principles of Combustion, Second Edition",
      wiley 2005,
45 Lennard-Jones potential data found in Table A.19, page 681-682, and the
      Chapman and Enskog's Method to calculate diffusion found as
      equation A-204, p679.

TURNS99 - Turns, Stephen R. "An Introduction to Combustion: Concepts and
50 Applications", 1999, 2nd ed. New York (New York): McGraw Hill;

ATKINS08 - Atkins, Peter, Jones, Loretta, "Chemical Principles, Fourth
      Edition", W.H. Freeman and Co., 2008, Back Cover

55 %}
% Calculate mixture temperature as the according to...?

% Assigning temperature and pressure can cause some real issues. The
% specific heat (Cp) comes in the fuel structures as a function of
60 % temperature, so re-assigning the temperature without updating that
% quantity will produce error in the mixture CP, R, gamma, etc... and so
% on. Ideally we should call the get_gas_properties for the constituents
% to get their Cp at the correct Temperature, but we'd lose the the
% information regarding the mass flow rate...

65 if nargin < 3
    mix.T = (fuel.mdot*fuel.Cp*fuel.T + oxidz.mdot*oxidz.Cp*oxidz.T) ...
            /(fuel.mdot*fuel.Cp + oxidz.mdot*oxidz.Cp);

70 % Set the pressures equal oxidizer pressure
% ROOM FOR EXPANSION - CALCULATE THE PARTIAL PRESSURES OF CONSTITUENTS...
    if fuel.P ~= oxidz.P
        warning('Fuel and oxidizer pressures are unequal in mix_properties.
Mixture properties are incorrect')
75 %fuel.P = oxidz.P;
    end
    mix.P = oxidz.P;

else

```



```

80         mix.T = T_in;
           mix.P = P_in;
       end

       % compute total mass flow rate (or total mass in the volume) TURNS99
85   mix.mdot = fuel.mdot+oxdz.mdot;

       % ROOM FOR EXPANSION: Implement Oxidizer qty and Oxidization qty in
       % get_gas_props, then calc the FAR as part of the mixture...

90   % compute equivalence ratio - assumes that the FAR_stoich is correct
       % REF: TURNS99
       mix.phi = (fuel.mdot/oxdz.mdot)/fuel.FAR_stoich;

       % compute mixture molar averaged molecular weight - molar average
95   % REF: TURNS99
       mix.MW = (fuel.mdot+oxdz.mdot)...
           /( fuel.mdot/fuel.MW + oxdz.mdot/oxdz.MW);

       % EXPANSION: Inclusion of Tcrit, Pcrit, see KU005, eq A-124 & A-41
100
       % approximate gas constant R
       % REF: TURNS99
       mix.R = 8314.47/mix.MW; %R: J/kgK Ref: ATKINS08

105 % Mix the specific heats using the mass fraction-weighted method
       % REF KU005, p650, Eq A-85
       mix.Cp = (fuel.mdot*fuel.Cp + oxdz.mdot*oxdz.Cp)/(mix.mdot);

       % Calculate specific heat ratio based off of the Cp and R values of mixture
110 mix.gamma = mix.Cp/(mix.Cp-mix.R);

       % approximate viscosity% molar average
       mix.mu = (mix.mdot) ...
           /( fuel.mdot/fuel.mu + oxdz.mdot/oxdz.mu);
115

       %{
       if fuel.constituents == TRUE
           % molar average
120     fprintf('averaging of viscosity by consituents not yet implemented');

       else
           fuel.r_i = fuel.mdot*fuel.MW/mix.MW; % (partial volumetric flow rate)
           oxdz.r_i = oxdz.mdot*oxdz.MW/mix.MW; % (partial volumetric flow rate)
125
           mix.mu = (fuel.r_i*fuel.mu*sqrt(fuel.MW*fuel.T_crit) ...
               + oxdz.r_i*oxdz.mu*sqrt(oxdz.MW*oxdz.T_crit) )...
               /(fuel.r_i*sqrt(fuel.MW*fuel.T_crit) ...
               + oxdz.r_i*sqrt(oxdz.MW*oxdz.T_crit) );
130 end
       %}

```

```

% approximate thermal conductivity, k    Density, rho    thermal
% diffusivity, alpha ....etc
135
% approximate the speed of sound (if given a temperature...)
mix.a = sqrt(mix.gamma*mix.R*mix.T);

% Calculate density with ideal gas law...
140 mix.rho = mix.P/(mix.R*mix.T);

% ROOM FOR EXPANSION:
% -- calculating mixture viscosity is complicated, the simple formulat
% here is insufficient to accurately capture multi-component mixtures.
145 % Refer to KU005, pp 673, A-172 thru A-174, requires reduced temperatures
% for each of the components...
% Calculate mixture thermal conductivity with mass averaging...
mix.k = (fuel.mdot*fuel.k + oxdz.mdot*oxdz.k)/mix.mdot;

150 % Calculate thermal diffusivity from other mixtue properties.
mix.alpha = mix.k/(mix.rho*mix.Cp);

% Use Chapman-Enskog model to calculate duffusion constant of the two
155 % gases, REF: KU005 Table A.19, page 681-682,equation A-204, p679

% Compute MW_AB
AB = [0.0 0.0 0.0 0.0];% initialize variable AB
AB(4) = 2/(1/fuel.LJ(4) + 1/oxdz.LJ(4)); % Eqn A-202 p679
160

% compute \sigma_AB - collision cross-section
AB(2) = (fuel.LJ(2)+oxdz.LJ(2))/2;

% Compute \epsilon_AB - energies - note the implied division of k_B...
165 AB(3) = (fuel.LJ(3)*oxdz.LJ(3))^0.5;

% Compute T* - Characteristic temperature
T_star = mix.T/AB(3);

170 % compute \Omega_D - Collision Integral
Om_D = 1.06036/T_star^0.15610 + 0.19300/exp(0.47635*T_star) ...
      + 1.03587/exp(1.52996*T_star) + 1.76474/exp(3.89411*T_star);

% Compute D_AB - diffusivity with the simplified formula (A-204), won't
175 % give particularly accurate answer for H2, buecause it's so much smaller
% than air

mix.D = 0.00266*mix.T^1.5/(mix.P*AB(4)^0.5*AB(2)^2*Om_D);

180 % approximate LJ props% molar average REF: KU005 Table A.19, page 681-682, and the
% Chapman and Enskog's Method found as equation A-204, p679. - NEED TO
% VERIFY MIXING RULES>>>
LJ(1) = (mix.mdot) ...

```

```

        /( fuel.mdot/fuel.LJ(1) + oxdz.mdot/oxdz.LJ(1));
185    LJ(2) = (mix.mdot) ...
        /( fuel.mdot/fuel.LJ(2) + oxdz.mdot/oxdz.LJ(2));
    LJ(3) = (mix.mdot) ...
        /( fuel.mdot/fuel.LJ(3) + oxdz.mdot/oxdz.LJ(3));
    LJ(4) = mix.MW;
190    mix.LJ = LJ;

```

end

2.3. Matlab Function StabVelGrad.m

The StabVelGrad function calculates the boundary layer velocity gradient using the Blasius formulation found in Grumer et al. (30). A full description of the derivation and intermediary calculations is found in Chapter II, Section 6 and Appendix II, Section 3.

