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High-Pressure LPRE Combustion Dynamics: Low-Cost Computation and Stochastic Analysis

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14. ABSTRACT The work has focused on improvements for modeling, descriptions, and understanding for liquid-propellant-rocket-engines (LPRE) with regard to turbulent combustion dynamics and instability, chaotic description, and improved sub-grid closure for reduced-order models. For the combustion dynamics, the use of the flamelet model for closure continues and has been extended to our three-dimensional code, saving computational resources compared to chemical kinetic modeling and better representing the sub-grid multi-physics by including sub-grid mixing with the chemistry. Deep learning neural networks (NN) have been used to represent the flamelet closure model and replace the look-up table, which is more costly in memory requirements and less accurate in interpolation. Successful modeling of the Continuously Variable Resonant Combustor (CVRC) combustion chamber for both initial transient behavior and the asymptotic dynamic equilibrium with near-constant amplitudes has been achieved. Optimization studies determine the number of deep NN layers, number of neurons per layer, and the use of separate NNs modeling each of the desired output variables. The training of the NN has been optimized by focusing on the most important parameter domains. Three-dimensional combustion instability has been examined in several multi injector engine configurations with 10-, 19-, 30-, and 82-injectors. Both one-step kinetics and the flamelet model have been used and compared. Some agreement with the Rocketdyne experimental results by Jensen et al. [16] is found. Both premixed and non-premixed flame structures are predicted through the combustor. Three-dimensional results show the determination of the dominant mode of oscillation is very sensitive to parameter choice. Accordingly, chaotic behavior can result in self-initiated change of the dominant instability mode occurring in an alternating fashion. The Flamelet Progress Variable subgrid model has been applied to our multi-injector computations. Results are compared to the more costly calculations where chemical kinetics are applied directly to the resolved CFD scale. While the existing flamelet theory is used in our CFD modeling, successful efforts have addressed improvements in the model through a greater inclusion of relevant physics. The theory has been extended to account for three-dimensional configurations that are multi-branched with both non-premixed and premixed flame structures. The effects of shear-strain rate and associated vorticity has been determined to be very important with critical interactions involving variable density, three-dimensional character and the centrifugal effect due to vorticity. The premixed-flame character need not follow classical behavior when the premixed flame exists with the nearby non-premixed flame. Heat diffusion from the non-premixed flame can be a controlling factor for the premixed-flame burning rate. The longer-term plan is to apply these new multi-physics flamelet models using NN directly without creating new lookup tables.			
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High-Pressure LPRE Combustion Dynamics:

Low-cost Computation and Stochastic Analysis

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Summary

The work has focused on improvements for modeling, descriptions, and understanding for liquid-propellant-rocket-engines (LPRE) with regard to turbulent combustion dynamics and instability, chaotic description, and improved sub-grid closure for reduced-order models. For the combustion dynamics, the use of the flamelet model for closure continues and has been extended to our three-dimensional code, saving computational resources compared to chemical kinetic modeling and better representing the sub-grid multi-physics by including sub-grid mixing with the chemistry.

Deep learning neural networks (NN) have been used to represent the flamelet closure model and replace the look-up table, which is more costly in memory requirements and less accurate in interpolation. Successful modeling of the Continuously Variable Resonant Combustor (CVRC) combustion chamber for both initial transient behavior and the asymptotic dynamic equilibrium with near-constant amplitudes has been achieved. Optimization studies determine the number of deep NN layers, number of neurons per layer, and the use of separate NNs modeling each of the desired output variables. The training of the NN has been optimized by focusing on the most important parameter domains.

Three-dimensional combustion instability has been examined in several multi-injector engine configurations with 10-, 19-, 30-, and 82-injectors. Both one-step kinetics and the flamelet model have been used and compared. Some agreement with the Rocketdyne experimental results by Jensen et al. [16] is found. Both premixed and non-premixed flame structures are predicted through the combustor. Three-dimensional results show the determination of the dominant mode of oscillation is very sensitive to parameter choice. Accordingly, chaotic behavior can result in self-initiated change of the dominant instability mode occurring in an alternating fashion. The Flamelet Progress Variable subgrid model has been applied to our multi-injector computations. Results are compared to the more costly calculations where chemical kinetics are applied directly to the resolved CFD scale.

While the existing flamelet theory is used in our CFD modeling, successful efforts have addressed improvements in the model through a greater inclusion of relevant physics. The theory has been extended to account for three-dimensional configurations that are multi-branched with both non-premixed and premixed flame structures. The effects of shear-strain rate and associated vorticity has been determined to be very important with critical interactions involving variable density, three-dimensional character and the centrifugal effect due to vorticity. The premixed-flame character need not follow classical behavior when the premixed flame exists with the nearby non-premixed flame. Heat diffusion from the non-premixed flame can be a controlling factor for the premixed-flame burning rate. The longer-term plan is to apply these new multi-physics flamelet models using NN directly without creating new look-up tables.

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List of Addenda

Addendum I: Z. Shadram, T. M. Nguyen, A. Sideris, and W. A. Sirignano, "Physics-aware Neural Network Flame Closure for Combustion Instability Modeling in a Single-Injector Engine," *Combustion & Flame* 240, 2022. <https://arxiv.org/abs/2108.05415>

Addendum II: J. Xiong, F. Liu, and W. A. Sirignano, "Combustion Dynamics Simulation of an 82-injector Rocket Engine", *AIAA Journal*, in press, 2022.

Addendum III: L. Zhan, T. Nguyen, J. Xiong, F. Liu, and W. A. Sirignano, "Triggered Tangential Instability of a Multi-Injector Rocket Engine Using the Flamelet Progress Variable Model," Internal Technical Report, an early stage of journal paper preparation.

Addendum IV: W. A. Sirignano, "Three-dimensional, Rotational Flamelet Closure Model with Two-way Coupling", invited revision, *Journal of Fluid Mechanics*, 2022.
<https://arxiv.org/abs/2111.11365>

Addendum V: W. A. Sirignano, "Inward Swirling Flamelet Model", submitted for journal review, 2022. arXiv:2203.06284, 2022 - arxiv.org

1. Introduction

The aims of our research are to improve analysis at various levels of fidelity and understanding of liquid-propellant rocket engine (LPRE) combustion instability and turbulent combustion dynamics and to identify methods for improved performance and stable operation. We attempt to reduce computational costs and increase accuracy of models, while gaining physical insight to the combustion dynamics, including the resonant and potentially destructive nonlinear acoustic oscillations.

Our work has covered three areas: (1) use of deep learning neural networks to present sub-grid flamelet models in large-eddy simulations (LES); (2) multi-dimensional, unsteady analysis of combustion dynamics and combustion instabilities, spontaneous and triggered, in multi-injector liquid-propellant rocket engines; and (3) development of superior flamelet models for future use in LES computations. More details on these topics will be presented in Sections 2, 3, and 4, as well as in the five papers and internal reports attached as Addenda in this Final Report. Substantial detail has been provided as Addenda to three prior Annual Reports.

The style here is to provide in summary fashion the material provided in greater detail in three prior Annual Reports. That detail is given in References [1-10] which were appended to prior reports. More attention will be given to the newer material contained in the five Addenda, i.e., References [11-15].

2. Neural Networks for Reduced-order Model of Combustion Process

There is considerable interest in using Neural Networks (NNs) for the development of closure models in fluid mechanics and in particular combustion. For example, [17] provides a survey of using machine learning in fluid mechanics, [18-21] discuss NN-based closure models for turbulence and flame modeling and [22, 23] have used NNs for the coupling of the linear eddy mixing (LEM) sub-grid model with the LES. It has been argued that flamelet models can provide a viable approach for integrating NNs into a CFD computation by first training them to reproduce the data stored in the flamelet table. Thus, in [24] a NN-based flamelet model has been developed for the Sandia flame D, in [25] NNs have been used for representing a flamelet model in a stably burning flame for the Sydney bluff-body swirl-stabilized flame, and in our previous work [2], NNs are trained on a pressure dependent flamelet table for a single injector rocket configuration exhibiting longitudinal instability. Such NNs are trained off-line and validated by comparing the flamelet-based CFD results with those where the NN replaces the flamelet table. The results in [2, 25] show that NNs are capable of capturing accurately the combustion dynamics while requiring much less computer memory than the flamelet table; however, NNs require higher computational cost than the look-up table representation suggesting deployment via GPUs to alleviate the increased computational cost [26]. At the same time, additional advantages of using NNs in place of flamelet tables include more sophisticated interpolation properties and thus potentially increased accuracy in the simulation results.

The ultimate goal in utilizing machine learning in combustion is the construction of NN models based on data from experiments and/or computationally expensive CFD simulations to be used as reduced-order models in place of detailed sub-grid models. Therefore, as an evolutionary step from our work in [2, 27, 28], we considered training NNs based on CFD data. The objective is to develop

new NNs for flame closure void of much of the limitations of our previous NN models and more universally applicable in reacting flow simulations. The challenge in realizing this objective derives from the fact that in a CFD simulation only a small portion (a manifold) of the dynamic behavior becomes available for training. Thus, assuming the table-based CFD simulation as the “truth model”, only a small portion of the data stored in the flamelet table is visited during the simulation. It is not clear at the outset if such a limited data set contains sufficient information to capture the combustion dynamics under various simulation conditions and maintain stability of the CFD simulation. This essentially requires that trained NNs are capable not only of interpolating but also of extrapolating to a sufficient degree. Our findings show that this is possible after restricting the NN models to observe certain physical constraints such as known boundary conditions; thus, we refer to such NN models as being physics-aware. Another physics-based source of information that leads to improved NN performance has been the inclusion of the flame temperature (which is an output of the flamelet table) as an input to the NNs predicting some of the other outputs of the flamelet table. Not surprisingly, NN models are more accurate in domains where training data is more readily available and to compensate for the lack of data, we have again used additional physical constraints as explained later to augment the training set. The designed NNs are verified by testing them as a part of the CFD where they replace the flamelet table under different simulation scenarios. They are also tested off-line on the whole flamelet table library, which includes also the unobserved parts besides the training data obtained from the CFD.

In summary, we obtained NNs with good accuracy overall that are “smaller” than the NNs trained previously on the whole flamelet table, thus requiring less computation for their training and operation. In the following, we describe our results more specifically and the reader is referred to Addendum I and [11] for additional details.

2.1 Summary of Previous Work on NN

In our previous work [2, 27, 28], we used as a testbed Purdue University’s Continuously Variable Resonant Combustor (CVRC) experiment [29, 30]. CVRC is a combustion chamber with a single-element injector/oxidizer post, in which the oxidizer post length can be varied, resulting in configurations with different stability characteristics. An axisymmetric LES is used without imposed swirl. Both spontaneous and triggered instabilities have been found in the past. The analysis resolves both types of unsteadiness: turbulent flow fluctuations and large-amplitude acoustic oscillations. The flamelet theory is used as a sub-grid model because it introduces the reasonable set of multi-physical phenomena that exist at sub-grid dimensions: e.g., chemical kinetics and molecular diffusion of heat and mass. Turbulence is treated using delayed detached-eddy simulation, whereas chemical reactions are modeled using a compressible flamelet progress variable method. The base case has spontaneous instability and emulates well the experimental evidence. Heat loss is introduced by imposing an isothermal boundary condition on the chamber wall. Various temperature values are used, with the spontaneous longitudinal-mode instability still occurring at the higher wall temperature (less heat loss). Stable but inefficient combustion occurs for the lowest wall temperature. Subsequently, triggered instability of the chamber with low wall temperatures is simulated by perturbing the propellant mass flow rates. Unsteady oscillations can be triggered to higher-amplitude limit cycles. The various triggers for instability are quantified through the definition of “triggered energy” and an unsteady Rayleigh-index analysis. More details about our results using look-up tables for this configuration can be found in prior Annual Reports and References [1, 31, 32].

We conducted two different simulations in the 14-cm oxidizer post CVRC configuration that is associated with a very high level of instability. We started the simulation at two distinct initial conditions. The first initial condition was selected at a time before the emerging instability and the second at a time after the instability had been fully developed. We refer to the first simulation as the “transient case,” and the second as the “dynamic equilibrium case.” Two different sets of NN structures, NNa and NNb, were trained for the transient and dynamic equilibrium cases, respectively, to learn the discretized mapping represented by the table. The training set used was a mere fraction (15%) of the 10,000,000 values stored in the table after careful selection. NNb was larger than NNa and required 40% more computation. Although both NNa and NNb provide similar accuracy for the dynamic equilibrium case, NNb was necessitated by the more demanding transient case. To validate the NN-based flame models, the results from each simulation were evaluated by investigating the similarity between pressure signals (as functions of time at a fixed location) from NN-based and table-based CFD simulations. We measured similarity based on a number of criteria, namely 1) the overall relative error between pressure signals calculated from each CFD, 2) their correlation (using Pearson’s linear correlation coefficient) to measure phase differences, and 3) the ratio of rms values of pressure fluctuation with respect to smoothed averages of the oscillating pressure signals. The mean and standard deviation of these measures over combustor locations for NNa and NNb are summarized in Table 1. We also successfully implemented the NNb model in the 9-cm oxidizer-post case, which is stable as pressure oscillations grow to a limit cycle with amplitude much smaller than the 14-cm case, to validate its generality. Also, comparisons were made between NN-based closure model for CFD and the table-lookup approach. The results correlate well with original CFD results, particularly for variables governed by acoustic behavior. Our study, established that NN can be used successfully as closure models in combustion simulations.

14-cm oxidizer-post cases	Model	Relative Error (%)		Correlation (%)		RMS Ratio (%)	
		mean	std	mean	std	mean	std
Dynamic equilibrium	NNa	7.18	2.47	78.50	12.69	93.71	4.58
	NNb	6.23	2.34	82.10	13.71	93.91	2.85
Transient	NNa	5.02	1.32	18.74	18.74	75.84	2.35
	NNb	5.02	1.40	79.61	14.89	103.63	2.89

Table 1 Accuracy of NN representation of Flamelet look-up table

2.2 Summary of Current Work on NN

The physical geometry and the flow field configuration in this work is again based on the Continuously Variable Resonance Combustor (CVRC) experiment of Purdue University [29, 30]. This fundamental single injector/oxidizer post rocket combustor produces different stability behaviors for different oxidizer post lengths. Similarly, varying the initial condition and wall boundary condition, leads to observation of various stability characteristics. Although the CVRC experiment uses gaseous injection, it is accepted as a valid benchmark for computational methods that address combustion instability in LPREs. The key factor in a model used in combustion instability is the capability of capturing the coupled relation between pressure and energy-related

flame variables such as the progress variable reaction rate (PVRR) or heat release rate (HRR). Pressure and thus the flame variables change drastically when instability occurs.

2.2.1 Flamelet Models: Flamelet models for turbulent combustion were introduced and further developed in [33] and [34]. These models assume a quasi-steady chemistry based on the fact that chemical time steps are shorter than flow and turbulent time scales. The quasi-steady assumption leads to the decoupling of chemistry-related calculation from the LES flow calculation. The analysis of a diffusion flame under normal compressive strain leads to the prediction of a complex chemical mechanism at a much lower computational cost [1, 31]. The flamelet model is used to generate look-up table libraries utilized in the CFD simulation. These libraries are collected in a block that is accessed during the CFD simulation via a set of inputs and provides a set of outputs describing the thermo-chemical properties of the flame. The inputs to the flamelet model are the flame state variables $\tilde{C}$, $\tilde{Z}$, $\tilde{Z}''^2$ and pressure $\tilde{P}$. $\tilde{Z}$ indicates the mixture state of fuel and oxidizer composition, $\tilde{Z}''^2$ is the mean variance that defines the deviation from the mean of Z and is important for turbulent combustion, and $\tilde{C}$ determines how much of the combustion process has been conducted at each time and point in space. Actually, the surrogate variable $B = \frac{\tilde{Z}''^2}{\tilde{Z}(1-\tilde{Z})}$ is used instead of $\tilde{Z}''^2$. A total of seven combustion variables are read off the table including reaction rate $\tilde{\omega}_C$ and flame temperature $\tilde{T}_f$. The set of inputs to the flamelet model is defined as a vector Ψ and the set of outputs as a vector Φ . In turbulent non-premixed modeling, it is assumed that the mixture fraction has a distribution that is generated by convolving the laminar flamelet solutions with a sub-grid beta PDF with mean $\tilde{Z}$ and (surrogate) variance B . A Dirac delta PDF is assumed to relate $\tilde{C}$ to the progress variable C , which is an indication of the progress of global reaction in the flow [34]. $\tilde{P}$ is also a significant element for describing the combustion state, particularly in the flow fields with unsteady pressure.