```

function [ velGrad ] = StabVelGrad( mdot, mu, epsilon, ht, wd , rho)
%StabVelGrad
% This function calculates the boundary layer velocity gradient for a
% mixture flowing through a rectangular channel.
5 % Inputs:
%   mix - structure containing mixture and channel properties
%       mdot - mass flow rate (kg/s)
%       mu - viscosity (N m/s)
%       epsilon -
10 %       ht - channel height (m)
%       wd - channel width (m)
%
%   Detailed explanation goes here

15 ReMix = mdot*2/(wd*mu); % Reynolds in Channl
    f_Darcy = Darcy_Weisbach_fric_factor( epsilon/ht, ReMix); % friction factor

    velGrad = f_Darcy*(mdot/rho)*ReMix/(16*pi*ht^3);

20 end

```

2.4. Matlab Function get_flame_props.m

The function get_flame_props returns the laminar flame speed, quenching distance, and reference conditions to allow an adjusted velocity gradient calculation to be

performed as outlined in Chapter II, section 3.3. Models for flame speeds and quenching distances are described in Appendix IV.

```

function [SL, dQ, SL_ref, dQ_ref, h_dQ, pcnt_vol] = ...
    get_flame_props( mix, fuel, oxdz, hexit )

% function get_gflame_props
% Author: Maj Ionio Q. Andrus in support of his PhD Dissertation
5 % This Matlab Function (v 2015b) is intended to calculate the flame speed
% and theoretical quenching distance for a mixture of fuel and oxidizer
% having the following properties (at a minimum)
%   mix.phi    -> Equivalence ratio
%   mix.P      -> mixture Pressure, Pa
10 %   mix.T     -> mixture Temperature, K
%   mix.alpha  -> mixture thermal diffusivity, w/mK
%   fuel.type  -> 'hydrogen' or 'ethylene'
%   fuel.MW    -> fuel molecular weight, atomic mass units
%   fuel.FAR_stoich -> stoichiometric fuel-to-air mass ratio
15 %   oxdz.MW   -> oxidizer molecular weight, atomic mass units
%   hexit      -> height of the channel through which mix is flowing, m
%
% Output: SL - modeled laminar flame speed, cm/s
%         dQ - modeled theoretical quenching distance, mm
20 %   SL_ref - laminar flame speed at 1 atm, 300K, cm/s
%   dQ_ref - theoretical quenching distance at 1atm, 300K, mm
%   h_dQ - ratio of slot height to theoretical quenching distance
%   pcnt_vol - percent fuel in mixture by volume

25
switch fuel.type
case{'H2'; 'hydrogen'; 'Hydrogen'}
    %   fprintf( 'H2 quenching:')
    pcnt_vol = 100*mix.phi ...
30         /(mix.phi+ (fuel.MW/oxidz.MW)/fuel.FAR_stoich);

    % =EXP(2.6378446-0.31739*N27+0.011698*N27^2...
    % -0.000186*N27^3+0.000001179*N27^4...
    % -2.143044*LOG10(R27)
    % -0.24292*(LOG10(R27))^2)
35     dQ = exp(2.826173 -0.342564*pcnt_vol +0.0127657*pcnt_vol^2 ...
        - 0.000205*pcnt_vol^3 + 0.0000012987*pcnt_vol^4 ...
        - 2.178311*log10(mix.P/101325)); % mm   expnnt = ;
    % =EXP(2.826173-0.342564*N27+0.0127657*N27^2
40     % -0.000205*N27^3+0.0000012987*N27^4
    % -2.178311*LOG10(R27))

    h_dQ = hexit*1000/dQ;

45     dQ_ref = exp(2.826173 -0.342564*pcnt_vol ...
        +0.0127657*pcnt_vol^2 - 0.000205*pcnt_vol^3 + ...
        0.0000012987*pcnt_vol^4 ...
        ); % mm   at 1 atm

```

```

50     SL = 0.0006272*(pcnt_vol)^4 - 0.1112*(pcnt_vol^3) ...
        + 6.713*pcnt_vol^2 - 157*pcnt_vol+1045.7+mix.T ...
        -22*log(mix.P/101325); %cm/s
    SL_ref = 0.0006272*(pcnt_vol)^4 - 0.1112*(pcnt_vol^3) ...
        + 6.713*pcnt_vol^2 - 157*pcnt_vol+1045.7+300; % cm/s
55
    case{'C2H4'; 'ethylene'; 'Ethylene'}
        % Constants for quenching distanc model (known data point)
        % REF Turns99
        % fprintf( 'C2H4 quenching:')
60        dqref= 1.3; %mm for reactants at @300k, 1atm
        alpha_SLref = (2.1290E-5)/64.0; %(w/mK) / (cm/s)
        pcnt_vol = mix.phi/(mix.phi+(fuel.MW/oxdz.MW)/fuel.FAR_stoich);

        SL = 47.711+259.86*(pcnt_vol)-47452.78*(pcnt_vol-0.07054)^2 ...
65        + 10245257*(pcnt_vol-0.07054)^4-24.767*log10(mix.P/101325);
            %cm/s

        dq = dqref*(mix.alpha/SL)/alpha_SLref; %mm
        h_dq = hexit*1000/dq;
70

        SL_ref =47.711+259.86*(pcnt_vol)-47452.78*(pcnt_vol-0.07054)^2 ...
        + 10245257*(pcnt_vol-0.07054)^4-24.767*log10(101325/101325);
            % cm/s

        oxdzREF = get_gas_props('air',300,101325);
75        fuelREF = get_gas_props('Ethylene',300,101325);
        oxdzREF.mdot = 1;
        fuelREF.mdot = fuelREF.FAR_stoich;
        mixREF = mix_properties(fuelREF,oxdzREF);
        dq_ref = dqref*(mixREF.alpha/SL_ref)/alpha_SLref; %mm
80

    case {'Ethane'; 'C2H6'; 'ethane'}
        pcnt_vol = mix.phi/(mix.phi+(fuel.MW/oxdz.MW)/fuel.FAR_stoich);
        SL = 0.0;
85        SL_ref = 0;

        dq = 0.1*(1.9486 -3.5677*mix.phi +1.6289*mix.phi^2 ...
            +0.1818*mix.P^(-0.901)); % mm
        dq_ref = 0.1*(1.9486 -3.5677*mix.phi +1.6289*mix.phi^2 ...
90        +0.1818*(101325)^(-0.901)); % mm
            % From an unpublished model see Predict_DQ_gft spreadsheet
            % No validation with data above 1 atm, errors at pressures
            % above and below 1 atm when equivalence ratio ~ 1.2 ...
            % gets bad pretty fast - only use as the roughest of guides
95        h_dq = hexit*1000/(dq);

    otherwise
        warning(['quenching distance for %s fuel is not '...
            'currently supported in RDE_PMI_read_TDMS_func'], ...
100        FlTyp );

```

```
105         dQ = 0; %mm
        h_dQ = 0;
        sL = 0;
        sL_ref = 0;
        dQ_ref = 0;
    end
```

Appendix VI Circumferential Variation in Wave Speed

1. Introduction

Integration of an RDE into an airbreathing engine presumes that the exhaust will be continuous and axially symmetric. However, variation in the circumferential wave speed was noted while reviewing the high speed video collected from the aft end of premixed RDE tests occurring in August, September, and October 2015. Variation in the detonation wave as it traversed the RDE was also noted in the banding of three sensor data by Russo (19, pp. 70-71) and the high speed video analysis of Shank (81, pp. 42-47; 63-67). Shank's analysis showed that the deceleration of the detonation wave was correlated with a port in the detonation channel but did not determine causality. He hypothesized that instrumentation and access ports presented physical obstacles that reflected shock waves within the detonation channel. This appendix captures additional analysis done using this premixed RDE, but does not reach any conclusions regarding causality, nor does it provide additional insights on how to mitigate the phenomenon. It does meet the intent of Objective 4 by providing characterization of the premixed RDE as it currently exists.

2. Methodology

Configuration of the detonation annulus changed slightly with each test; camera angle also changed. An image collected with the high speed video camera at approximately 0.089 s after the trigger for the test event on August 31, 2015 at 14:44:42 (hereafter referred to as test event 8) local time is shown in Figure A6.1. The camera was

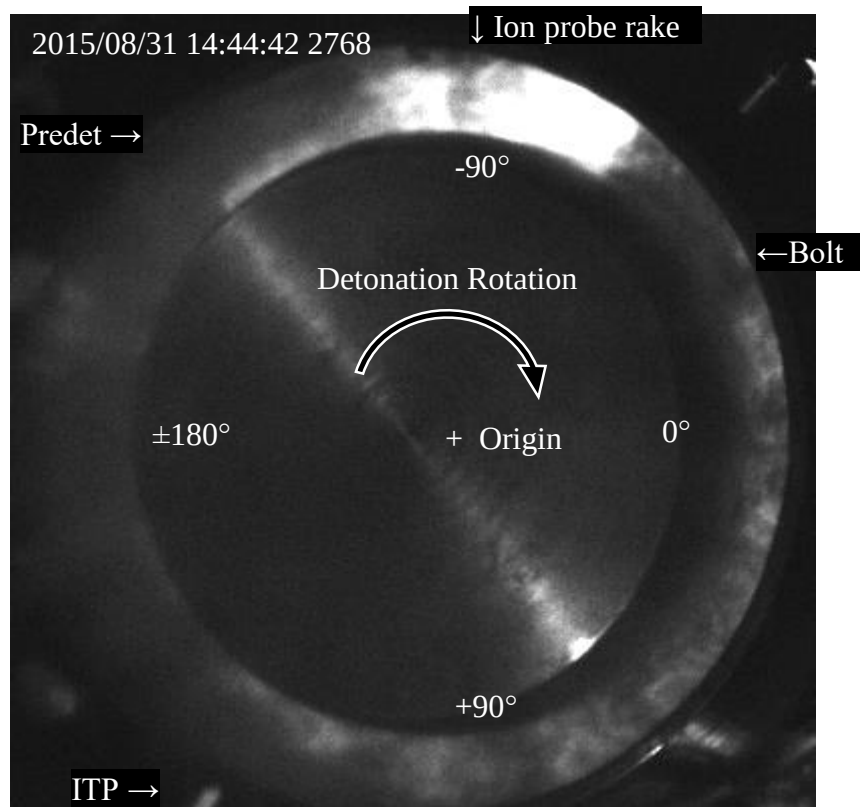


Figure A6.1 Diagram of the detonation channel annulus for varying wave speed investigation

situated about 18 degrees off-center, giving a shallow angle to the perspective view. The exit of the channel was bounded on the inside by the centerbody, which appears as an ellipse that fills the center of the image. The channel was bounded on the outside by the outerbody, which appears as a larger elliptical frame around the centerbody. The gray fog residing between these outerbody and inner body ellipses was chemiluminescence emitted from the reacting ethylene-air. The combustion had already transitioned to a detonation event, and the bright spot at the 1:00 position was the detonation wave moving in the clockwise direction, as noted with the circular arrow. The detonation propagated near the base of the annular channel, and measurements taken from the video were

defined by the coordinate system adjusted slightly to the right due to the perspective view of the camera.

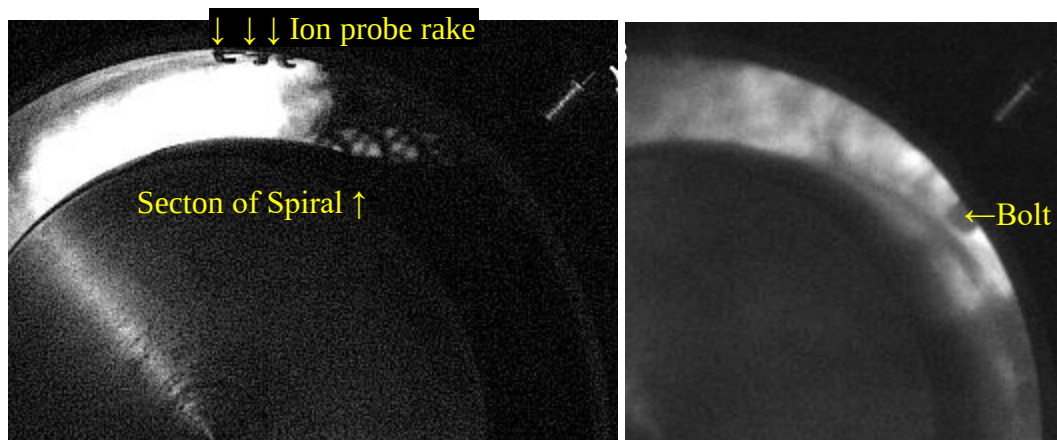


Figure A6.2 close-ups of the annulus channel showing the barb of the ion probes inserted into the channel (left) and the single 3/8-inch bolt inserted into the detonation channel (right)

Two lines of four threaded holes existed in the centerbody at the 12:00 and 2:00 positions and were intended as instrumentation ports. Into the set of holes at the 12:00 position, a single CTAP was inserted into the hole closest to the base of the channel and a set of three re-threaded automotive spark plugs was inserted to serve as ion probes in the remaining holes. Four bolts were threaded into the bolt holes at the 2:00 position to serve as either a large obstacle or simply a cap to the hole, as highlighted in Figure A6.2. The CTAP located in the port closest to the base of the detonation channel consisted of 2 m of 1.5 mm tubing mounted with an opening flush to the inner wall of the outerbody and capped with a pressure transducer. The ion probes were inserted so that the hook of the probe extended into the channel. Three of the four bolts were inserted so that they filled the hole and provided a flush wall. The fourth bolt was nearest the base (reactant injection point) of the channel and was inserted radially so that it extended approximately half-way across the channel, as shown in Figure A6.2. An ITP probe was connected to

the detonation channel at the 7:00 position and consisted of a 3 mm tube inserted so that the end was flush with the inside wall of the outerbody. A spiral that looked like a coil spring whose ends were connected to make a large circle was inserted at the bottom of the channel, as seen in Figure A6.3. The spiral did not have a uniform helix angle, so the spacing of the spring-coils varied. The location where the two ends were joined is shown



Figure A6.3 Photograph of the spiral inserted into the base of the detonation channel at the two o'clock position in the photograph and references to a 'spiral angle' indicate the location of this junction in the channel.

Wave speed measurements were made using two different methods to track the leading edge of the detonation wave as it propagated around the annulus. The first method tracked the leading edge of the detonation wave as it appeared in each frame using the Phantom Cv software (181). The leading edge locations were post-processed using Microsoft Excel to calculate angular wave speeds with a finite difference scheme. The finite difference calculated the angular location of the wave front in two frames relative to the center of the RDE, and the difference in angle was divided by the

difference in elapsed time between the frames. Angles were calculate using the ATAN2 function in Excel, using the user-selected origin and detonation wave position. When tracking the wavefront in individual frames, the wave front was identified by flipping between frames and identifying changes in intensity or chemiluminescence structure. Significant levels of chemiluminescence occasionally saturated the image in one region making tracking frame-to-frame difficult since intensity changes were difficult to identify in the region of saturation. Recognizing that this first method really involved looking for differences between frames, a slight modification was made to create a second method.