2.2.2 Neural Network Design: Feedforward Neural networks (NNs) employed in this work consist of connected layers of computational units called neurons and are used to implement a target function between certain input and output variables known in terms of possibly noisy samples. The output of each neuron is a nonlinear function (activation) of a linear combination of the outputs of neurons in the previous layer via weights that collectively constitute the parameters of the NN. The inputs are applied to the neurons of the first layer while the neurons in the final layer generate the output(s) of the NN. The layers between the first and final layers are called hidden layers and Deep Learning Neural Networks are characterized by having (many) more than one hidden layer. The objective is to find the NN parameters minimizing the squared error between the outputs of the NN and the target outputs corresponding to the inputs (training samples). Solving the optimization problem iteratively constitutes the NN training process that typically is accomplished by the method of Backpropagation, which is an efficient implementation of gradient descent.

In this work, we design NNs (one for each of the flame variables) to replace the flamelet table in the CFD simulation, thus the input set to the NN is Ψ and the output set is an element of Φ . We use only data generated from a single-injector configuration, which during a table-based CFD simulation utilizes only part of the table. A challenge with learning from large data sets (simulation and/or experimental data) is the selection of a sufficiently representative training set that does not lead to an excessive computational cost for the training process. For example, a CFD simulation of spontaneous instability (referred above as the transient case) with the pressure signal growing from a relatively low value to a large limit cycle, requires a simulation time of 10ms to capture it

completely. Sampling this simulation at 200 kHz leads to 2000 snapshots of the combustor. A snapshot of the combustor has around 137500 grid points in our axisymmetric set-up. Thus, the pool of data generated by such simulation has around 275 million points. Handling such a large data set and selecting the most informative points for training is a challenging task. We accomplished this as follows. In the table-based CFD set-up, the flame variables are calculated by linear interpolation of the values stored in the flamelet table. Since, our objective at this stage is to replace the flamelet table by a NN trained only on the part of the table accessed during the CFD simulation, we created a reduced training set based on the table values that are accessed during the simulation. We mainly use the transient case configuration with 14 cm oxidizer post, which is a highly unstable case. While the flamelet table stores 10,342,800 data points, the observed table points from the transient case amount to only 338,283 points. This data set turns out to be sufficiently rich for developing good models for all output variables except PVRR due to the lack of a sufficient number of samples from high pressure regions. To remedy this, data from another simulation (referred above as the dynamic equilibrium case) that starts after high limit cycles have set in, has been also included in the training set for PVRR. Another limitation of the observed training set during the CFD simulation has to do with adequate coverage of the boundary points in the flamelet table. The boundary points are the ones that define the flame dynamics of the sub-grid counterflow model. For example, for every pressure, turbulence level, and progress variable values, the species mass fractions and temperature are known when the flow is purely oxidizer or purely fuel, indicated by $Z = 0$ and $Z = 1$, respectively. Accordingly, the value of all other flamelet outputs is known at these extreme cases and can be added as additional training points even though they have not been observed so that our model meets the physics-related constraints of the system. Another physical assumption that can facilitate the NN-based model development is the inclusion of the values for each variable when the progress variable $C=0$. In this case, there is no combustion, and the flamelet model is governed by the flow dynamics. Therefore, the training set can be reinforced by adding the parts of flamelet table associated with the points having $C=0$, again relying on physics-informed considerations.

Separate NN are developed for modeling the flamelet table outputs based on three NN structures specified by the number of layers and number of neurons in each layer. NN structure design is aimed at increasing accuracy while decreasing the data retrieval computational cost. A NN with the lowest number of neurons and layers that results in sufficiently small error is desired for each variable. In all NNs, the activation function of hidden layers is selected to be the leaky Rectified Linear function [35] and the output layer activation function is taken to be linear. The NN parameters (weights) are initialized by the Xavier initialization [36] algorithm and are updated via the ADAM algorithm [37] within the back-propagation procedure. Mini-batch training, as it is helpful to avoid local-minima in the training process, and regularization to avoid overfitting and improve NN performance on the test sets have been also used [38].

The flamelet model assumes second order PDEs for the species mass fractions and flame temperature. The PDEs are defined in the domain of time (unsteady flamelet) and mixture fraction. Other outputs of flamelet model are essentially functions of species mass fractions and flame temperature $\tilde{T}_f$. Thus, in developing NN-based models for those variables flame temperature is also considered as an input. Accordingly, we managed to significantly improve the accuracy of our NN-based models for certain of the output variables. Including flame temperature as an input not only helps to improve accuracy, but also provides a means to keep flamelet outputs consistent

within the CFD simulation. However, one disadvantage is that the error in the model for $\tilde{T}_f$ propagates in other variables as well.

2.2.3 Results: The training error and testing error for these variables and PVRR are provided in Table 2. The NN designed for PVRR is the most expensive structure among all variables and was selected after testing many other smaller structures that failed to capture its full dynamics. Due to the very nonlinear dynamic and large scale of PVRR, finding a converging solution is a challenging task; at the same time our study did not indicate considerable improvement in using temperature $\tilde{T}_f$ as an additional input for the PVRR NN. In the third column of Table 2, the computational cost of generating the output from each of the proposed NNs is listed in terms of floating points (FLOP). Implementing these NNs inside CFD costs around 5815 FLOP representing the least NN-related computational cost we have been able to achieve for the same or worse accuracy including our previous work [2]. As discussed in the literature, the computational cost issue related to the NN can be alleviated by the utilization of GPUs. However, in this work, CPU is used as the computational resource.

	# of neurons in each layer	FLOP	training error (%)	test on table (%)
$\tilde{T}_f$	4-15-10-15-1	375	0.59	4.83
$\tilde{e}_f$	5-15-10-15-1	390	0.0566	0.57
$\tilde{R}$	5-15-10-15-1	390	0.0526	0.65
$\tilde{\lambda}$	5-15-10-15-1	390	0.21	3.57
$\tilde{\gamma}$	5-15-10-15-1	390	0.0371	0.48
$\tilde{\alpha}_\gamma$	5-15-10-15-1	390	0.22	1.41
$\tilde{\omega}_C$	4-15-20-25-35-25-20-15-5-1	3490	1.49	32.86

Table 2 Selected NN structures for each flame variable

We also tested the NN-based models by incorporating them into the CFD simulations in place of the flamelet models. In addition to the dynamic equilibrium and the transient cases, another simulation, the triggering case, exhibiting a triggered instability is studied. In this configuration, the wall thermal boundary condition is assumed to be isothermal at 1030 K, while in the other two cases an adiabatic wall is considered. Simulations with the 14-cm oxidizer post length CVRC configurations describing the dynamic equilibrium and triggering cases are performed and the results of the NN-based simulations are compared with the table-based ones. Since the NN models were trained based on a set of data from the transient CFD simulation, as a first step, we implemented the model for the transient simulation. The pressure signal at two points in the oxidizer post and the shear layer are compared in Figure 1. The NN is more accurate where the pressure signal reaches the high amplitude limit cycle, albeit the amplitude of the limit cycle is underestimated during the transient. Our NN-based model has been able to follow pressure well while growing from low values to reaching a high amplitude limit cycle.

Next, we consider the dynamic equilibrium scenario, in which the simulation starts from an initial condition with the dynamic instability already set in. We plot in Figure 2, the pressure time waveforms at two representative locations, one in the oxidizer post and another in the shear layer.

At both locations, there is great consistency between the table-based and NN-based simulations. We also plot in Figure 3, the overall relative error calculated for each spatial point as the norm of the difference of the pressure signals time waveforms from the NN and table-based simulations normalized by the norm of the signal from the table simulation.

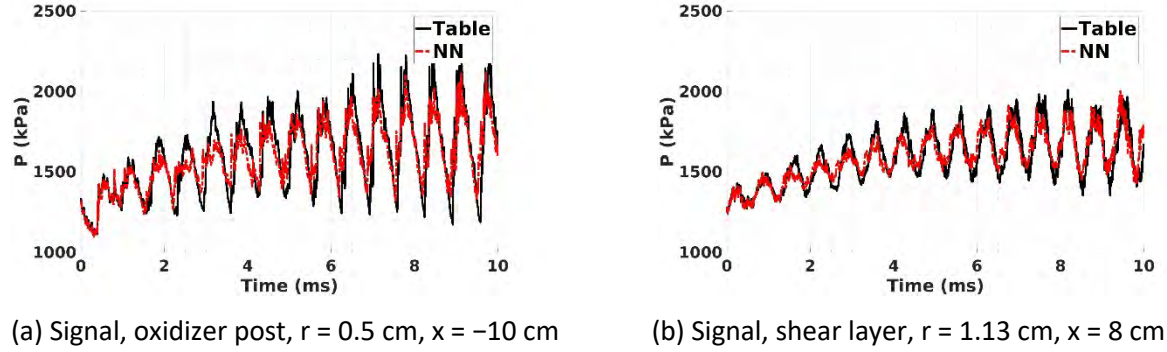


Fig. 1 Transient Case: comparison between NN and table of pressure time signals at representative points

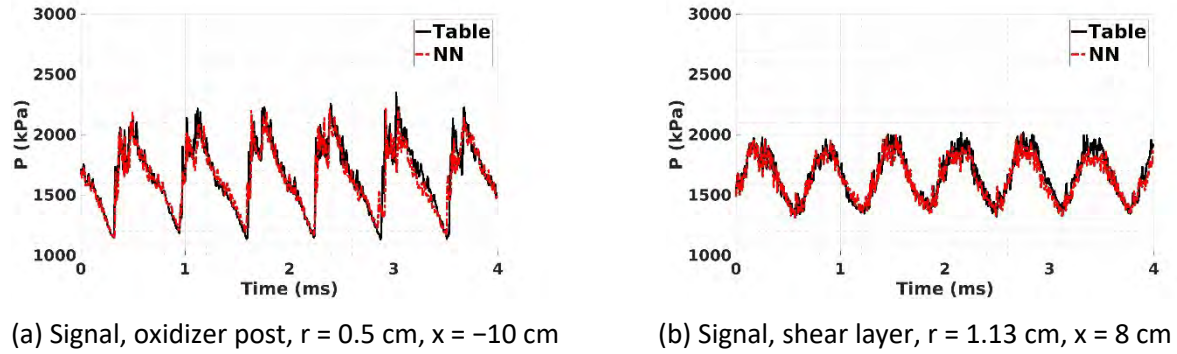


Fig. 2 Dynamic Equilibrium Case: comparison between NN and table of pressure time signals at representative points

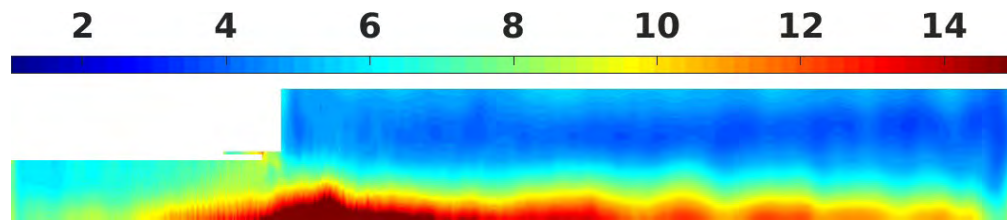


Fig. 3 Dynamic Equilibrium Case: Relative error between NN and table pressure signals at each spatial location

In the triggering scenario, two periods of sine wave perturb the mass flow rate. The top wall is modeled to be isothermal at 1030 K. The pressure signals at the two representative locations (one

in the oxidizer post and another in the shear layer) are plotted in Figure 4 showing again great consistency; in particular, the pressure response to the perturbation in the mass flow rate can be observed in both simulations, where the response has been damped after 2.5ms.

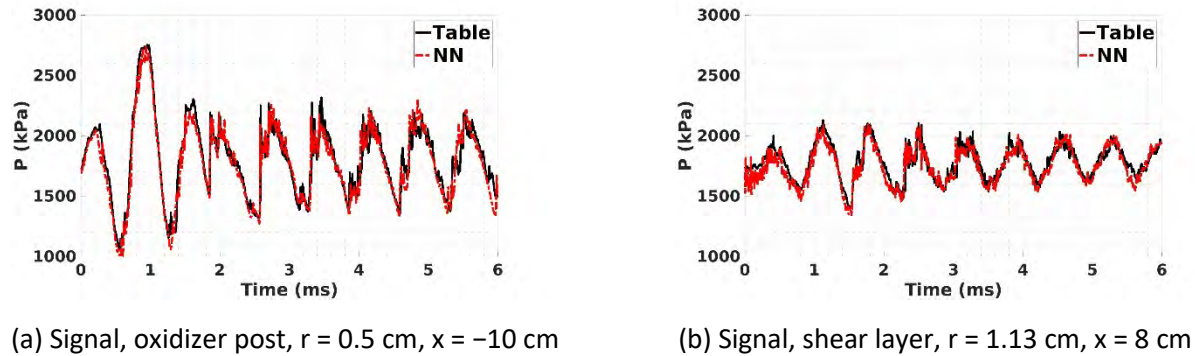


Fig. 4 Triggering Case: comparison between NN and table of pressure time signals at representative points.

3. Three-dimensional Large-Eddy Simulations of Multiple-injector Rocket Engines

Computational studies [3, 4, 12, 13] are presented of the nonlinear combustion instability of several multi-injector rocket engines. The study addresses configurations with a choked nozzle and a combustion chamber with 10-, 19-, 30-, and 82-coaxial injector ports. The 82-injector study models an experimental rocket chamber used by Rocketdyne [16]. Computations using a three-dimensional unsteady $k - \omega$ shear-stress transport delayed detached-eddy simulation method provide detailed time-resolved information about the combustion instability. We address unsteady interaction between neighboring injector-jet streams to understand where premixed flames prevail and where non-premixed flames prevail. We pursue understanding of the chaotic character when energy is exchanged between two resonant modes. Triggering is deliberately used to change the resonant mode to a less energetic and less consequential mode; here, a method of control could be developed.

The report on three-dimensional LES is divided below into three parts which appear in the three following subsections: (3.1) analysis of the 10-, 19-, and 30-injector chamber, (3.2) analysis of the 82-injector chamber, and (3.3) inclusion of the Pierce-Moin flamelet model for the ten-injector chamber

3.1 Analysis of 10-, 19-, and 30-injector Rocket Chamber

We reported on References [3] and [4] in previous Annual Reports that the spontaneous longitudinal-mode instability is observed for the 10- and 19-injector geometries with a combustion-chamber diameter of 28 cm. The triggered tangential and longitudinal instability modes occur for the 19-injector geometry with a combustion-chamber diameter of 43 cm by pulsing the injector mass flux. An oscillating combustion-chamber flow can be triggered to a

new mode with a larger disturbance amplitude. The streamwise vorticity created by the instability impact the heat release in a manner that supports the instability. For the 28-cm-diam combustion chamber, a similar combustion instability with 10- and 19-injector geometries is obtained by preserving the mixing rate parameter of $K = D/(\Delta U)^{1.25}$ where D is the injector diameter and ΔU is the relative velocity between the core axial oxygen jet and the annular fuel jet in the co-axial injector.

The Rocketdyne 82-injector experimental rocket chamber [16] is mimicked by a 30-injector rocket engine combustor. The computational model with 30 injectors avoids the high cost for an 82-injector combustion analysis. The experiment model had a chamber length of 24 cm. In addition to that length, we examine a shorter length (18cm) and a longer length (30cm) in the present study. Figure 5 shows the 30-injector and 82-injector combustor geometries. The combustion chamber diameter is 14.38cm. P1-P6 marks six pressure probes around the combustion chamber wall. Figure 6 shows the combustor geometry. The individual co-axial injection for the 30-injector design matches the injection geometry for the 82-injector engine. The radial distribution of the inlet mass flow rate of the 30-injector combustors is designed to match that of the 82-injector combustor. Figure 7 shows the comparison of the radial distributions. In the simulation, the total mass flow rate and the mixture ratio match those in the experiments. So, the solution for 30-injectors is expected to be similar to that of the 82-injector combustor. The total number of computational nodes is about 12.1 million for the 24cm length combustion chamber.