The best solution to tracking the changes between frames was to subtract one frame from another in a pair of adjacent frames. This subtraction method removed most of the persistent background noise and highlighted the significant changes in intensity from frame to frame. This second method calculated wave speed based on the angular velocities just as the first method, but locating the detonation wave front could be done with increased reliability.

Tracking the front of the wave avoided uncertainty in the wave speed that was induced in a centroid tracking scheme by eclipsing or changes in size of the chemiluminescing region. One drawback of the leading edge tracking was that the wave front was only visible for approximately 60 percent of the cycle, and location was inferred for the last portion of the cycle (from about the 7:00 position to the 10:00 position) from subtle changes in the uneclipsed portion of the channel. Inference of the location included looking for reflections off of the outerbody wall and illumination within the visible portion of the channel. In some cases, when the detonation wave was completely obscured, the wavefront movement was detected by locating the spatial

averaging of the chemiluminescent deflagration structures that occurred within a single exposure and was caused when the detonation wave forced significant movement of the fluid while the video shutter was open.

Error was introduced in the measurements by the user as well as the finite resolution of a video frame. The image was a small region of pixels. Based on the size of the image and the radius of the circle, there was a minimum angular resolution that could be achieved. Since the ratio of the pixel arc size to the radius was approximately 1:60, the angular uncertainty was estimated at 1/60, or about one degree. A much larger error was encountered by inconsistency of the user-selected leading edge. For each pixel of inconsistency, the user introduced 1 degree of uncertainty. Also, there was generally some interpretation of where the leading edge was, since the wave front does not generally take the form of a straight line extending across the annulus. Uncertainty due to selection of the wave front by the user was estimated at 7° on average. An ensemble of measurements was taken to mitigate the effects of user induced error in the wave speed measurements. All data shown in this appendix included at least 22 cycles per ensemble, while some utilized as many as 27 cycles. Using an ensemble average may obscure some of the detail on variation within a single lap of the detonation, but frame rates between 15 frames per cycle and 20 frames per cycle would only be able to identify cyclic trends on the order of 1/7th to 1/10th of the cycle if tracking were perfect.

3. Results and Discussion

The average velocity for multiple runs was computed as a function of azimuth angle for a minimum of 22 complete cycles of RDE operating on premixed ethylene-air. The combined data is shown in Figure A6.4, and a summary of results appears in Table

A6.1. The mass flow rate for these runs varied between 0.185 kg/s and 0.346 kg/s, with equivalence ratios between 0.977 and 1.50. The azimuth angle in Figure A6.4 refers to the angle in the detonation frame of reference and will be identical to that shown in Figure A6.1 for detonation waves propagating in a clockwise motion. The time component of the detonation wave movement moves from left to right in Figure A6.4 regardless of which direction it moves in the laboratory frame of reference.

The data of each line is an average of approximately 25 measurements within each 20 degree sector. In the legend there are several abbreviations which describe the data set from which the measurements were taken. The direction of wave movement is abbreviated as CW for clockwise and CCW for counter-clockwise movement in the video. A test identification number comes next, corresponding to the numbers found in Table A6.1. The position of the helical spiral joint (depicted in the 2 o'clock position of Figure A6.3) is noted by a clock position in the laboratory frame of reference, or the term

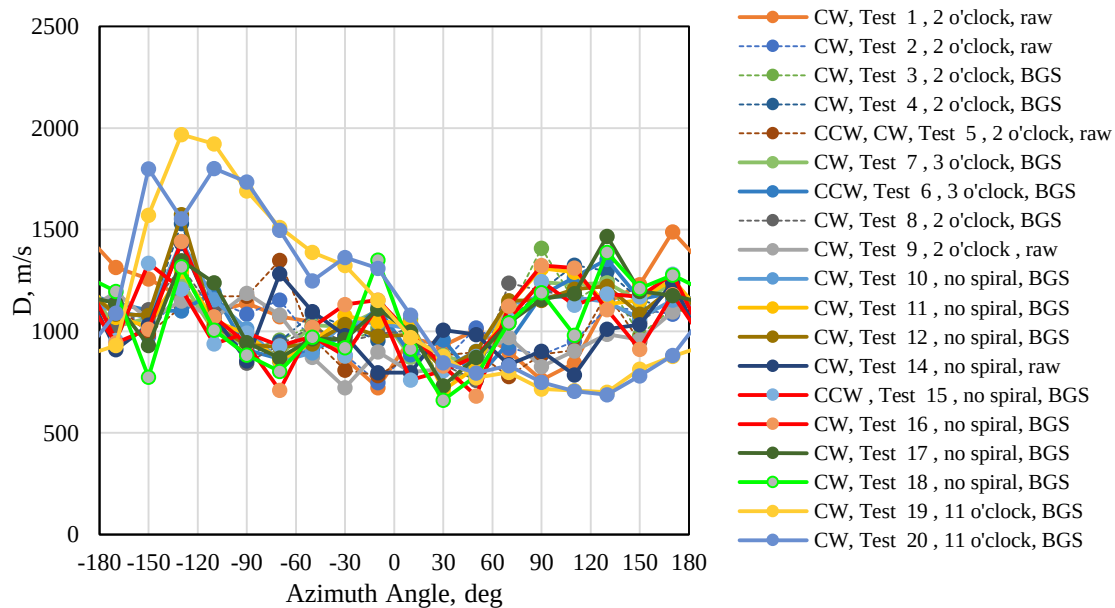


Figure A6.4 Discrete wave speed measurements as a function of azimuth angle measured for 20+ consecutive cycles during 20 separate tests

“no spiral” indicates that the spiral was removed from the channel. Finally, an indication of whether the single frame (raw) imagery, or a frame subtracted imagery (BGS) was used for tracking is included last.

A single cycle might have experienced large variations in wave speed at every azimuth. Three lines were selected from Figure A6.4 and plotted with the standard deviation of the measurements in Figure A6.5. The data sets from Test 8 and 16 were typical of the data from Tests 1 through 17, and while the mean of the data showed a definite trend, the standard deviation at each azimuth allowed a single horizontal line to be drawn through the entire data set. The data set from Test 19 followed a different trend and had a more repeatable cycle with significantly less variation as noted by the smaller error bars. The large standard deviation associated with the data in Tests 1 through 17 was attributed to the error selecting wave front measurements. The video was collected so that there were about 15 frames per cycle, and the detonation wave moved about 24°

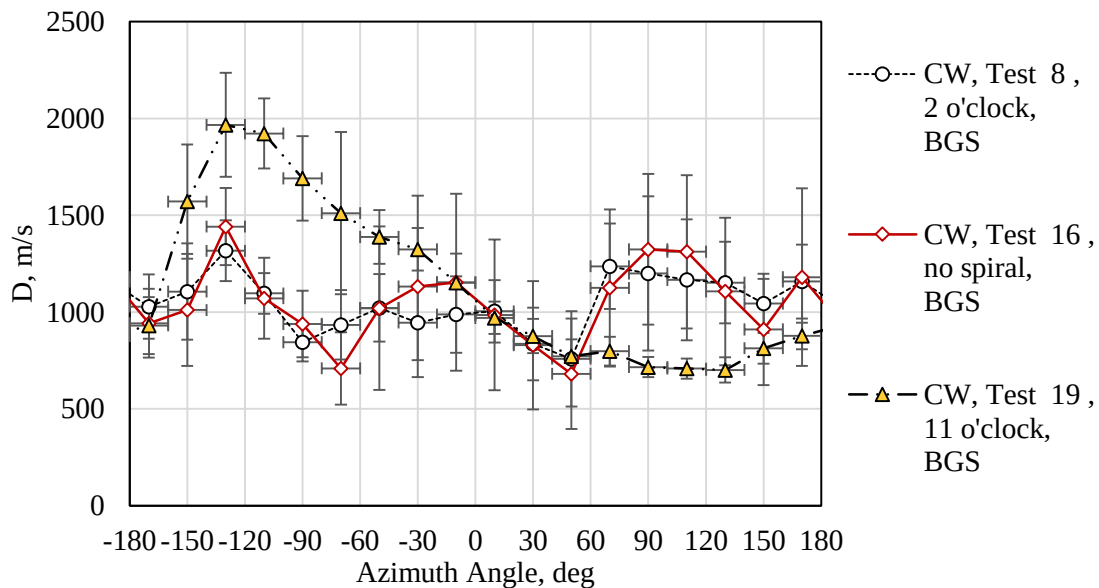


Figure A6.5 Three selected azimuth cycle wave speeds averaged over 25 cycles with standard deviations included

during each frame on average. As noted in the methodology section, each pixel of circumference translated to roughly 1° , and locating the wave front with 5 circumferential pixels of error produced a 20% error. Assuming the wave speed variation was consistent with each cycle, the time-averaged wave speed should average out the error in wave front location measurements. Wave front selection for tests 1 through 17 was inhibited by the angle at which the video was taken. A clear view of the detonation wave was only available in the two sectors between the 11 o'clock and 2 o'clock positions on the upper half of the video and between the 4 o'clock and 7 o'clock positions in the lower portion of the image. The data from tests 18 and 19 was collected after the camera was moved to a position that allowed a clear view of the detonation wave front for almost the entire cycle, and showed less variation at all phase angles.

The data set shown in Figure A6.4 was described in Table A6.1 and had several configuration variables, hereafter referred to as treatments, that affected the wave speed profile as a function of phase angle (or azimuth). Three wave speed profiles were identified in the premixed RDE data of Figure A6.4, and a fourth profile was found in the wave speed profile of a non-premixed RDE that will be discussed later. Each treatment will be discussed briefly with its impact on the wave speed profile.

Mass flow rate was varied between approximately 0.19 kg/s and 0.35 kg/s. Wave speed profiles were not seen to change between runs at the two different mass flow rates, and the A, B, and C profile shapes may all be seen in the 0.34 kg/s to 0.35 kg/s range.

Equivalence ratios were varied between 0.98 and 1.5. Although wave speed profile A was separable from B and C due to higher equivalence ratios, there was a more distinct separator for profile A: the method of tracking.

The tracking method using the single image without prior-image subtraction produced profile A. When the same set of data was tracked using prior-image subtraction, the wave shape cycle was of the type B or C. This represents variability and uncertainty associated with the wavefront tracking method and not variability in the detonation engine configuration.

Table A6.1 Summary of results and experimental treatments for the azimuthal wave speed review

Test Event	Results		Treatments							Mixing
	Cycle Shape	Wave Speed, m/s	Total Mass Flow, kg/s	Equiv. Ratio	Track Method	Spiral Or.	Bolt	Ion Probe	Direction	
1	A	1015±307	0.35±0.05	1.50±0.20	raw	2	1x45	3@90	CW	Pre
2	A	988±241	0.35±0.02	1.28±0.07	raw	2	1x45	3@90	CW	Pre
3	B	1028±247	0.34±0.06	1.17±0.21	BGS	2	1x45	3@90	CW	Pre
4	B	1059±408	0.32±0.04	1.27±0.17	BGS	2	1x45	3@90	CW	Pre
5	A	966±293	0.31±0.04	1.14±0.15	raw	2	1x45	3@90	CCW, CW	Pre
6	B	1041±364	0.31±0.04	1.14±0.15	BGS	3	1x45	3@90	CCW	Pre
7	B	1040±274	0.30±0.03	1.02±0.12	BGS	2	1x45	3@90	CW	Pre
8	B	1031±252	0.30±0.03	1.02±0.12	BGS	2	1x45	3@90	CW	Pre
9	A	955±283	0.30±0.04	1.05±0.14	raw	2		3@90	CW	Pre
10	B	1055±382	0.30±0.03	1.05±0.12	BGS			3@90	CW	Pre
11	B	1045±281	0.30±0.04	1.05±0.13	BGS			3@90	CW	Pre
12	B	1057±356	0.31±0.04	1.09±0.15	BGS			3@90	CW	Pre
13	A	985±317	0.19±0.03	1.35±0.18	raw			3@90	CW	Pre
14	B	1037±324	0.19±0.03	1.35±0.18	BGS			3@90	CCW	Pre
15	B	1032±434	0.19±0.03	1.35±0.18	BGS			3@90	CW	Pre
16	B	1046±275	0.19±0.03	1.22±0.18	BGS			3@90	CW	Pre
17	B	1010±449	0.19±0.03	0.98±0.14	BGS	11		3@90	CW	Pre
18	C	1024±406	0.35±0.03	0.98±0.09	BGS	11		3@90	CW	Pre
19	C	1043±472	0.34±0.05	1.02±0.14	BGS	11		3@90	CW	Pre
20	D	1006±145	0.65	0.98	BGS				CW	Non
21	D	989±184	0.64	0.96	BGS				CW	Non
22	D	906±170	0.79	0.97	BGS				CCW	Non

Spiral orientation effects could not clearly be separated, but both A and B wave forms were seen with the spiral oriented at the 2 o'clock position and with no spiral at all. Wave speed profiles B and C were noted with the spiral in the 11 o'clock positions. It is concluded that the spiral had no effect upon the wave speed profile since the wave speed shape remained the same with the spiral regardless of orientation and whether or not it was in use.

Similarly, the RDE produced the same wave speed profile whether or not the bolt at the 2 o'clock position was present. Also, there was no noticeable influence on the total cycle speed with the bolt treatment.

Within this data set, the ion probe treatment was changed simultaneously with the following factors: mixing scheme (moving from premixed to non-premixed), mass flow rate (< 0.35 kg/s to > 0.64 kg/s), outerbody material (steel with ports to seamless quartz), predetonator configuration (2 ports at 10 o'clock and 5 o'clock to single port from centerbody), and centerbody shape (convergent nozzle to no nozzle). Thus, the individual effect of the ion probe cannot be separated from all of the other effects that allowed a movement from the highly cyclic wave speed profiles of A, B, and C to the very uniform, only slightly varying profile D.

The direction of the detonation in the wave speed frame of reference was seen to have no effect on the wave speed profile. An important point to remember is that although the wave direction changed in the laboratory frame of reference, the wave speed was tracked in the wave frame of reference, where 0° azimuth was at the 3 o'clock position in the laboratory frame of reference, and the azimuth angle increased as the detonation wave moved away from that position, regardless of the direction of movement

in the laboratory frame of reference. This would indicate that none of the physical protrusions, gaps, or cavities had any influence on the wave speed profile. If the explanation for the variation in wave speed profiles were tied to the geometry, it must have existed at the 0 or 180 azimuth locations that were common in the laboratory frame of reference for the different wave directions. One possible explanation is the presence of a local variation in fuel, oxidizer, or total mass flow rate at those locations. Another possible explanation is that the variation is an artifact of the video tracking that cannot accurately track the detonation wave front when the wave front is eclipsed by the sidewalls of the detonation channel.

Wavespeed profile C was only noted in Table A6.1 for test events 18 and 19, which occurred on a separate day, and from a different angle, than the events 1 through 17. The camera angle for test events 18 and 19 had a better view with less eclipsing of the detonation channel, and the detonation wave was easily tracked for most of the cycle. The larger variation across the cycle and the smaller variation at each angle in the cycle strongly suggest that the overall variation within the cycle is a real phenomenon. As such, the simple explanation of cycle variation being an artifact of a camera angle that eclipses the detonation wave is rejected.