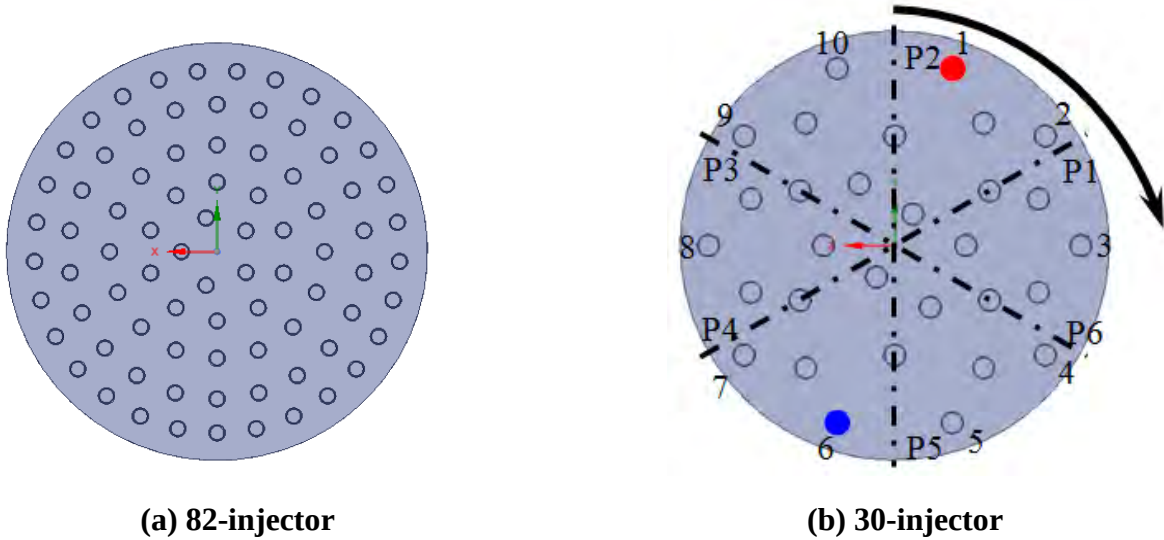


Fig. 5. Front view of the injector plate

Computations using a three-dimensional unsteady $k-\omega$ shear-stress transport delayed detached-eddy simulation method provide detailed time-resolved information about the combustion instability. Our flame-index analysis explains why the premixed-flame structures dominate over diffusion flame-structures in the driving mechanism for the instability. This causes the engine to become more unstable as the mixture becomes more fuel rich. Spontaneous longitudinal mode and tangential-mode instabilities are observed, in general agreement with the experiment. The oscillation amplitude of each of the two instability modes vary in alternating fashion during the simulation time. The alternating behavior of the two instability modes can be modified by pulsing the injector mass-flux on the mixture ratio at a particular frequency.

More details are provided in Reference [13].

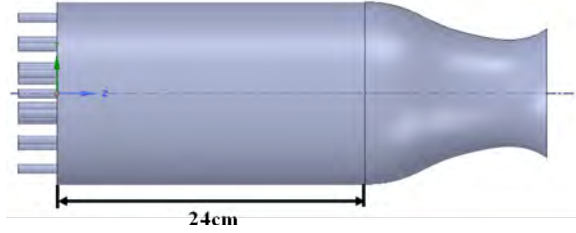


Fig. 6. 30-injector combustor geometry.

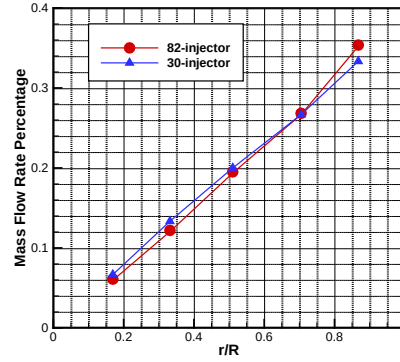


Fig. 7. Inlet mass flux radial variation.

3.2 Analysis of Rocketdyne 82-injector Rocket Chamber

A computational study of the nonlinear rocket-engine combustion instability is presented for the Rocketdyne experimental engine with 82 coaxial methane-oxygen injector ports, a choked nozzle, and a combustion chamber. The configuration is shown in Figure 5a. Computations used a three-dimensional unsteady $k-\omega$ shear-stress transport delayed detached-eddy simulation method. Comparisons are made with the experimental results and with the 30-injector simulation that uses the same chamber and nozzle designs, mass flux, mixture ratio, injector velocities, and pressure. Four different combustion rates are simulated. When the normalized combustion rate is one, only the longitudinal-mode instability is observed. As the combustion rate decreases, the tangential-mode instability occurs and the longitudinal-mode instability becomes weak.

In comparison with the 30-injector configuration, the sizes of the injector ports and the distance between ports are reduced; thus, we expect that the jet mixing rate is enhanced for the 82-injector configuration for the same injection velocities, global mass-flux rates, and mixture ratios. This result is confirmed by examining the mass fractions for reactants and products, which indicate burning rates are higher with 82 injectors, given the same chemical kinetic rates and pathways. By reducing the one-step kinetic rate for the 82-injector computations, the burning rates for the two configurations match better.

See Figure 8 where the reaction rate for the 82-injector engine has been reduced by a factor of greater than 2. That is, a reduction coefficient of 0.375 is multiplied with the chemical kinetic rate at all points in space and time to give a reduced rate for chemical reaction and thereby for the burning rate. Without the adjustment, the 82-injector case showed that the longitudinal mode, rather than the tangential mode, was dominant. The faster burning rate brings the larger portion of the combustion zone and the associated heat release to the pressure antinode adjacent to the injector plate. Reduction of the burning rate and movement of the major portion of heat release in the downstream direction reduces the Rayleigh index for the longitudinal mode but not for the

tangential mode. The tangential mode is theoretically insensitive to the streamwise location point of the heat release.

The longitudinal mode appears alone at the normal chemical kinetic rate with a resonant frequency in the range of 2000-2500 cps. At a reduction coefficient of 0.500 as shown on the left in Figure X11, the tangential mode at about 4400 cps also appears but the lower frequency longitudinal mode still dominates. With a reduction coefficient of 0.375, the tangential mode comes to dominate, which agrees better with the experiment and the 30-injector simulation.

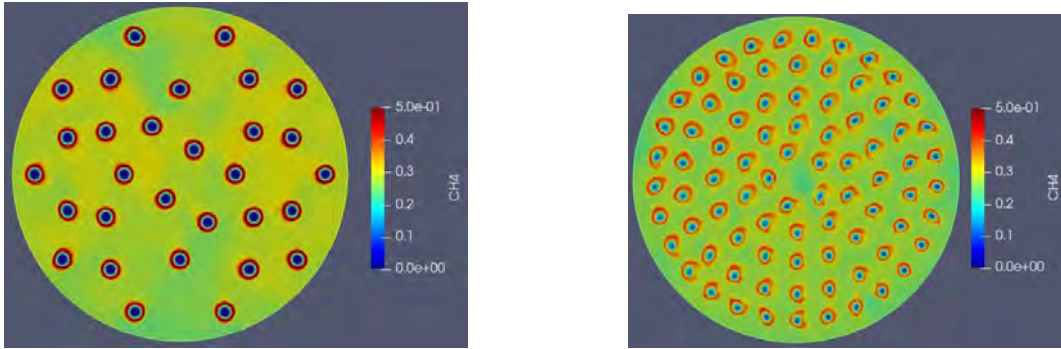


Fig. 8 (Figure 9 in Addendum IV.) Comparison of methane mass fraction at 1.0 cm downstream of injector. 30 injector engine on left, 82-injector engine on right.

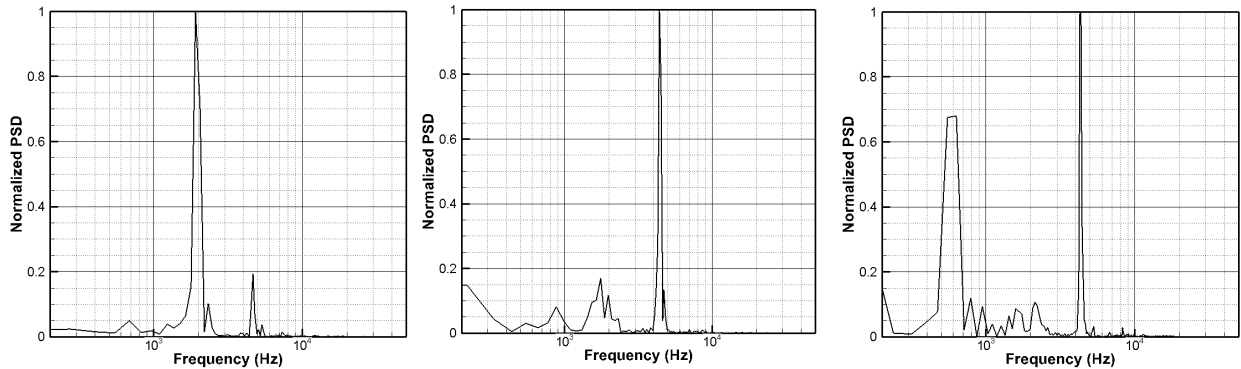


Fig. 9 (Figure 7 in Addendum II). 82-injector engine with simultaneous longitudinal (lower frequency) and tangential oscillations (higher frequency). Chemical-kinetic-rate reduction coefficient of 0.50 on left, 0.375 in middle, and 0.25 on right.

One may conjecture several possibilities for the 82-injector simulation over-predicting the burning rate compared to the experiment. (i) The one-step kinetics law which was designed by Westbrook & Dryer [39] for premixed flames might not work well for our combination of premixed and non-premixed flames in the turbulent rocket combustor. (ii) At the supercritical pressures considered, the equation of state and the describing relations for diffusivity need corrections. (iii) The imperfect representation of the flow inside the injector ports could be consequential on downstream mixing and burning rates. Notwithstanding various needs for improvement in the model, the analysis has shown the substantial sensitivities that can result in a change of the oscillation mode with a small parameter change.

In ongoing work, the Soave-Redlich-Kwong real-fluid equation of state is being applied to the 82-injector configuration for improving the physical representation. It is expected that the better representation of gas density, especially near the injectors where temperatures are low, will improve the flow field computations.

3.3 Use of Flamelet Model for Multi-injector Rocket Chamber

Our prior multi-injector studies [3, 4, 11] have used one-step chemical kinetics at the resolved scale of the LES while our CVRC-configuration, single-injector studies [1, 2, 11, 31, 32] have employed the sub-grid flamelet progress variable (FPV) model [34], either through look-up tables or neural networks. The direct use of one-step kinetics avoids computational-storage costs but can require smaller time-steps at additional computational time costs. Direct use of more detailed kinetics would add substantially to the multi-time-scale costs. FPV gives both the multi-species character of the detailed kinetics and the more precise determination of the flame temperature without the computational time costs. For that reason, we have extended the use of FPV to both the 10-injector configuration and the 19-injector configuration. Look-up tables are used in this first approach with an intent to use neural networks in the future.

3.3.1 Ten-injector Configuration: For our CVRC configuration, axisymmetric large-eddy simulations are the approach. Our large-eddy simulations for multi-injector configurations [3, 4, 12] using one-step chemical kinetics are three-dimensional. Recently, we have been developing a three-dimensional model using FPV. The same Open-FOAM based 3D computational code is utilized for the new approach with the flamelet model. The axisymmetric code used previously in the single-injector-engine computations was not an OpenFOAM code. The intricacies of connecting the flamelet table with the CFD code are very different, especially with regard to the connection with the energy equation and the determination of enthalpy and temperature.

Specifically, for the analysis of the 10-injector, 28-cm-diameter rocket combustor and nozzle system, we add the partial differential equations for the averaged mixture fraction, rms mixture fraction, and the progress variable to the system of flow equations as before. The solutions to these equations, together with the pressure are the instantaneous inputs to the table lookup process for each point in the three-dimensional space. The progress variable reaction rate and the species mass fractions are the major outputs. The energy equation resolves the total energy, i.e., both chemical and thermal components. The code, with the use of the mass fractions and the species heats of formation, determines by subtraction of the chemical energy the enthalpy and the temperature. In prior use of the flamelet model with the CVRC simulations, species mass fractions were not utilized; temperature came directly from the table; and then a modest correction to that temperature was made by the code to reflect compressibility effects of the flow.

In addition, the multi-injector engines are operating at pressures an order of magnitude higher than the CVRC engine. Pressure is a key input to PVF look-up table. Thus, we had to create a new table. Even more importantly, we needed a chemical kinetics scheme that can be trusted for methane oxidation at very high pressures. Professor Hai Wang of Stanford provided us with his 12-species, 39-reaction system for CHO systems at high pressures. With this new information, the Flamemaster code, which creates the table given the kinetics description, generated a new table

that was used with the multi-injector CFD. In the future, neural networks can replace the look-up table.

In Figure 10, spectral analyses for the pressure oscillations are shown and compared for the simulations with the flamelet progress variable model on the left and the one-step kinetics model on the right. Both simulations show a 1500-cps first-longitudinal mode and a 2500-cps first-tangential mode. The longitudinal mode dominates with one-step kinetics while the tangential mode dominates with the flamelet approach.

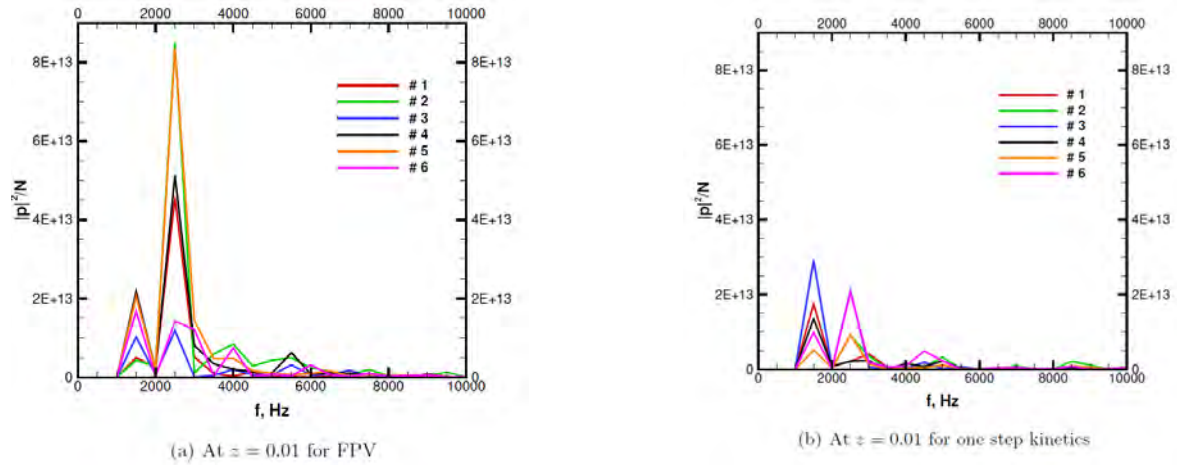


Figure 10. Spectral analysis of pressure in unstable combustor: (a) with flamelet progress variable. (b) with one-step chemical kinetics.

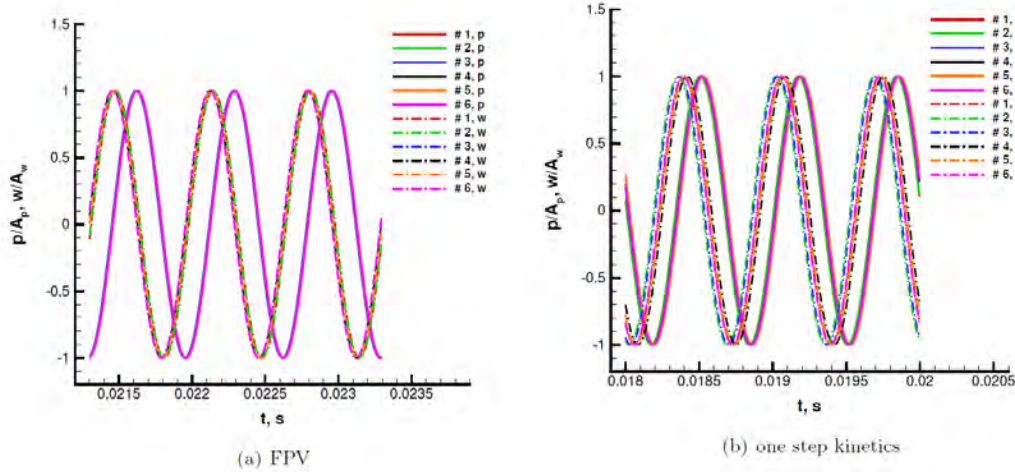


Figure 11. 1500-cps Fourier component for longitudinal mode pressure and axial velocity: (a) with flamelet progress variable. (b) with one-step chemical kinetics.

Figure 11 presents normalized pressure and axial velocity for the 1500-cps Fourier component at the nozzle entrance, a region close to the expected pressure antinode for the first longitudinal mode. The pressures at six azimuthal positions are in phase, indicating a longitudinal-mode behavior,

which is verified because the axial velocity oscillations at six azimuthal positions are in phase with each other but out of phase with the pressure.

Figure 12 presents normalized pressure and tangential velocity for the 2500-cps Fourier component very near the injector plate. The pressures at six azimuthal positions are not in phase, but rather two pressure recordings 180 degrees apart in the azimuthal direction are out of phase, indicating a tangential-mode behavior. A first-tangential standing-wave behavior is found by showing that tangential velocity and pressure are not in phase with each other. In these issues for both modes, the behaviors with the two combustion models are shown to be in agreement in Figures 11 and 12.

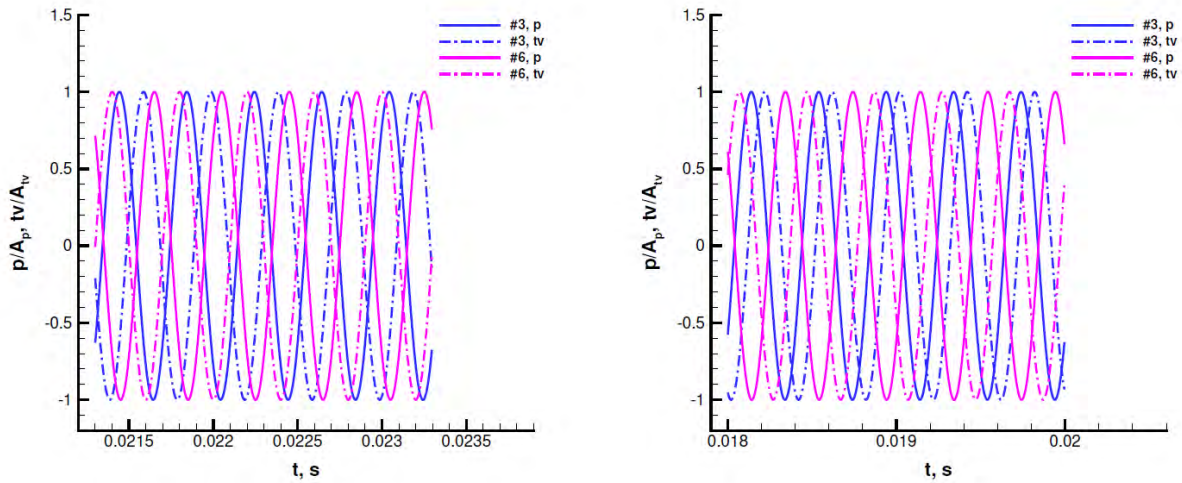


Figure 12. 2500-cps Fourier component for tangential mode pressure and axial velocity: (a) with flamelet progress variable. (b) with one-step chemical kinetics.

We have been successful in extending the use of the flamelet model to the three-dimensional analysis and addressing both longitudinal and tangential-mode behaviors. The one-step-kinetics approach and the flamelet-model approach give qualitatively similar results. However, there are differences. The flamelet approach removes any characteristic time associated with chemistry which appears to have some consequence concerning the resonant mode that is most strongly supported by the combustion. The flamelet model accounts for more chemical species and more reactions without reducing the computational time-step below the required level demanded by advective and diffusive processes. While the table lookup process requires more computational memory resources, we have shown in Section 2 that deep learning neural networks can solve that resource problem.

In this ten-injector analysis, we resolve better the flow within the injector ports compared to resolution for configurations with a larger number of injectors. The position $z = 0$ is at the injector-plate face and injector exit. So, positions inside the injector ports have $z < 0$. The injector port has a length of 0.05 m with z position varying within the port from $z = -0.05$ m to $z = 0$. Figure 13 shows the oscillatory behavior in the central port from an analysis using the progress-variable flamelet model. Similar oscillatory behavior occurs with the one-step kinetics model. A similar

resonance phenomenon is also found in each of the injectors. However, the oscillation magnitude reaches a maximum value in the central injector with decreased values in the surrounding injectors.

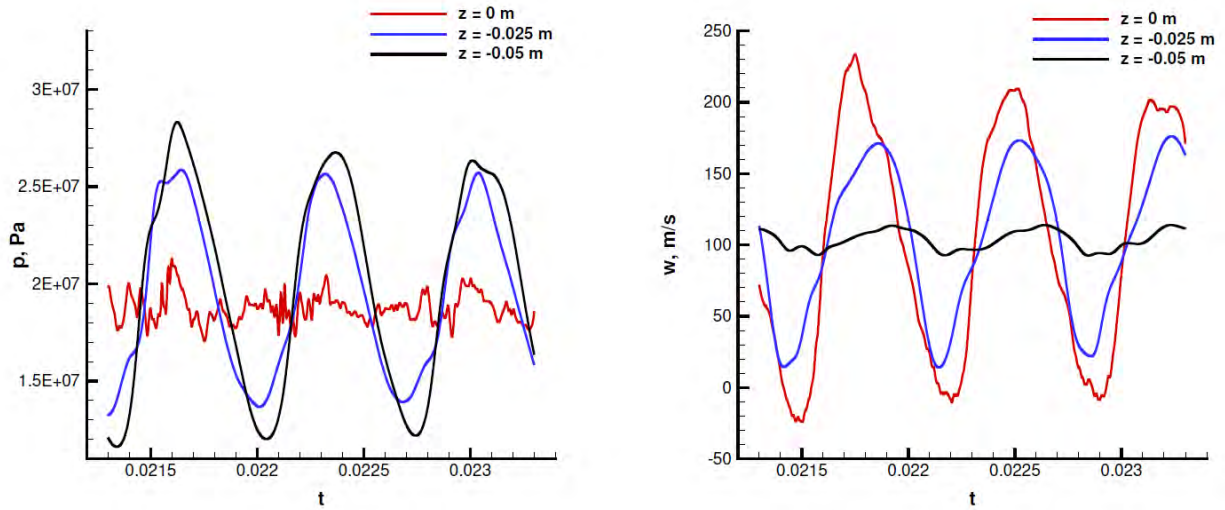


Figure 13. 1500-cps oscillations for pressure and axial velocity in the center injector with flamelet-progress-variable analysis.

A pressure antinode (velocity node) occurs at $z = -0.05$ m, the injector-port entrance, and a pressure node (velocity antinode) occurs at $z = 0$, the injector exit. At $z = -0.025$ m, the phase angle difference between pressure and the axial velocity is about 90 degrees. All these features suggest that the injector is behaving as a quarter-wave-length tube. Here, the exit of the injector behaves as the open end while the inlet is partially closed and behaves as the closed end. For pure oxygen at 400 K, the speed of sound is about 379 m/s. The theoretical frequency of this 5-cm quarter-wave-length resonance is 1895 Hz. The actual resonance frequency here is 1500 Hz, deviating slightly from the theoretical value. The oscillation at 1500 cps is expected since it is driven by the longitudinal-mode oscillation in the combustion chamber.

3.3.2 Nineteen-injector Configuration: The study of the nineteen-injector configuration is based on the same theoretical approach and computational code. Without triggering, stable combustion is predicted. This differs from the case where OSK was used [3] resulting in a weak longitudinal mode. The difference is not surprising; OSK predicts a faster burning rate and a higher flame temperature. Thus with OSK, more of the combustion occurs upstream near the longitudinal-mode pressure anti-node and the burning is more energetic; both characteristics increase the support of the longitudinal mode. With appropriate triggering, it is possible to obtain first-tangential-mode oscillations, either of the travelling or standing type.

Figure 14 shows results for the triggered tangential-travelling-wave case with the largest pulsing amplitude, i.e., $\epsilon = 1.00$. The travelling wave or standing wave was induced by pulsing mass flux in the twelve outermost injectors but with appropriate phase in time. Testing with values of $\epsilon = 0.25, 0.50, 0.75$, and 1.00 was done where ϵ is the ratio of injector-mass flux amplitude to mean

injector mass flux. The resulting oscillation amplitude in the chamber for pressure and other quantities increases as ϵ increases.

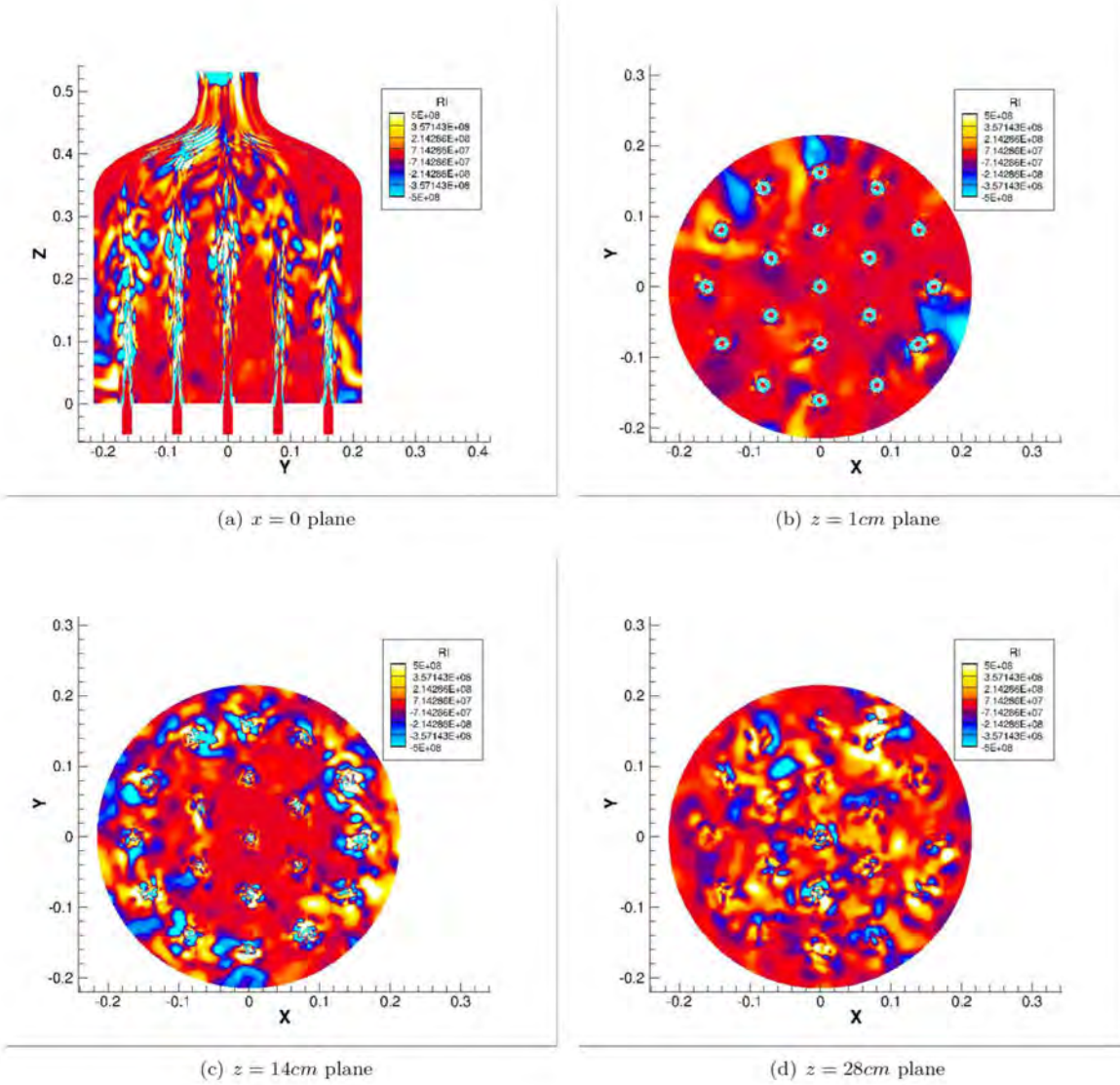


Figure 14. Time-averaged Rayleigh Index for 19-injector rocket engine with triggering of a transverse travelling wave with large-amplitude mass-flux perturbation: $\epsilon = 1.00$.

The Rayleigh index is commonly used to evaluate the severity of the instability. It involves an integral over time of the product of burning rate perturbation and pressure perturbation. Positive numbers indicate that the pressure oscillations and the burning rate oscillations are mutually reinforcing.

In Figure 15, the Rayleigh index results are provided for the triggered tangential-standing-wave case. For both standing and travelling waves, the regions of high burning rate, and therefore high Rayleigh index values, are not distributed uniformly over the combustor. The lack of smoothness is a consequence of the turbulent combustion process.

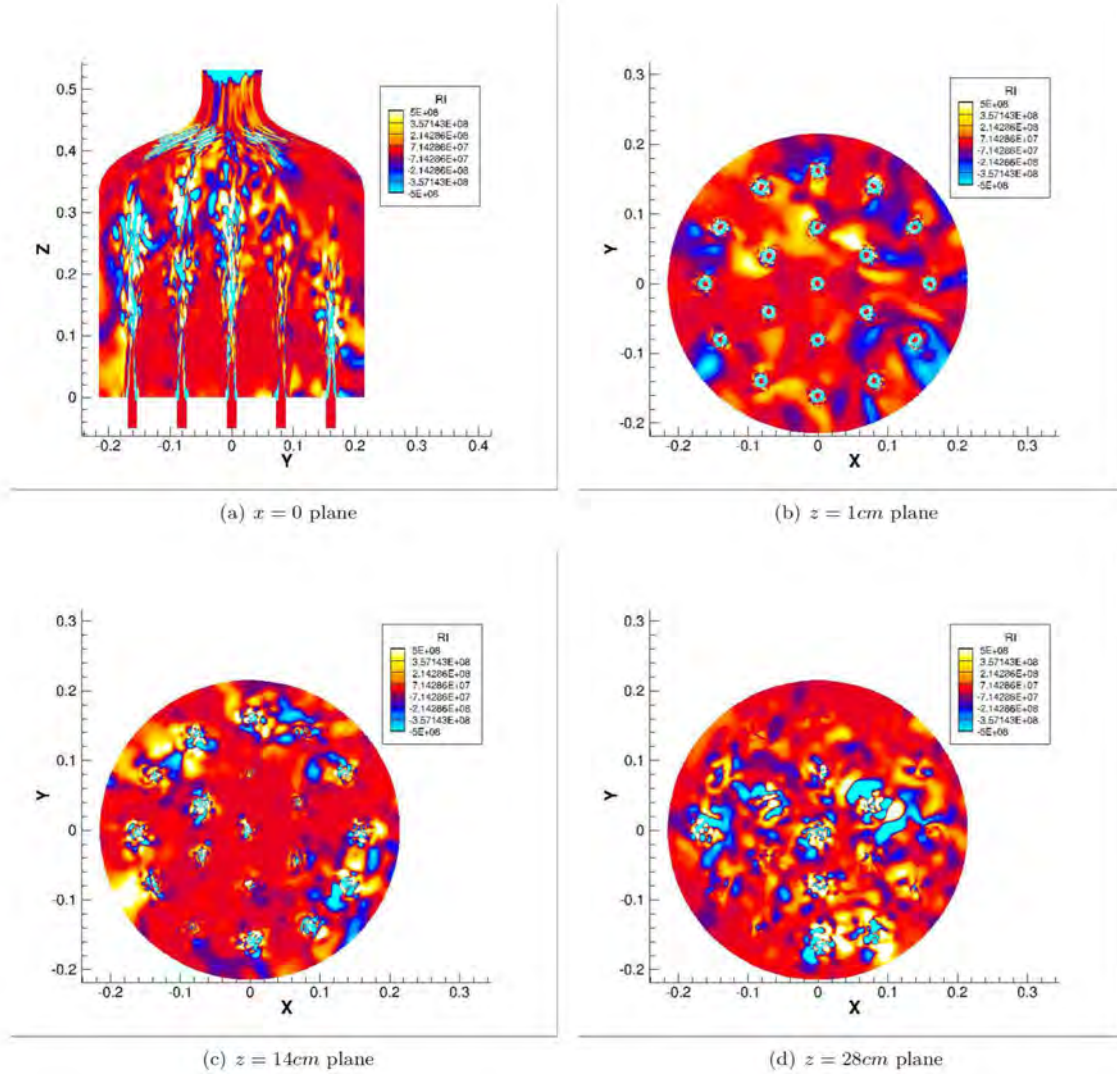


Figure 15. Time-averaged Rayleigh Index for 19-injector rocket engine with triggering of a transverse standing wave with large-amplitude mass-flux perturbation: $\epsilon = 1.00$.