Additional testing of the influence of the physical treatments could be done by removing them from the detonation channel, leaving only a smooth wall in their location. If local slow spots continue to occur, then it could be assumed that the physical discontinuities were the source of the wave speed variation. Replacing the steel outerbody with a smooth quartz outerbody would be a very simple way to do this. If the variation in wave speed continues to exist, and is correlated to the physical geometry,

then the irregularities of the channel wall could be eliminated as the root cause.

Fortunately, video data does exist of an ethylene-air RDE configured with a quartz outerbody, operating without premixing, and collected in a similar fashion as for the non-premixed RDE. The non-premixed quartz outerbody operating results are reported as test events 20 through 22.

Overhead imagery collected by Cho et al. (82) provided an opportunity to evaluate circumferential wave speeds in a clean channel. He configured the RDE with a quartz outerbody so that there were protrusions or holes in the detonation channel due to sensors or initiator. The imagery of this detonation in Figure A6.6 shows three chemiluminescent waves, one detonation wave rotating clockwise, and two acoustic waves rotating counter-clockwise. This smooth channel had nothing to reflect the detonation wave. Figure A6.7 shows the evaluated wave speeds to be very repeatable when averaged over 23 cycles of the 2003 Hz detonation. Figure A6.7 shows the wave speed for the detonation wave and the counter-rotating acoustic waves. The error bars in

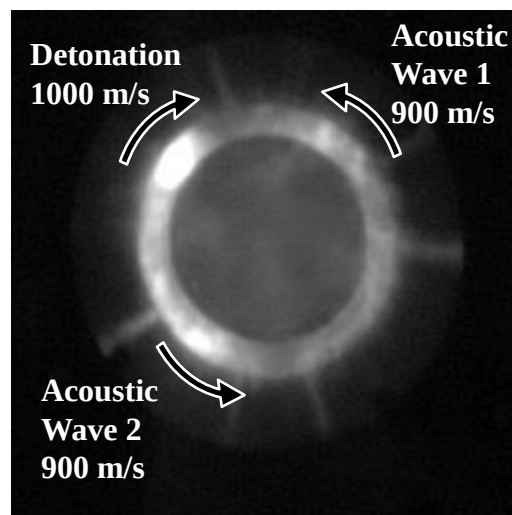


Figure A6.6 View of the detonation annulus showing a 1000 m/s detonation wave at the 11 o'clock position and two acoustic waves moving in the opposite direction at 900 m/s and located at the 1 o'clock and 7 o'clock positions

both plots represent one standard deviation of the wave speed measurement. The detonation wave speed has correlations to both the geometry of the channel and the acoustic waves. The normalized power spectral density of the detonation wave speed variation from Figure A6.7 (a) is shown in Figure A6.8 (a). The frequency spike at 2000 Hz matches the laboratory frame of reference wave speed of 2003 Hz and is therefore a variation once per cycle in the laboratory frame of reference. This variation is relatively small and may be noted in Figure A6.7 (a) as a slight variation of the mean wave speed. The wave speed profiles of Figure A6.7 are referred to as cycle shape D, and the detonation is test event 20 in Table A6.1. The slight variation in the average wave speed is unlikely to be due to a camera that was slightly off-center, but no effort was made to correct for the elliptical wave path in the camera field of view. The spike at 4000 Hz is a

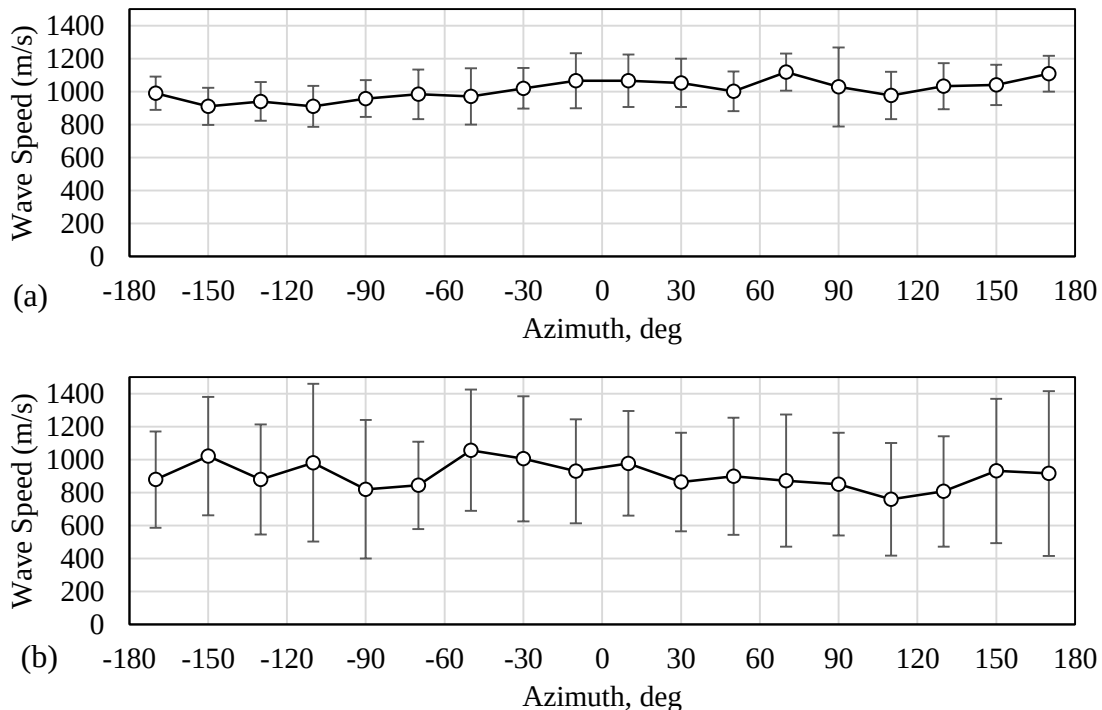


Figure A6.7 Azimuth wave speeds for (a) clockwise detonation and (b) counter clockwise acoustic waves averaged over 23 detonation cycles from an ethylene-air detonation in an RDE configured with a quartz outer body, 0.65 kg/s total mass flow, and $\phi = 0.98$

second harmonic of the detonation wave indicating a subtle change in velocity twice per cycle. The spike at 7600 Hz results from the double acoustic wave modulating the detonation wave approximately 4 times per cycle. The acoustic wave speed was tracked and plotted in Figure A6.7 (b), and the spectral decomposition of the variance is shown in Figure A6.8 (b). The acoustic wave was moving slower, at approximately 900 m/s. The spectral decomposition of the acoustic wave speed again shows a modulation associated with the cycle as indicated by the peak at 1800 Hz. The primary peak at 3800 Hz denotes the modulation of the acoustic wave by the counter-rotating detonation wave and provides the same information as the 7600 Hz wave which appears in both Figure A6.8 (a) and (b). This modulation of the acoustic wave speeds by the detonation wave speed is

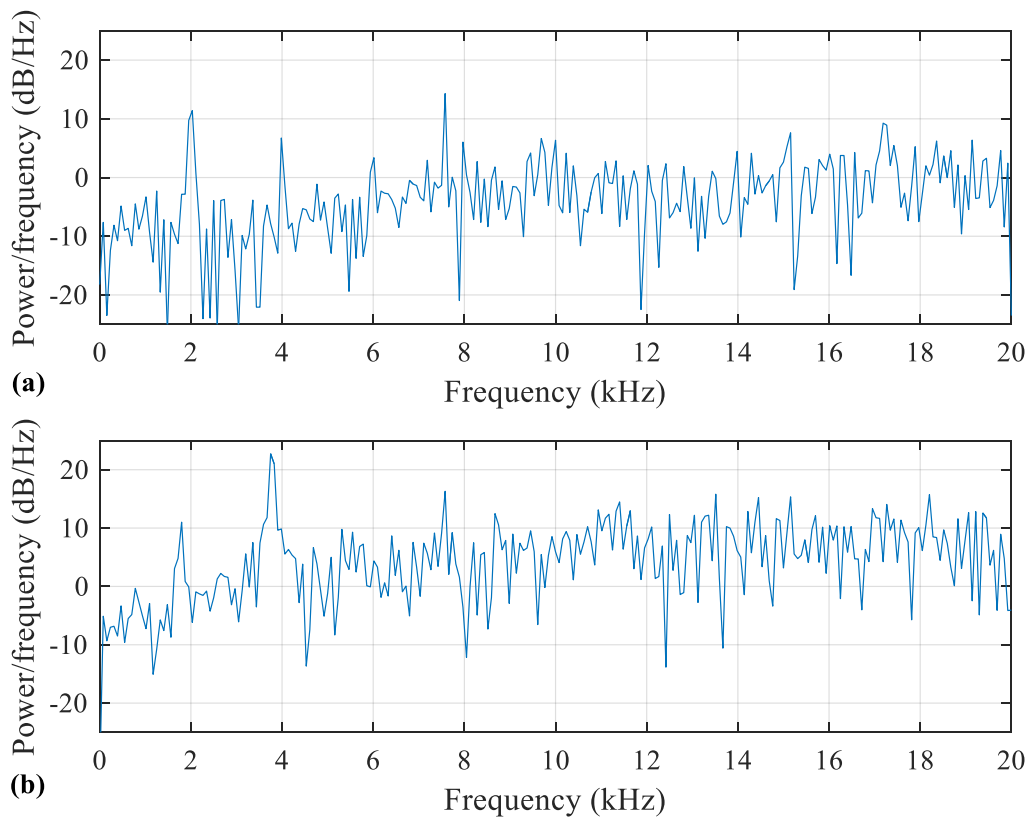


Figure A6.8 Periodogram of the variation of the (a) detonation wave speed and (b) counter rotating acoustic waves with time for an ethylene-air detonation in an RDE configured with a quartz outer body, 0.65 kg/s total mass flow, and $\phi = 0.98$

due to more than just difficulty in tracking the independent waves as they pass each other. After each encounter, the acoustic waves travel noticeably less than just before the wave hits. This may be in part to circumferential swirl induced in the detonation zone of the RDE as the hot combustion gases trailing the detonation wave expand. Taken as a whole, the analysis indicates that the detonation wave is modulated first by some effect tied to the geometry of the channel, and second by the interaction of other waves present in the channel.

The final finding from this test event is that the circumferential variation is greatly minimized with the non-premixed RDE configured with the smooth walled outerbody. This finding does not provide a conclusive indication of where the wave speed variability originates since mixing methodology, total mass flow rate, and channel configuration were all changed simultaneously.

4. Conclusion

Wave speeds vary within the detonation channel as tracked by the chemiluminescence associated with the detonation wave. Errors associated with locating the detonation front relative to the chemiluminescence can cause issues with accurately tracking the variation, but ensemble removes some of the uncertainty. Numerous high speed videos were reviewed to ascertain if the cyclic variation was caused by a particular physical configuration or flow conditions. A steady wave speed profile was measured in a non-premixed ethylene-air RDE operating at an equivalence ratio near one and mass flow rates between 0.65 kg/s and 0.79 kg/s. The changes between the remaining runs with high variance in the azimuth-averaged wave speeds were 1) non-premixed, 2) higher total mass flow rates, and 3) a smooth walled detonation channel configuration. There is