4. Improvements and Extensions for the Flamelet Model

The flamelet theory developed by Peters [33] and Pierce & Moin [34] is widely used both for table-lookup and NN approaches [1, 2, 11, 25, 27, 28]. It is based on axisymmetric or planar configurations with a single non-premixed flame and only normal strain (i.e., it is irrotational). Multiple flames in one counterflow structure and the effects of shear strain and vorticity on the flame structure have not been considered in the current model. We have been seeking extensions of that model since our rocket combustion analysis has shown clear signs of three-dimensional flame structures with both premixed and non-premixed flames appearing in the presence of shear

strain and vorticity [1]. Our extensions [5, 7-10, 14, 15] account for (i) three-dimensional configurations, (ii) multi-branched flame structures with co-existing non-premixed and premixed flames, (iii) effects of shear-strain rate and associated vorticity (i.e., extension of current irrotational flamelet models), (iv) variable density, and (v) physics-based connection (i.e., without a contrived progress variable) between the sub-grid level flamelet model and the resolved-scale quantities in the large-eddy simulations. The results show that the premixed-flame character need not follow classical behavior when the premixed flame exists with the nearby non-premixed flame. A new finding is that heat diffusion from the non-premixed flame with a higher temperature can be a controlling factor for the premixed-flame burning rate. Another key finding is that the synergy between three-dimensional behavior, variable density, and vorticity is essential and must be allowed in the analysis to capture the correct behavior. The longer-term plan is to apply these new multi-physics flamelet models using NN directly without creating new look-up tables.

4.1 Consideration of Multi-Flame Structure

Structures with multiple flames, non-premixed and premixed, in strained flow representative of turbulent combustion are analyzed with reacting, viscous, three-dimensional counterflows [7-10, 14, 15]. There can be differing normal strain rates in each of the three directions. For example, we have studied configurations with a diffusion flame plus one or two partially premixed flames with reduction of the equations to a similar mathematical form. In steady, variable-density configurations, results for the velocity and scalar fields are found as functions of two tensile normal strain rates between the two transverse directions, a range of Damköhler number based-on strain rate, and various Prandtl number values. With increasing strain rate and/or decreasing pressure, the multiple flames will merge into a single diffusion flame and with further changes of those types, extinction will occur. In the three-flame case, the fuel-rich premixed flame merges first with the diffusion flame as Da decreases; with further decrease, the fuel-lean premixed flame merges with the diffusion flame, leaving a diffusion flame to extinguish with further decrease. Velocity overshoots occur in the viscous layer, yielding an important correction of theories based on constant-density. Advection and convection are important in the flame neighborhood.

In the most recent works [14, 15], we analyze steady laminar flow structures with vorticity, mixing, chemical reaction, and normal strain representative of turbulent combustion at the small scales. A counterflow configuration is examined to focus more easily on the premixed flames that are known to occur in multiple flame structures; the premixed flame can be driven by a controlled heat source, which is a surrogate for the diffusion flame in the practical multi-flame structure. Reduction to a one-dimensional similar form is obtained with density and properties variations.

In addition to introducing two strain rates for flamelet models, we broaden the choice of the conserved scalar to be used. Flamelet theory as a closure model for turbulent combustion has been based on the tracking of two variables: a normalized conserved scalar and the normal strain rate; the latter may be given either directly or through a progress variable. Mixture fraction has traditionally been used for the conserved scalar. A new normalized scalar is presented which is built on the Shvab-Zel'dovich conserved scalars. Another choice for the normalized scalar that has been developed is a functional of the velocity field.

More details can be found in References [7-10].

4.2 Flames with Both Normal Strain and Shear Strain

Three-dimensional, steady laminar flow structures with mixing, chemical reaction, normal strain, and shear strain qualitatively representative of turbulent combustion at the small scales are analyzed in Reference [10] for a mixing layer with compressive counterflow in the transverse y -direction and tensile strain in the z -direction for both non-reactive and reactive flows. This three-dimensional configuration for a mixing layer with imposed normal strain in the transverse plane has been analyzed through a similar solution for both non-reacting and reacting configurations. A system of the Navier-Stokes equations coupled with equations for scalar transport was developed and solved. More recently, in work yet to be published, the similar solutions have been compared favorably with new multi-dimensional computations of the same configuration. Of course, the similar solution will be more useful for sub-grid models in the future because of its lower computational costs. Variable density, temperature, and composition are considered. One bounding stream for the mixing layer is pure oxygen or sometimes a fuel-lean combustible mixture while the other stream is pure propane or sometimes a fuel-rich combustible mixture. The enhancement of the mixing and combustion rates by imposed normal strain on a shear layer can be very substantial. Furthermore, the imposition of shear strain and thereby vorticity on the counterflow can be substantial indicating the need for flamelet models with both shear strain and normal strain.

Density and properties variations are considered. Results for the velocity and scalar fields are found for ranges of Damköhler number Da , normal strain rate due to the counterflow, streamwise-velocity ratio across the mixing layer, Prandtl number, and Mach number. A conserved scalar is cast as the independent variable giving an alternative description. The imposed normal strain decreases mixing-layer thickness and increases scalar gradients and transport rates. Diffusion control is possible for partially premixed flames in the multi-branched flame situation. There is substantial enhancement of the mixing and combustion rates by imposed normal strain on a shear layer. Also, the imposition of shear strain and thereby vorticity on the counterflow can be substantial indicating the need for flamelet models with both shear strain and normal strain.

The Damköhler number Da is an important parameter in the reacting case, which has been varied over a range of one order of magnitude here. In the definition of Da here, the reaction rate is normalized using a residence time x/u_∞ . The diffusion flame becomes thinner with increasing Da but its position does not change in either the single-flame or multi-flame configurations. The premixed flames show some diffusion control, especially at lower values of Da and less flammable inflowing mixture ratios. In some cases, we can expect at least the fuel-rich premixed flame to fit the similar solution format with no change in location as Da varies.

The shear-strain rate and the normal-strain rate have opposing effects on mixing layer thickness and thereby on scalar gradients, mixing rates, and burning rates. Increased shear-strain rate increases slightly both the displacement of streamlines and the width of the mixing layer. Increases in the normal strain rate can profoundly decrease the mixing layer width and increase transport rates.

In another study [8], methane-air counterflow simulations are presented, in computationally efficient similar form, allowing combustible mixtures to flow from one or both directions to learn more about multi-branched propagating flame structures (e.g., a triple flame). These structures with both premixed and non-premixed flames are commonly seen in more practical combustion analyses. Our findings here with methane and detailed kinetics show that the multi-flame structures found for counterflow with propane and one-step kinetics are not confined to one fuel choice or to simplified kinetics. The diffusion-control aspect for the partially-premixed flame appears with different chemical kinetic approaches and with different fuels.

A range of realistic mass mixture fractions and asymmetric chemical rate laws are examined while avoiding the commonly forced unreal symmetric behavior with one-step second-order kinetics. Moreover, a survey of critical parameters is performed varying pressure and normal strain rate to define the flame structure and detect different characters. Three flames can co-exist if the strain rate is low enough and the pressure is high enough. Additional details are given in Reference [8].

4.3 Rotational Flamelets in Multi-Dimensional Counterflow

A new flamelet model is developed to be used for sub-grid modeling and coupled with the resolved flow description for turbulent combustion. The model differs from current models in several critical ways. (i) Non-premixed flames, premixed flames, or multi-branched flame structures are determined rather than prescribed. (ii) The effects of shear strain and vorticity on the flames are determined. (iii) The strain rates and vorticity applied at the sub-grid level are directly determined from the resolved-scale strain rates and vorticity without the use of a contrived progress variable. (iv) The flamelet model is three-dimensional without need for assuming axisymmetry or planar geometry. (v) The effect of variable density is addressed in the flamelet model. Solutions to the Navier-Stokes equations and the associated scalar equations governing the flamelet model are obtained without the boundary-layer approximation. By appropriate coordinate transformation, a similar solution is found for the rotational flamelet model, reducing it to a system of ordinary differential equations (ODEs). Vorticity is shown to create a centrifugal force on the sub-grid counterflow that modifies the molecular transport rates and burning rate. Sample computations of the rotational flamelet model without coupling to the resolved flow are presented first to demonstrate the importance of the new features of the model. Scaling laws are presented for relating strain rates and vorticity at the sub-grid level to those quantities at the resolved-flow level for coupling with large-eddy simulations or the time-averaged mean-flow level for Reynolds-averaged flows. The time-averaged behavior of a simple turbulent flow is resolved with coupling to the rotational flamelet model. Specifically, a two-dimensional, multicomponent, time-averaged planar shear layer with variable density and energy release is employed using a mixing-length description for the eddy viscosity. Needs for future study are identified.

Combustion in high mass-flux chambers is the practical and major method for energy conversion for mechanical power and heating. Inherently, the high mass-flow rate leads to turbulent flow. Thereby, many length and time scales appear in the physics making serious challenges for both computational and experimental analyses. For computations where the smallest scales typically cannot be resolved, the method of large-eddy simulations (LES) is employed wherein the smaller scales are filtered via integration over a window size commensurate with the computational mesh

size that allows affordable computations. Consequently, the essential, rate-controlling, physical and chemical processes that occur on shorter scales than the filter size must be modelled. Those sub-grid models must be properly coupled to the resolved LES flow field.

Current flamelet models that are used for LES or Reynolds-averaged Navier-Stokes (RANS) methods have some advantages. Typically, the flamelet equations are a system of ordinary differential equations (ODEs) that can be solved offline with solutions available in tabular form or through neural networks (NN). The flamelet models can handle multi-species, multi-step oxidation kinetics without requiring small time steps during the solution of the resolved-scale fluid dynamics. Thus, for several reasons, savings of computational resources can be huge compared to direct numerical simulation. We aim here to retain these very attractive features while removing some less desirable features. Already, some progress has been made in extending the fundamental flamelet theory beyond its long-term limitation of a single-flame structure, two-dimensional (or axisymmetric) configuration, and use of the uniform-density assumption. However, those advances still must be applied to LES or RANS. In addition, the flamelet theory must be advanced to consider shear strain and vorticity at the small scale of the flamelet; these are the vital forgotten physics in current flamelet modeling. Furthermore, the strain rates in the flamelet model are far from properly connected to the strain rates at the resolved scale. Attempts at corrections of these weaknesses are made here.

The focus here is on the types of turbulent flames found in the shear-driven flows of practical combustors. Thereby, we address flamelets as originally described by Williams [41], namely “highly sheared small diffusion flamelets” and “forming a turbulent flame brush which appears on the average to fill” the flow domain. Our discussion will not cover some interesting work on corrugated or wrinkled flames. The goals of this work are to improve the flamelet model by including several important physical effects that are commonly neglected in present models and to identify other issues that require further study, e.g., such as related to the coupling between the sub-grid-scale physics and the resolved-scale (or time-averaged) physics..

There is need to understand the laminar mixing and combustion that commonly occur within the smallest turbulent eddies. These laminar flamelet sub-domains experience significant strain of all types: shear, tensile, and compressive. Some important works exist here but typically they are restricted for either counterflows with only normal strain or simple vortex structures in two-dimensions or axisymmetry and often with a constant-density approximation. See, for example, Peters [33] and Pierce & Moin [34]. Linan [40] and Peters focused on the counterflow configuration. Williams [41] first established the concept of laminar flamelets in the turbulent diffusion flame structure. Karagozian and Marble [43] examined a three-dimensional flow with radial inward velocity, axial jetting, and a vortex centered on the axis. The flame sheet wrapped around the axis due to the vorticity. An interesting review of the early flamelet theory is given by Williams [42]. Generally, flamelet studies have focused on either premixed or non-premixed flames; a unifying approach to premixed, non-premixed, and multi-branched flames has not been developed. That unifying approach is taken here.

Most flamelet studies have not directly considered vorticity interaction with the flamelet. Williams [41] first recognized the advantage of separating rotation (due to vorticity) and stretching by transformation to a rotating, non-Newtonian reference frame. He did not however examine the

momentum consequences in the new reference frame, which will be examined later here. The other works that have examined vortex-flame interaction have not separated the effects of stretching and rotation. See Marble [44], Karagozian & Marble [43], Cetegen & Sirignano [45, 46], and Meneveau & Poinso [47].

A new flamelet model is developed for use in sub-grid modeling for analysis of turbulent combustion by RANS and LES. This flamelet model presents certain key advances: (i) non-premixed flames, premixed flames, or multi-branched flame structures are allowed to appear naturally without prescription; (ii) the impacts of shear strain and vorticity (and associated centrifugal effects) on the flames are determined; (iii) the applied sub-grid strain rates and vorticity are directly related to the resolved-scale strain rates and vorticity without the use of a contrived progress variable; (iv) the flamelet model is three-dimensional without need for assuming axisymmetry or planar geometry, allowing the physically correct counterflow under the vorticity constraint; and (v) variable density is addressed in the flamelet model. The results indicate that each of these five features introduces consequential, vital physics that is missed by current two-dimensional, irrotational, constant-density flamelet models that assume a priori a non-premixed- or premixed-flame structure and make no direct connection to shear strain or vorticity on the larger turbulence scales.

Information from direct numerical simulations concerning the relative alignments of the vorticity vector, scalar gradients, and principal strain axes provides a basis for a set of assumptions. The analytical framework allows for multi-step, detailed kinetics although the calculations here are limited to one-step propane-oxygen kinetics. The quasi-steady assumption used in previous flamelet models is maintained here.

A similar solution is found for the flamelet model. Sample computations of the flamelet model without coupling to the resolved flow are presented first to demonstrate the importance of the new features of the model. The rotation due to vorticity creates a centrifugal force that generally decreases the mass-flux through the flamelet counterflow. Thereby, an increase in residence time and a decrease in burning rate occur. Rotation can thereby allow flames, which would otherwise extinguish, to survive. Premixed flames can only exist with orders-of-magnitude larger values of Da compared to diffusion flamelets or multibranched flames. Thereby, we can expect that premixed flames will be less likely to survive extinction in a turbulent situation with high strain rates. The partially premixed flames in a multibranched flame structure are driven by heat flux from the diffusion flame; thereby, they survive at lower values of Damköhler number Da .

Scaling laws relate sub-grid strain rates and vorticity to resolved-scale quantities for coupling with large-eddy simulations or Reynolds-averaged flows. Given these relations, the burning rate is determined by the rotational-flamelet physics and the energy release rate and rate of change of species mass fraction are given to the resolved scale by the rotational-flamelet algorithms. The theory does not introduce any new contrived variable such as a flamelet progress variable. Connection between the two scales is made using long established variables.

For this initial study, a highly challenging turbulent flow is deliberately avoided. Rather, a simple turbulent flow is resolved with coupling to the rotational-flamelet model in order to explore the interaction across the different scales. A two-dimensional, multicomponent, time-averaged planar

shear layer with variable density and energy release uses a mixing-length description for the eddy viscosity and is coupled to the new rotational-flamelet model. The eddy diffusivity is proportional to the local magnitude of the velocity gradient and grows with downstream distance. These simplifying assumptions are only used in this first demonstration of the application of the sub-grid flamelet model. They should not be generalized to be an inherent component of the approach.

The profiles for velocity and scalar properties are seen to broaden with downstream distance in the shear layer, indicating the growing width of that layer. With increasing downstream distance, the zone where burning occurs moves towards the oxygen-rich side (for the chosen propane-oxygen kinetics) whether or not it is the faster stream. That burning zone becomes narrower with increasing downstream position.

Some results are shown for three types of flame configurations: a diffusion (non-premixed) flame, a multi-branched flame structure, and a premixed flame. We reference to a certain value of Da by defining $K = Da / Da_{ref}$.

4.3.2 Diffusion Flame: We treat a situation with a three-dimensional diffusion-flame structure at the sub-grid level. Figure 16 shows the influence of vorticity on the flamelet stability near the extinction limit. The rotation of the flamelet due to vorticity causes a centrifugal effect on the counterflow velocity and thereby on the residence time in the vicinity of the reaction zone. The dash red and solid red curves represent K values of 0.195 and 0.196, respectively, both without vorticity. Despite the very modest difference in K , one survives as a strong flame and the other is basically extinguished. By applying $K = 0.195$ and normalized vorticity $\omega = 1.0$ and therefore rotational speed of value 0.5, the solid blue curve is obtained, indicating a strong flame with regard to both reaction rate and peak temperature or enthalpy is induced by the rotation. Actually, the $K = 0.196$, $\omega = 1.0$ curve falls right on the solid blue curve as well. The rotation causes a lower mass flux than what was obtained without rotation. The inflow rate is diminished because the centrifugal effect creates a more adverse pressure gradient. However, the slower flow rate allows a longer residence time and modifies the extinction limit. As K is lowered to values of 0.180 or 0.185, the flame is essentially extinguished in spite of the increased residence time due to the rotational effects.

The rotation also causes a decrease in the x-component of velocity and an associated increase in the z-component of velocity. Basically, the low-density products of combustion more easily flow in the z-direction wherein no centrifugal effect is applied. Specifically, when reaction and energy release occur, the outflow for the counterflow configuration will have the greater extensional strain rate in the principal direction aligned with the vorticity. The outflow velocity in the principal direction orthogonal to the vorticity might still experience a higher magnitude than the inflow velocity in the compressive-strain direction due to the density decrease in the flow. However, its increase will be less profound than for the velocity component aligned with the vorticity. Clearly, the combination of fluid rotation, variable-density, and three-dimensional structure have major consequences for flamelet behavior.

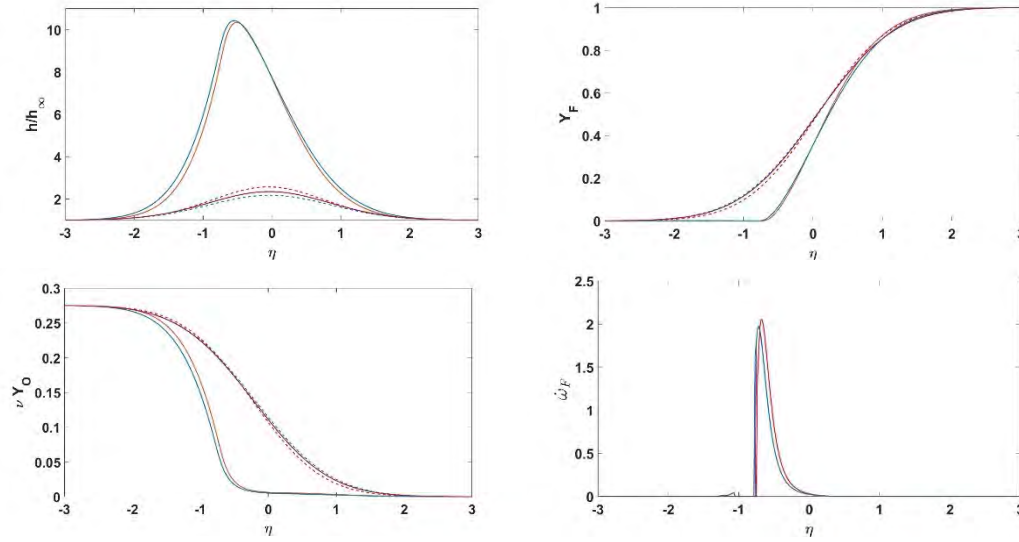


Figure 16. Diffusion flame with varying vorticity and Da . Dash red, $K= 0.195$, $\omega = 0$. Solid red, $K= 0.196$, $\omega = 0$. Solid blue, $K= 0.196$, $\omega = 1.0$. Solid purple, $K= 0.185$, $\omega = 1.0$. Dash blue, $K= 0.180$, $\omega = 1.0$. The $K = 0.195$, $\omega = 1.0$ case is covered by the solid blue curve.

4.3.2 Premixed Flame: The premixed flame is treated with consideration of a mixture that is 12% propane by mass and 43.5% oxygen by mass (stoichiometric proportion), with the remainder an inert gas. This flame structure requires a much larger Da to exist when compared to the diffusion flame. It extinguishes under high strain rate (i.e., low residence time in the counterflow). In Figure 17, Da and/or ω are varied. K varies between 15 and 40 while ω varies between 0 and 1. At lower values of the imposed vorticity, the flame extinguishes. Increased vorticity strengthens the centrifugal effect, increasing the efflux of the counterflow in the z -direction aligned with the vorticity vector.

Figure 17 shows that modest changes for the Da can result in differences in burning rate. As Da increases, the flame shifts to a position in the counterflow with higher incoming velocity and mass flux. All three components of the velocity generally increase as Da increases. There is an increase in the chemical reaction rate leading to an increase in the premixed flame speed and a flame position farther from the counterflow interface where the incoming velocity is larger in magnitude. At the lowest value of Da shown in the plots, the flame extinguishes as the reaction rate decreases because, in the spatially varying velocity field, it cannot obtain the needed residence time. The higher velocities result from the combination of an increase in mass burning rate and a decrease in density.

Vorticity produces the centrifugal effect that decreases outflow rate in the y -direction while increasing the outflow rate in the z -direction. It also causes the flame to stabilize at a larger distance from the interface. The inflow mass flux decreases as ω increases, implying an increase in the residence time.

It is noteworthy that the premixed flames require Da values that are orders of magnitude larger than required for diffusion flames. We can expect that they therefore are less likely to appear in highly strained turbulent flows.

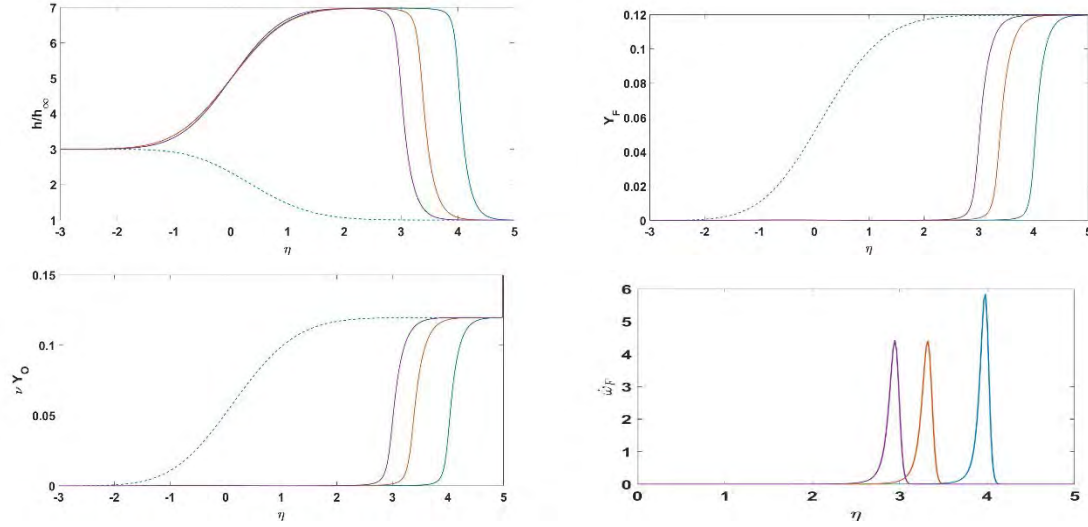


Figure 17. Premixed flame: influence of Da and vorticity. Blue, $\omega = 1.0$, $K= 40$. Red, $\omega = 1.0$, $K= 30$. Dash blue, $\omega = 1.0$, $K= 15$. Purple, $\omega = 0$, $K=30$.

4.3.3 Multi-flame Structure: For the multi-branched flame as well as the simple diffusion flame, fluid rotation, variable-density, and three-dimensional structure combine to have major consequences for the behavior.

In Figure 18, results are shown for a configuration with a fuel-rich mixture on one side of the inflow and a fuel-lean situation on the other side. The fuel-rich mixture exists with fuel mass fraction $Y_F = 2/3$ and oxygen mass fraction $Y_O = 1/3$ and flows inward on one side of the swirling flame. A fuel-lean mixture with $Y_F = 1/12$ and oxygen mass fraction $Y_O = 11/12$ flows inward from the other side.

Three flame structures can appear based on this new theory: a fuel-lean premixed flame on the left, a diffusion flame in the center, and a fuel-rich premixed flame on the right. The two premixed flames are not independent structures but rather depend substantially on heat flux from the diffusion flame [9]. As vorticity and rotation rate increase, the burning rate for each of the three flame branches and mass-flux through the counterflow decrease. The location of each of the flames shifts towards the fuel-lean side as rotation rate increases. Also, the fraction of the outflow in the direction aligned with the vorticity increases substantially with increasing rate of rotation.

For both the multi-branched flame and the single diffusion flame, values of the rates of normal strain, S_1 in the x -direction and S_2 in the z -direction, have consequence on the behavior. As S_1 decreases and S_2 increases, the flame zone moves slightly, the integrated burning rate decreases, and the normalized mass flux through the counterflow decreases. As S_1 decreases, the velocity

component in the x -direction increases while the velocity component in the y -direction decreases and velocity reverses direction in the region of highest temperature and lowest density. So, again in that low-density region, there is inflow (compressive strain) in two directions with outflow (tensile strain) only in the z -direction. In some cases, an inflowing particle of material enters at first with decreasing magnitude of y with Lagrangian time and increasing values of x and z in time. However, a reversal for the x -direction is seen with the entire outflow going in the z -direction. This behavior is consistent with DNS findings concerning alignment of vorticity and principal strain axes for reacting flows.

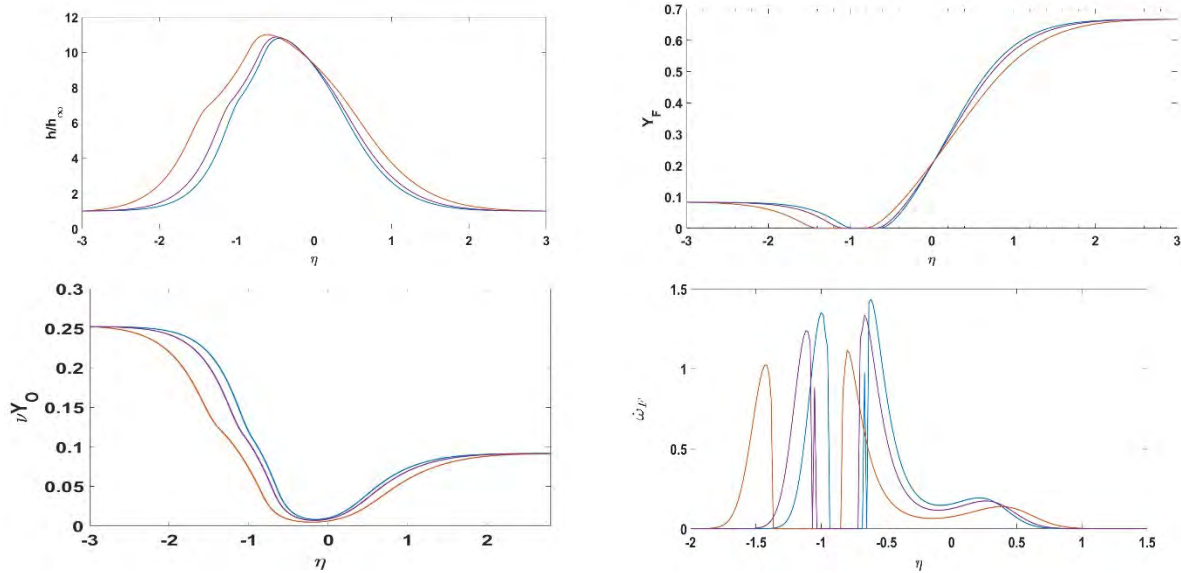


Figure 18. Multi-branched flame with $K = 0.200$ and varying vorticity. Blue, $\omega = 0$. Red, $\omega = 1.50$. Purple, $\omega = 1.0$.

In the future, multi-step kinetics should be utilized with the rotational-flamelet model. The model can be used to produce look-up tables or neural networks that can be employed with LES or RANS calculations.

There are several important issues that should be addressed in future studies to allow better matching between the closure model for the sub-grid mixing and combustion with the resolved-scale (or time-averaged) flow: (1) the lags, due to the turbulence cascade, in spatial position and time for the coupling between the large-scale strain and the energy release that it affects; (2) the degree of partial mixing of reactants during the cascade; (3) the proper choice of the parameter to represent the optimal sub-grid volume-size for averaging; and (4) relative magnitudes of the vorticity and normal principal strain rates on the sub-grid scale. These matters can be examined through carefully designed DNS and perhaps clever experiments. Attention is needed to improve our knowledge of the statistical relations between resolved-scale quantities for vorticity, strain rates, and scalar gradients and those quantities on the flamelet scale. Of course, flamelets can in principle exist across a range of the smaller scales, not just the smallest scales. Also, better determination is needed of the range of scales where mixing and reaction are prominent.

More details are found in Addendum IV.

4.4 Inward Swirling Flamelets

A new rotational flamelet model with inward swirling flow through a stretched vortex tube is developed for sub-grid modeling to be coupled with the resolved flow for turbulent combustion. The model is built upon the same theoretical foundations as the work described in Sub-section 4.3. Therefore, it has the same critical new features: (i) Non-premixed flames, premixed flames, or multi-branched flame structures are determined rather than prescribed. (ii) The effects of vorticity and the related centrifugal acceleration are determined. (iii) The strain rates and vorticity applied at the sub-grid level can be directly determined from the resolved-scale strain rates and vorticity without a contrived progress variable. (iv) The flamelet model is three-dimensional. (v) The effect of variable density is addressed. Here, the inward swirl is created by vorticity combined with two compressive normal strain components; this feature distinguishes the model from counterflow flamelet models, including the work in Sub-section 4.3.

Solutions to the multicomponent Navier-Stokes equations governing the flamelet model are obtained. By coordinate transformation, a similar solution is found for the model, through a system of ordinary differential equations. Vorticity creates a centrifugal force on the sub-grid counterflow that modifies the molecular transport rates, burning rates, and flammability limits. Sample computations of the inward swirling rotational flamelet model demonstrate the importance of the new features. Premixed, non-premixed, and multi-branched flame structures are examined. Parameter surveys are made with rate of normal strain, vorticity, Da , and Prandtl number. Again, the centrifugal effect has interesting consequences when combined with the variable-density field. Flow direction can reverse; burning rates can be modified; flammability limits can be extended.

4.4.1 Diffusion Flame: Without rotation and also with $\omega = 0.5$, there is negligible reaction rate and heat release, essentially yielding extinction as shown in Figure 19. Fuel and oxidizer just diffuse and mix without significant exothermic reaction. Further increase of the rotational rate with $\omega = 1.0$, however, yields a strong flame with a narrow reaction zone.

The heat release causes a decrease of the density in the vicinity of the flame. A plane still exists in the rotating reference frame where two different mixtures come together in a direction aligned with the scalar gradient while turning into the z -direction aligned with the vorticity. The expanding gas can cause a flow reversal of the inward flow from the x -direction, orthogonal to the scalar gradient. The increased rotational rate produces the centrifugal acceleration that inhibits radially inward flow of the heavier gas and allows the expansion and velocity reversal for the lighter, hotter gas.

The combination of fluid rotation, variable density, and three-dimensional structure have major consequences for inward swirling flamelet behavior. The specific mechanism is not immediately obvious but can be inferred from the results. The strong swirl causes the reversal of the x -component of velocity and an increase in the z -component of velocity, both now being outward flows from the combustion zone. However, the fractional decrease in density is significantly larger than the fractional increase in outward velocity. So, the outward mass flow rate is reduced, which is consistent with the reduction of the inward mass flow rate when the inward flow ceases to come from both the x - and y -directions and is limited to only the y -direction. Thereby, an increase in residence time of the flow in the reaction domain is allowed. This increase in vorticity and thereby in swirl rate changes the flammability limit.