insufficient information in this data set to clearly separate the influence each experimental treatment had upon the wave speed variation. Wave speeds were seen to vary in all configurations, and both detonation and acoustic waves were seen to modulate the other's wave speed in the laboratory frame of reference.

5. Recommendations

The finite difference method used for most of the wavefront tracking was fairly noisy. Future work should consider using a different method that re-samples the individual observations over two or three frames so that wave speed estimates with lower noise can be obtained. Also, future work should use mirrors, if necessary, to obtain imagery that does not eclipse the detonation wave front. A simple clocking scheme of the outerbody could further separate the influence of any irregularities associated with the detonation channel. A final effort might be to intentionally cause one portion of the flow to be richer or leaner to see if that affects wave speeds.

List of Symbols

<u>Symbol</u>	<u>Description</u>
A	Area
a	Length of the major axis of a rectangle
a	Speed of sound in a gas
a	Mass fraction of air in a combustible mixture
atm	atmospheres
b	Constant fuel-specific correction factor for thermal quenching theory
b	Narrow dimension of the cross section of a rectangular channel
B	Material type of Brass
$c_1, c_2, \dots c_n$	Constant coefficients
c_f	Fanning friction factor
C	Phase angle matrix
C_D	Discharge coefficient
C-C	Bicarbon or Ethenediylidene
CH	Methylidyne
CJ	Chapman-Jouguet
cm	Centimeters
CN	Cyano radical
CO ₂	Carbon dioxide
c_p	Specific heat at constant pressure
C_p	Calibration offset uncertainty for a pressure transducer
C_T	Calibration offset uncertainty for a thermocouple
d	distance between two plates (or diameter for tubes)
d_c	Critical minimum diameter for sustained multi-headed detonation in a tube
d^*	Minimum limiting diameter for single-headed spin detonation in a tube
$\mathcal{D}$	Molecular diffusivity
D	Detonation Wave Speed
D_{CEA}	Detonation Wave Speed calculated using NASA's CEA code
D_{CJ}	Chapman-Jouguet calculated detonation wave speed
D_h	Hydraulic diameter
d_Q	Theoretical quenching distance
d_{QB}	Quenching distance at blowoff for a combustible mixture
d_{QF}	Quenching distance at flashback for a combustible mixture
$d_{Q_{obs}}$	Quenching distance calculated using observed or experimental temperature and pressure of a combustible mixture

$d_{Q_{ref}}$	Quenching distance at reference temperature and pressure of a combustible mixture
d_{RDE}	Mean diameter of an RDE detonation annulus
dT	<i>Differential change in temperature</i>
$\partial u / \partial y$	Gradient of a flow velocity profile orthogonal to the flow direction
dx	Differential change in distance along the primary axis
$E_{initiation}$	Minimum initiation energy for a detonation
F	Darcy friction factor
F	Frequency
f	Fuel mass fraction
$\left(\frac{f}{o}\right)$	Fuel-to-oxidizer mass fraction
$\left(\frac{f}{o}\right)_{stoich}$	Fuel-to-oxidizer mass fraction at stoichiometric conditions
F	Individual video Frame
ft	feet
fps	Frames per second
g	Area normalized mass flow rate (used in Russian RDE literature)
g	Critical wall boundary layer velocity gradient
g_b	Critical wall boundary layer velocity gradient in a combustible mixture (e.g. maximum to avoid blow-off)
g_c	Critical wall boundary layer velocity gradient in a combustible mixture
g_f	Critical wall boundary layer velocity gradient in a combustible mixture (e.g. where flashback is likely to occur)
g_{fex}	Experimentally observed wall boundary layer velocity gradient
Ga	Gauge
g-mol	Gram-mole
h	Slot height
Δh_c	enthalpy of combustion
h_i°	Enthalpy of formation at state i
h_r	Reactant refill height in an operating RDE
H_o	Null hypothesis
H_a	Alternate hypothesis
Hz	Hertz
in	Inch
I_{sp}	Specific Impulse
k	Thermal conductivity
K	Degrees Kelvin
K_a	Pre-exponential factor for a chemical reaction rate

kg	kilogram
kHz	Kilo Hertz
L	Length of a laminar flame passing along a wall
Le	Lewis number, ratio of thermal diffusivity to molecular diffusivity
l	Slot length
lbm	Pound mass
Le	Lewis number
m	meters
$\overline{\dot{m}}'''_F$	reaction rate in a combustng gas mixture
$\dot{m}$	Mass flow rate
M	Mach number
M_{pl}	Mach number of the reactants flowing through the feed plenum
MHz	Mega Hertz
mm	millimeters
ms	milliseconds
mV	milli Volts
n	Exponential constant of experimental flame speed variation with temperature
n	Integer number of detonation waves
N_2	Nitrogen
o	Oxidizer mass fraction
OH	Hydroxyl radical
nm	Nanometers
p_i	Pressure at location i
P	Static pressure
P_{amb}	Ambient pressure
P_0	Stagnation pressure
psi	Pounds per square inch
q	Thermal heat release
Q	Material type of Quartz
$\dot{Q}'''$	Heat generation within the volume V of the flame front
$\dot{Q}_{cond}$	Heat conducted from the burning gas by a conductive wall
r	radius
R	Specific gas constant
R_f	Fuel specific gas constant
R_o	Oxidizer specific gas constant
R_u	Universal gas constant
R^2	Coefficient of Determination
rad	Radians, ratio of arc length to radius

Re	Reynold's Number, ratio of momentum forces to viscous forces
RGB	Red-Green-Blue, generally a vector space to define visible color
s	Second
s_i	Enthalpy at state i
S	Sparse phase angle and video frame segment matrix
S	Material type metal (generally steel)
S	Combustion reaction speed
S_L	Laminar flame speed
S_{Lref}	Laminar flame speed of a combustible mixture at the reference temperature and pressure
S_{obs}	Observed combustion reaction speed
S_T	Turbulent combustion reaction speed
S_u	Combustion reaction wave speed relative to the unburned gases
sec	Seconds
T	Temperature
t_b	Time during an RDE cycle that the feed system pushes combustion products from flashback into the channel
T_b	Temperature of the burned gases
t_c	Time within an RDE cycle that detonation is combusting reactants
t_{cycle}	Time for one RDE cycle to complete
t_{ind}	Time during an RDE cycle that reactants are being inducted to the reaction front
t_r	Time during an RDE cycle that the feed system refreshes reactants
T_o	Total temperature
t_q	Time during an RDE cycle that the feed system quenches flashback
T_u	Temperature in the un-burned gases
u	Velocity in the direction of the primary axis of a flow