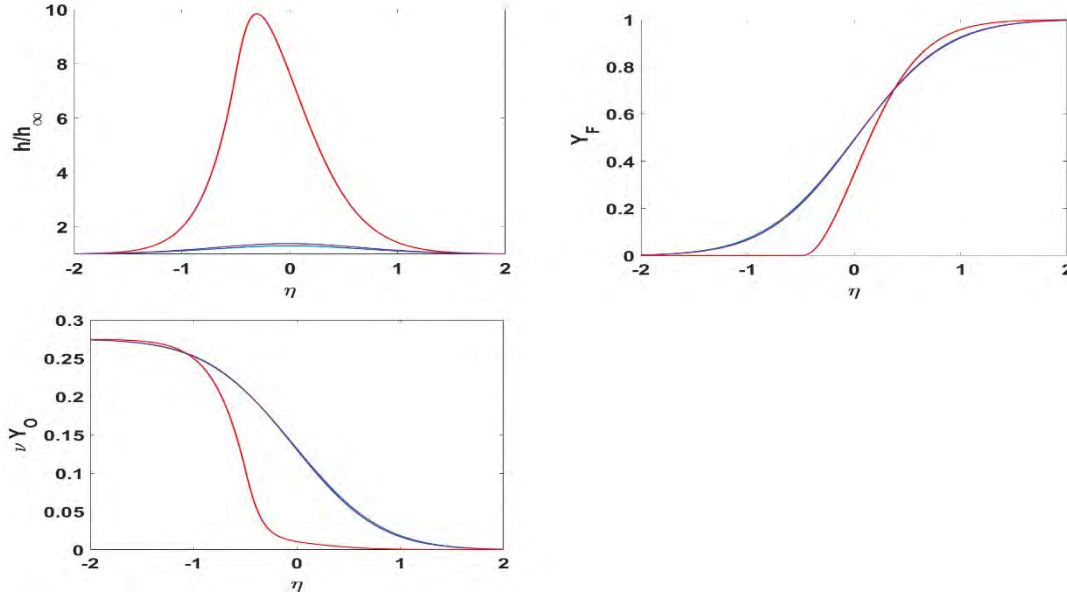


Figure 19. Scalar properties for inward swirling diffusion flame with varying vorticity. $K = 0.275$. Blue, $\omega = 0$, no flame. Purple, $\omega = 0.5$, no flame. Red, $\omega = 1.0$, flame.

4.4.2 Premixed Flame: The analysis here can apply to a situation where the inward swirling fluid has opposing streams of a combustible mixture and a hot inert gas (likely combustion products). A premixed flame can be established. As noted for the rotational flamelet in Sub-section 4.3, the premixed flame requires a Da value that is orders of magnitude larger than the required value for a diffusion flame. We expect therefore that the premixed flame is less likely to appear in turbulent combustion than the diffusion flame or the multi-flame structure. The vorticity and centrifugal motion can have consequence, especially near a flammability limit. Figure 20 has some interesting results. At a sufficiently high Da value, a strong premixed flame is shown to exist with or without a vorticity field. Application of swirl through the vorticity results in the same peak enthalpy or temperature and flame speed. The x -component of velocity is seen to reverse direction with or without imposed vorticity. However, the increase in rotational rate and centrifugal acceleration decreases the magnitude of the reversal. The premixed flame moves slightly farther upstream as a greater swirl rate or vorticity is applied. It likely occurs because, with less reversal in the x -direction, the expansion in the y -direction is enhanced.

4.4.3 Multi-flame Structure: For a sufficiently high value of Da , a strong diffusion flame and a weak, fuel-rich premixed can co-exist without a rotational flow. See the case with $K = 0.180$ and $\omega = 0$ in the Figure 21. The weak premixed flame is indicated by the region of negative second derivative for enthalpy on the right-side of Figure 21. (A negative second derivative also exists on the right-side of Figure 21 but is more difficult to detect.) The diffusion flame contributes to the region with the largest first derivative (the reaction rate which is the integrand) while the premixed flame contributes in the region where the first derivative is still positive but smaller. The existence of multiple flames is also indicated by consumption of oxygen to the right of the diffusion flame in the figure. The weak premixed flame is driven by heat diffusion from the strong diffusion flame. More information about these multi-flame structures is provided by [7, 8, 9, 15].

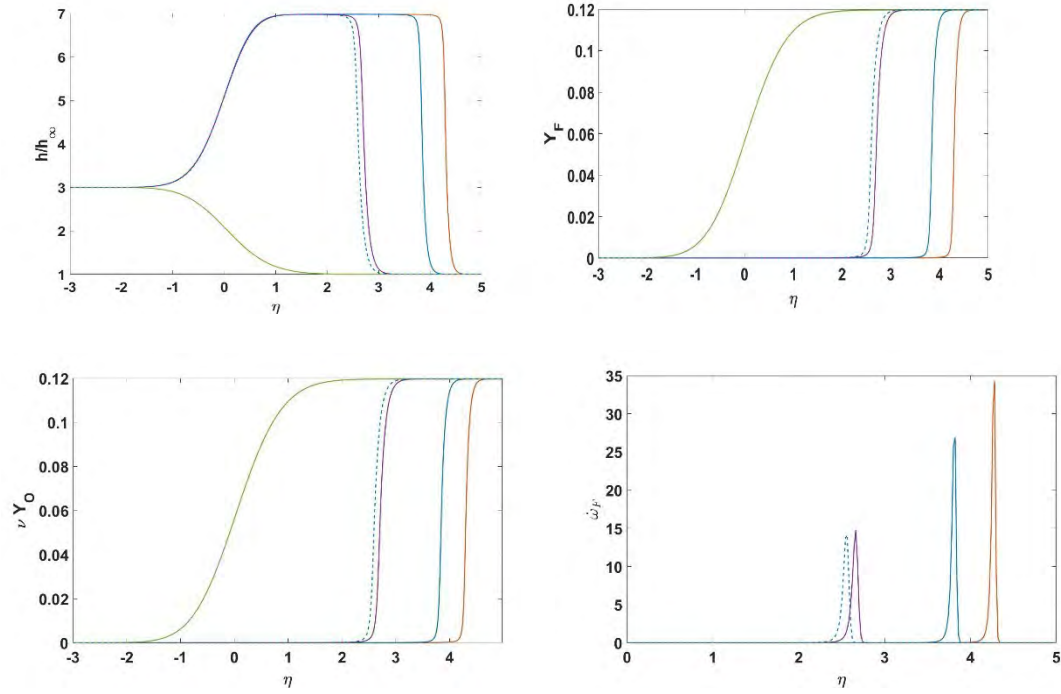


Figure 20. Scalar properties for premixed flame with varying Da and vorticity. $K = 250$, $\omega = 1.0$, red, flame. $K=200$, $\omega = 1.0$, blue, flame. $K=100$, $\omega = 1.0$, purple, flame. $K = 100$, $\omega = 0$, dashed blue, flame. $K = 20$, $\omega = 1.0$ green, no flame.

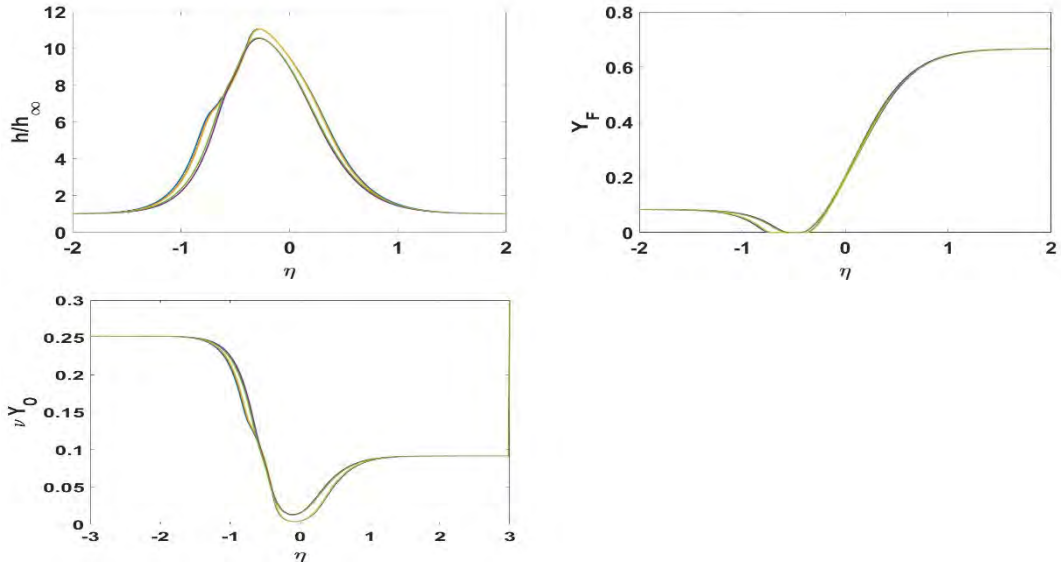


Figure 21. Scalar properties for multibranched flame with varying Da and vorticity. $K=1.00$: $\omega = 1.0$, blue; $\omega = 0.50$, red; $\omega = 0$, orange. $K=0.300$: $\omega = 1.0$, green; $\omega = 0$, purple.

More details about the inward swirling flamelet can be found in Addendum V.

5. Concluding Comments and Future Plans

Several improvements have occurred for modeling, descriptions, and understanding for liquid-propellant-rocket-engines (LPRE). Attention centers on turbulent combustion dynamics and instability, closure for reduced-order models using deep learning neural networks, chaotic behavior for the combustion instability, potential to use triggering for control of instability, the relevance of premixed flames versus non-premixed flames on the combustion instability, and the advancement of flamelet models.

The work described in Section 2 has demonstrated the usefulness of deep-learning neural networks (NN) for flamelet closure model and its ability to combine with CFD to capture the turbulent combustion dynamics and combustion instability. Our ability to design the neural network better for the range of tabular values needed has been shown for the type of computations under consideration. The CVRC combustion chamber has been modeled well for both the initial transient behavior and the asymptotic dynamic equilibrium. Also, the neural network can address changes in geometry which have large consequence on the stability of the combustor, such as the change in the oxidizer-injector port-length. The inclusion of the flamelet model for the three-dimensional rocket motor code demonstrates a future opportunity for the use of neural networks to replace the look-up table. Note that the flamelet model, the look-up table, and/or the neural network used for the subgrid flamelet model need not change as the configuration or its number of spatial dimensions varies.

Three-dimensional combustion instability has been examined in several multi-injector engine configurations with 10-, 19-, 30-, and 82-injectors. Chaotic behavior and sensitivity to small changes for the favored resonant mode have been identified. This gives interest to the use of deliberate triggering to serve as a control mechanism for changing the unstable mode to a less damaging mode. Some agreement with the Rocketdyne experimental results by Jensen et al. [25] has been explained. Needs for better resolution of the details of injector-port design and the supercritical thermodynamic behavior have been identified. The use of an engine configuration with fewer injectors to examine instability in an engine of the same size and shape and with the same mass flux but more and smaller-diameter injector ports has been examined. The method has some merit if care is taken to obtain the same burning rate. The use of flamelet theory for sub-grid models has been examined for multi-injector engines and comparisons have been made with results from the use of chemical kinetics directly at the resolved scale.

While the existing flamelet theory is used in our CFD modeling, successful efforts have addressed improvements in the model through a greater inclusion of relevant physics. Our extensions account for three-dimensional configurations that are multi-branched with both non-premixed and premixed flame structures. The effects of shear-strain rate and associated vorticity have been determined. Heat diffusion from the non-premixed flame can be a controlling factor for the premixed-flame burning rate. There is a future need to bring these improvements into use for the sub-grid modelling used with large-eddy simulations of liquid-propellant rocket engines.

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Physics-aware neural network flame closure for combustion instability modeling in a single-injector engine

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ABSTRACT

Neural networks (NN) are implemented as sub-grid flame models in a large-eddy simulation of a single-injector liquid-propellant rocket engine with the aim to replace a look-up table approach. The NN training process presents an extraordinary challenge. The multi-dimensional combustion instability problem involves multi-scale lengths and characteristic times in an unsteady flow problem with nonlinear acoustics, addressing both transient and dynamic-equilibrium behaviors, superimposed on a turbulent reacting flow with very narrow, moving flame regions. Accurate interpolation between the points of the training data becomes vital. A major novel aspect of the proposed NNs is that they are trained to reproduce relevant portions of the information stored in a flamelet table by using only limited data from a few CFD simulations of a single-injector liquid-propellant rocket engine under different dynamical configurations. This is made possible by enriching the training set with contrived data resulting from the physical characteristics of the combustion model and also by including the flame temperature as an extra input to the NNs that are trained to model other flame variables of interest. These physics-aware NN-based closure models are first tested offline by comparing them directly with the flamelet table and then are successfully implemented into CFD simulations in place of the flamelet table and verified on various dynamical configurations. The results from those tests compare favorably with counterpart table-based CFD simulations. Computational advantages of the approach are discussed.

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1. Introduction

In today's research world, huge availability of data has one eminent benefit, which is the use of machine learning to generate data-driven models. By means of machine learning and exploitation of this data, it is possible to explore potentially more descriptive models that help us achieve a better understanding of any phenomena. In recent years, there are numerous works exploring the application of different machine learning techniques in fluid mechanics for reactive as well as non-reactive flow modeling. Different techniques such as classification, clustering, and regression analysis have been applied to various problems in fluid mechanics and combustion studies [1]. Clustering is used mainly in the tabulation of probability density function (pdf)-based turbulent flame models through self-organizing maps algorithms [2–4]. Principal

component analysis (PCA) algorithms have been used for chemistry reduction in turbulent flame models [5–7]. The Neural Network (NN) approach, which is a regression based machine learning method, has been applied to model turbulence flow with chemical reactions in [8–10]. Convolutional NNs have been developed to estimate unfiltered variables from filtered ones from LES simulation with turbulent combustion [11]. The same technique has also been used to estimate the sub-grid reaction scale rates in [12]. The modeling of sub-grid quantities such as scalar dissipation rate is also discussed in [13]. More specifically, in combustion modeling, [14,15] used NN for the coupling of the linear eddy mixing sub-grid model with the LES. Owoyele et al. [16] developed a set of NNs to model diesel spray flame.

The ultimate goal of utilizing machine learning is to use the data from experiments and computationally expensive CFD simulations to develop low-cost NN-based models. Among initial steps toward this goal, articles like [17–19] developed NN-based models utilizing data from CFD simulations with flamelet closure. Flamelet, first introduced analytically by Williams [20], is defined as the thin reactive diffusive layer embedded in an otherwise non-reacting flow field. Peters [21] later proposed the idea of generating flamelet libraries based on presumed sub-grid distribution to

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Nomenclature

a_γ	ratio of specific heat capacity coefficient, K^{-1}
C	progress variable
e_f	flame internal energy, m^2s^{-2}
P	pressure, kPa
R	gas constant, $Jkg^{-2}K^{-1}$
T	flow temperature, K
T_f	flame temperature, K
U	axial velocity ms^{-1}
Z	mixture fraction
Z'^2	mixture fraction variance from the mean
γ	ratio of specific heat capacity
λ	thermal conductivity, $Wm^{-1}K$
ρ	density kgm^{-3}
$\dot{\omega}_C$	progress variable reaction rate (PVRR) $Kgm^{-3}s^{-1}$
$\dot{\omega}_i$	i-th species reaction rate, $kgm^{-3}s^{-1}$
χ	Scalar dissipation rate
Φ	flamelet input set
Ψ	flamelet output set

Superscripts

$\sim$	density-weighted Favre average
$-$	Reynolds average
$\hat{\sim}$	empirical mean of a set

treat turbulent combustion closure. From a data science perspective, these flamelet libraries are essentially sets of input/output blocks that can be isolated and replaced by NN-based models. Thus, the flamelet model provides a proper stepping stone for exploring the use of machine learning in the combustion studies. The NN-based models developed in [17–19] successfully replace the flamelet table in their CFD testbeds. In particular, the NN-based flamelet model in [19] has been developed to be used with the Sandia Flame D. NNs have been used in [17] for representing a flamelet model in a stably burning flame in Sydney bluff-body swirl-stabilized flame.

Recently, Shadram et al. [18] explored NN capability of replacing flamelet libraries as a sub-grid flame closure model to simulate longitudinal combustion instability in a single injector rocket configuration called the Continuously Variable Resonance Combustor (CVRC) [22,23]. Highly turbulent flow field, with a Reynolds number of 400,000 based on the mean oxidizer mass flow rate, occurs in the CVRC test-bed. The flame is also subjected to intense acoustical fluctuation that significantly alters its behavior depending on the cycle [24–26]. Pressure and thus the flame variables change drastically when the instability occurs. The NN training process presents an extraordinary challenge due to the multi-scale lengths and characteristic times in an unsteady flow problem with nonlinear acoustics, addressing both transient and dynamic-equilibrium behaviors, superimposed on a turbulent reacting flow with very narrow, moving flame regions. Accurate interpolation between the points of the training data becomes vital. Shadram et al. [18] addressed these challenges by using relatively large NNs, and proposing a training set selection method that requires full access to the pressure-dependent flamelet table. In that work, the NNs were validated by testing on the table, and verified in multiple stability configurations of CVRC. Similar to previous work, the results in [18] suggests that although NN requires a higher computational cost than a look-up table representation of a flamelet table, it requires much less memory. This feature provides the flexibility of using graphics processing unit (GPU) to reduce the associated computational cost [27]. The accuracy of the NNs in [18] are limited by the training data derived for the flamelet combustion model and thus inherent all the limitation associated with the model assumptions.