u_{av}	Average velocity in the direction of the primary axis of a flow
$\bar{u}_{pl}$	Bulk velocity of flow in a plenum
v	Vibrational level of an energy state
V	Volume
V	Video frame matrix
$\dot{V}$	Volumetric flow rate
V_{CJ}	Chapman-Jouguet detonation velocity
V_{T_0}	Thermocouple voltage signal
W	Watts
w	Slot width
x	Horizontal distance
x_D	Horizontal location of the detonation wave front

x_c	Horizontal location of a cylinder's main axis
z	Mass fraction of oxygen
α	Thermal diffusivity
β_0	Linear model intercept coefficient
β_1	Linear model slope coefficient
Δ	Finite difference
Δ	Measurement uncertainty
ϵ	Ratio of surface roughness to pipe diameter
ϵ_a	Activation energy
ϕ	Mass fuel-to-air equivalence ratio
ϕ	Elevation angle
ϕ^*	Adjusted fuel-to-air equivalence ratio
γ	Ratio of specific heats
δ	Laminar flame thickness
λ	Detonation cell width
μ	Dynamic viscosity
μm	Micrometers
μs	Microseconds
ν	Molar fraction of a component gas
π	Ratio of the diameter of a circle to its circumference
ψ	Lateral expansion angle of a con-annular segment
ρ	Density
ρ_i	Density at location i
ρ_u	Density of unburned gases
σ	Standard deviation
θ	Azimuthal angle between two vectors
τ_w	Wall shear stress
τ_r	Ratio of RDE reactant refill time to total cycle time
v	Measurement uncertainty
ξ_p	Pixel to distance conversion factor

List of Acronyms

AF	Air Force
AFB	Air Force Base
AFIT	Air Force Institute of Technology
AFRL	Air Force Research Laboratory

AFIT	Air Force Institute of Technology
CA	California
CCW	Counter clockwise
CEA	Chemical Equilibrium Analysis, a NASA computational program
CFD	Computational Fluid Dynamics
CJ	Chapman-Jouguet
CTAP	Capillary Tube Attenuated Pressure
CW	Clockwise
DDT	Detonation to Deflagration Transition
DERF	Detonation Engine Research Facility
DLL	Dynamically Linked Library, an executable computer code
EELV	Evolved Expendable Launch Vehicle
ITP	Infinite Tube Pressure
JP	Jet Propellant
NACA	National Advisory Committee for Aeronautics
NASA	National Air and Space Administration
NIST	National Institute of Standards and Technology
NPS	Naval Postgraduate School
NRL	Naval Research Laboratory
PDE	Pulsed Detonation Engine
PLIF	Planar Laser Induced Fluorescence
RDE	Rotating Detonation Engine
RQTC	Combustion Branch, Turbine Engines Division, Aerospace Systems Directorate
USAF	United States Air Force
ZND	Zel'dovich, von Neumann, and Döring

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Vita

Major Ionio Q. Andrus received his Bachelor of Science degree from Utah State University in December of 2002. While earning his undergraduate degree he worked as a student researcher for Dr. Tom Wilkerson at the Space Dynamics Laboratory where he was able to co-author several conference papers discussing wind speed and direction measurements collected from conically scanned lidar.

Major Andrus was commissioned through Detachment 860 AFROTC at Utah State University. His first assignment was to the National Air and Space Intelligence Center located at Wright-Patterson AFB. He provided engineering analysis on several foreign threat aircraft systems.

In August of 2005 he began Master's studies at the Graduate School of Engineering and Management, Air Force Institute of Technology. His research used the National Propulsion Simulation Software (NPSS) to model a pulsed detonation combustor, which was then used to compare the theoretical combustor embedded in a high-bypass turbofan to the current technology.

After graduation, he was assigned to work with the Airborne Laser (ABL) Combined Test Force (CTF), representing the 412th Test Wing Engineering group at Edwards AFB, CA. During his time at the ABL CTF, the Airborne Laser team successfully demonstrated tracking, beam compensation, High Energy Laser Installation, and Lethality Demonstration. He was able to co-author a results paper that was presented at the Directed Energy Professional Society in 2011.

Major Andrus was next assigned to work in the Program Management division of the Evolved Expendable Launch Vehicle (EELV) program office. His duties included

management of a small portfolio of research and development projects for the ongoing EELV program, which included the EELV Secondary Payload Adapter, ULA Dual Launch initiative, and implementation of additively manufactured parts.

In 2013, Major Andrus was re-assigned to AFIT to pursue a PhD in aeronautical engineering. His research has returned to detonation engines, focusing this time on experimental work with rotating detonation engines. He has successfully demonstrated a feed system for injecting premixed fuel and oxidizer into a detonation channel and is projected to graduate in the summer of 2016.

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14. ABSTRACT Desire for a more efficient air breathing engine has shifted research attention to the Rotating Detonation Engine (RDE). Detonation is a more efficient combustion process than deflagration and provides a pressure gain. The RDE detonation cycle occurs in a compact volume to produce a high specific impulse engine. Computational fluid dynamic (CFD) models predict comparable specific impulse and faster detonation wave speeds than measured in experimental RDE. The CFD models frequently assume premixed reactants to facilitate computation. A premixed experimental RDE was designed, constructed, and operated to test if premixing fuel and oxidizer caused the discrepancy between computational and experimental results. The premixed RDE required a feed system that simultaneously arrested flashback and fed the detonation. Flashback arresting feed designs were explored with single injector tests. Application of modified flame quenching and burner stability theories produced in a feed system design with feed slots 2.5 cm long by 0.5 mm high. With an ethylene and air mixture, the premixed RDE operated in a narrower band of equivalence ratios than non-premixed RDE. Chemiluminescence suggest that premixing without modeling deflagration caused CFD wave speeds to be faster than experimental results. Future CFD studies should assume unmixed reactants and model injection geometry.					
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