In a novel step closer toward this goal, the NNs in this work are trained directly using the CFD data, which only observes parts of the flamelet space. Our model are then verified by testing the NNs on a number of different simulations. The designed NNs are also tested on the whole flamelet table library, which includes the unobserved parts as well as the training data. The objective is to develop new NNs flame closures that can be more universally applicable in any reacting flow simulations while removing as much possible limitations found in our previous work.

Section 2 provides background on the flamelet model and the numerical scheme for our CVRC CFD analysis. Section 3 discusses the NN design and testing process in detail. In Section 4, first, the proposed NN-based flamelet models are validated by comparing them to table-based flamelet models, see Subsection 4.1. Then, the NN-based models are verified by comparing the NN-based CFD simulations with the table-based ones at different stability configurations in Subsection 4.2. The paper is concluded in Section 5.

2. Computational setup

Combustion instability is a potentially destructive acoustical phenomenon inside a combustion chamber, where an unstable high-amplitude pressure oscillation is excited and sustained by a high rate of combustion energy release. Study and theorization of liquid-propellant rocket engine (LPRE) combustion instabilities have been a major research subject for decades [28–32]. One key component of these studies is the numerical analysis done through CFD simulations, which requires the development of descriptive models that can represent a complicated phenomenon such as combustion in a turbulent reacting flow with unsteady pressure. Research has been conducted to generate such descriptive models [26,33].

In this work, we focus our modeling efforts on the combustion instability phenomenon, which occurs in the single element model rocket combustor called CVRC. A schematic of the CVRC experiment is shown in Fig. 1a together with the CFD solver's outline. Different stability behaviors are observed for different oxidizer post lengths. At its most unstable operation, CVRC consists of a 14-cm oxidizer post with a 38-cm combustion chamber. In this configuration, methane is injected through the outer concentric tube at 300 K, and the oxidizer, composed of 58% H_2O and 42% O_2 , is injected through the inner tube at 1030 K. The equivalence ratio in this globally fuel-lean flow is 0.8, which results from a constant mass flow rate of fuel and oxidizer at 0.027 kgs^{-1} and 0.32 kgs^{-1} , respectively. Although the CVRC experiment uses gaseous injection, it is an accepted benchmark for computational methods that address combustion instability in Liquid Propellant Rocket Engines (LPREs).

Both spontaneous and triggered instabilities in this single-injector coaxial dumped combustor have been analyzed using CFD simulations in the past [24,34,35]. The analysis resolves both types of unsteadiness, turbulent flow fluctuations and large-amplitude acoustic oscillations. In our work, the flamelet theory is used as a sub-grid model because it introduces the reasonable set of multi-physical phenomena that exist at sub-grid dimensions, such as chemical kinetics and molecular diffusion of heat and mass. Turbulence is treated using delayed detached-eddy simulation. Due to the intense local extinction and reignition observed in the CFD calculations [25], the Compressible Flamelet Progress Variable (CFPV) [36] is implemented. For all simulations performed in this work, we use an in-house structured finite-difference solver, as shown in Fig. 1b. The mesh structure is based on the mesh used in the 3D calculations in [26] and consists of 137,494 grid points. The smallest radial and axial grid sizes are 0.05 mm and 0.2 mm, respectively, which are located around the mixing shear layer or near any walls. The overall accuracies in time and space are fourth-

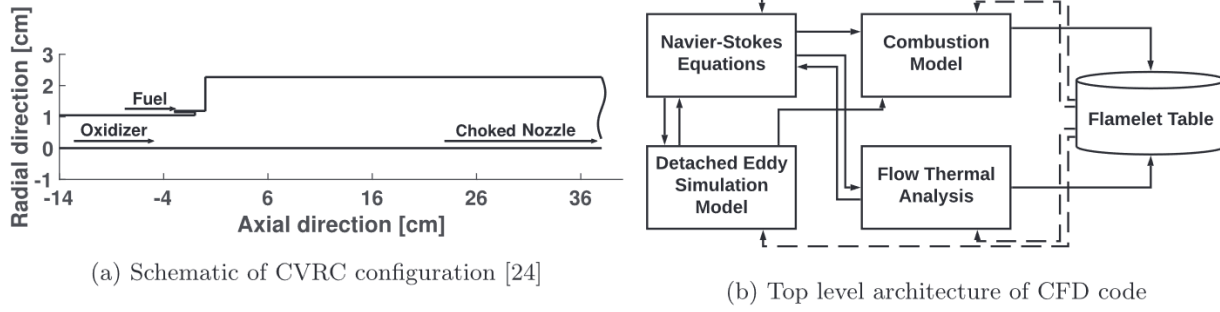


Fig. 1. Overview of the computational domain for the CVRC experiment and the CFD code architecture.

order and second-order, respectively. At both reactant inlets, a constant mass flow rate boundary condition is implemented using the Navier-Stokes characteristic boundary conditions [37]. A computationally efficient short-choked-nozzle [38] outlet boundary condition is used. The walls are assumed impermeable with the no-slip boundary condition. For the thermal aspect, two different boundary conditions are analyzed; in one case leading to spontaneous instability, the walls are assumed to be adiabatic. The second case assumes an isothermal wall temperature, which leads to triggering instability behavior [35] [35,39]. give a complete description of the current solver and numerical setup validation.

2.1. Flamelet and NN modeling

In the flamelet concept, the chemical time scales are shorter than the turbulent time scales so that the flame can be viewed as a collection of laminar flamelets [40]. This definition allows the chemistry computation to be performed independently of the main flow simulation and pre-process as flamelet libraries/tables. Since Peters [21] first proposed the turbulent flamelet closure method, there has been intense focus on developing flamelet models for non-premixed combustion with the most popular examples being the Steady Laminar Flamelet (SLF) [21], Representative Interactive Flamelet (RIF) [40], and Flamelet Progress Variable (FPV) [41] models. Regardless of the implementation strategy, one must first obtain the flamelet solutions. In this work, we solve the second order quasi-steady laminar flamelet equations in the mixture fraction space:

$$-\frac{\rho \chi}{2} \frac{\partial^2 \psi_i}{\partial Z^2} = \dot{\omega}_i \quad (1)$$

where ψ_i can be any reactive scalar quantities such as species mass fractions and temperature.

In the current CFPV model [42], presumed PDFs are used to relate the laminar flamelet solutions in the mixture fraction space to their Favre-averaged/mean counterparts. The β PDF is assumed for the mixture fraction while the Dirac δ PDF is assumed for both the progress variable and pressure. The Favre-averaged thermochemical quantities ($\tilde{\psi}_i$) at each pressure value are pre-processed as lookup libraries using the convolution:

$$\tilde{\psi}_i(\tilde{Z}, \tilde{Z}''^2, \tilde{C}, \tilde{p}) = \int_0^1 \int_0^C \int_{p_0}^p \psi_i(Z, C) \beta(Z, Z''^2) \delta(C) \delta(p) dZ dC dp \quad (2)$$

where Z is the mixture fraction, C is the progress variable. During the LES calculations, the solver only requires transporting a reduced set of governing equations for $\tilde{Z}, \tilde{Z}''^2, \tilde{C}$, with $\tilde{C}$ being the only reactive scalar. Therefore, flamelet model avoids the well-known stiffness problem associated with finite rate combustion models, especially for skeletal mechanisms such as the 27-species

and 72 reactions one used in this work. This presents no physical error in the expected situations where mixing is generally the rate-controlling process, but detailed chemistry is needed to determine accurately the flame temperature and product composition. Complete description of the flamelet governing equations as well as in-depth examination of the CFPV model impact in predicting combustion instability in the CVRC are given in [25].

There are 7 flamelet tables, which describe the flame thermochemical properties, needed for the CFD calculations: $\tilde{\Psi} = [\tilde{\omega}_c, \tilde{T}_f, \tilde{e}_f, \tilde{R}, \tilde{\lambda}, \tilde{\gamma}, \tilde{a}_\gamma]$. From a data science perspective, the seven flamelet libraries as formulated above are a set of well characterized outputs needed for CFD calculations with a reasonably well defined set of inputs: $\Phi = [\tilde{Z}, B, \tilde{C}, \tilde{P}]$, where parameter $B = \frac{\tilde{Z}''^2}{\tilde{Z}(1-\tilde{Z})}$ is a surrogate variable that resembles the variance of the mixture fraction to describe the combustion state in the turbulent flow. Therefore, reduced manifolds such as flamelet libraries are well suited for Neural Network closure model development.

Note that despite their advantages, the flamelet models still possess many limitations. The first weakness of the flamelet model is its turbulent closure approach, where sub-grid Probability Density Functions (PDF) are assumed for transported variables. Furthermore, flamelet theory usually assumes either an axisymmetric or planar strain field, while three-dimensional structure exists in realistic flow field. In addition, flamelet theory assumes that fuel or oxidizer would only exist on one side of the flame, yet, combustible mixtures can exist on both sides in a diffusion flame. Detailed discussions on the challenges toward improving flamelet models are provided in [43,44,45,46,47].

Fully regression-based data-driven models such as NNs, are designed to predict the output data provided to them as training examples, with the least error. Therefore, their predictive capability is limited by the properties of this data. Selecting the richest and most informative training data set is a crucial step in developing NN-based models. At current stages of exploring the potential of using NNs in combustion, where the NNs are trained based on currently available models, one should note that the predictive accuracy of the resulting models is limited by the accuracy of the target model.

One such way to improve the NN model proposed in this work is to provide it with higher fidelity training data, such as the table data coming from the Transported PDF method [48] together with In-Situ Adaptive Tabulation (ISAT) method [49]. The Transported Probability Density Function (TPDF) [50,51] is arguably the best closure model for chemistry-turbulence interaction, as it does not require any additional model for the chemical source terms. However, because of the high dimensionality of its argument, the model requires Monte-Carlo simulations of at least 30–50 notional particles in a cell. The PDF simulations are, thus, usually very computationally expensive even with a simple chemistry model [50]. Fortunately, ISAT can be used to accelerate chemistry calculation in a TPDF calculation by generating on-the-fly ta-

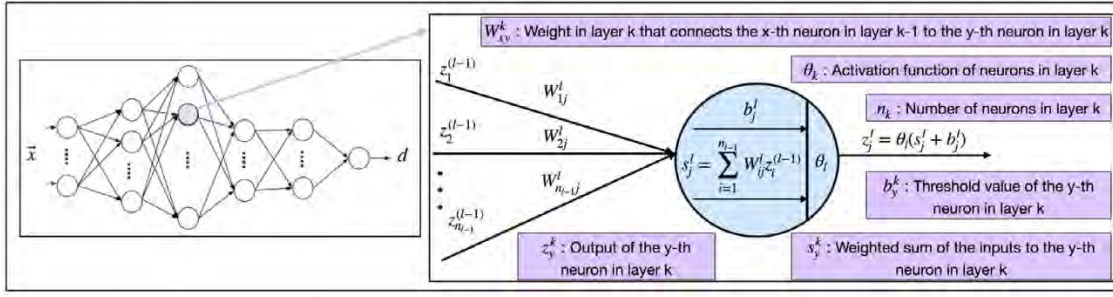


Fig. 2. Single output NN structure and schematic of a neuron as a computing unit in the NN.

bles that store thermo-chemical states from the previous timestep. Therefore, manifolds produced from such calculations do not suffer from simplifying assumption of the flamelet model. Furthermore, because of the adaptive tabulation strategy, we can eliminate the need to design sample selection strategy, as presented in Section 3.1 below. Furthermore, successful NN models generated from such dataset can significantly reduce the computational cost while maintaining reasonable accuracy compared to the TPDF method.

3. Neural network design

Neural networks are trained to emulate an input-output mapping based on a provided set of samples. Feed forward neural networks consist of connected layers of computational units called neurons. Each neuron performs a nonlinear function (activation) on a linear combination of the outputs of neurons in the previous layer via weights that collectively constitute the parameters of the NN. Fig. 2 provides a schematic of a neuron as a computational unit. The neurons in the final layer generate the output of the NN. Regression-type NNs, which are of interest in this work, minimize a cost function, which is the difference between the outputs of the NN-based model and the targets (training samples), in a least mean squared error sense over the parameters of the NN. This minimization is accomplished via the iterative Backpropagation method, which is an efficient implementation of gradient descent [52]. The cost function, R , of the regression NN for N training samples is defined as: $R = \frac{1}{N} \sum_{i=1}^N (d_i - y_i)^2$, where d_i is the sample output associated with an input x_i , and y_i the predicted output calculated by the NN. To find appropriate weights W_l for layer l , one minimizes R with respect to W_l , requiring that:

$$\frac{\partial R}{\partial W_l} = 0 \Rightarrow \frac{1}{2N} \sum_{i=1}^N (d_i - y_i) \frac{\partial y_i}{\partial W_l} = 0 \quad (3)$$

The Backpropagation algorithm recursively computes $\frac{\partial y_i}{\partial W_l} = 0, l = L, L-1, \dots, 1$ in Eq. (3). In its simplest form, this iterative algorithm starts from assigning a random initialization of the weights and proceeds with calculating the cost function and updating the weights in the direction of the negative gradients, i.e. $-\frac{\partial R}{\partial W_l}$, with a step size $\alpha > 0$ that is called the learning rate. More specifically,

$$W_l(k+1) = W_l(k) - \alpha \frac{\partial R(W_1, W_2, \dots, W_L)}{\partial W_l} \quad (4)$$

Using a random subset of the training dataset at each iteration results in the method of stochastic gradient descent (SGD). More advanced methods for selecting the step size at each iteration are comprehensively discussed in [53].

Here, the designed NNs (one for each of the flame variables) are meant to replace the flamelet table in the CFD structure shown in Fig. 1b; thus, the input set to the NN is Φ and the output set is

from Ψ . As discussed in Section 1, the ultimate goal of using NN is to develop a fully data-driven model from experimental and numerical data. This goal can be achieved if a rich enough data set of training samples is provided that covers different regions of flame dynamics. Since each NN is essentially designed to learn the pattern among these samples, the richer the training data set is the more comprehensive model can be developed. In this work, we use only the data that are generated from a single injector configuration. However, in a multi-dimensional system like combustion, one configuration observes only a manifold or a subset and not the whole dynamic. The availability of comprehensive data is essential in developing data-driven models. However, comparing the NNs trained on limited data helps to test the extent of the modeling power of NN beyond the training region and paves the way for further and more complicated methods.

3.1. Sample selection

A challenge that is particularly associated with learning from large data sets (numerical and or experimental data) is the selection of a sufficiently representative training set that does not lead to a high computational cost for the training process. As an example, a CFD simulation of spontaneous instability, in which the pressure signal grows from a relatively low pressure amplitude to a large amplitude limit cycle, requires simulation of 10 ms of the system to capture the whole dynamic. This simulation, the so-called transient case [18], is used mainly as the training set source. Storing data from this simulation at 200 kHz leads to a pool of data with around 275 million points.

In order to select the best training set at this stage, the framework of the flamelet table is utilized. In the table-based CFD set-up, the flame variables for a given input vector are calculated by linearly interpolating the values stored in the flamelet table. We then form the training set from the table values and corresponding inputs that have been called through the CFD simulation of each configuration. As mentioned above, by adding more simulations and experiments to the main pool of data, a richer set can be developed at the cost of more complex data management at the training stage. Here, we mainly use the transient simulation of CVRC with 14-cm oxidizer post. This data set leads to developing a relatively good model for every variable except for PVRR, due to lack of data in very high pressure regions. To remedy this situation, data from another simulation that is started after the occurrence of the instability, i.e. after high limit cycles have set-in, the so-called dynamic equilibrium case is also included in the training set for PVRR.

The observed points by the transient case amount to less than 3.3% of the flamelet table. Using only the transient case, significant regions of the table are not observed in the training set. To have a more reliable model, it is important that our model meets the physics-related constraints of the system. The training set generated from sampling the CFD simulation data does not necessarily

include the boundary points of the flamelet table, and these points define the flame dynamics of the sub-grid counterflow model. For example, for every pressure, turbulence level, and progress variable, the species mass fractions and temperature are known when the flow is purely oxidizer or purely fuel, which are indicated by $\tilde{Z} = 0$ and $\tilde{Z} = 1$. Accordingly, the value of all other flamelet outputs is known at these two points, regardless of the availability of training data from these regions. Moreover, the training set can be enriched by our knowledge of the flow when the progress variable is zero. At this point, there is no combustion, and the flamelet model is governed by the flow dynamics. Therefore, the flow data can be added to the training set.

3.2. Algorithm and structure

The training set based on the transient CFD simulation is used to train the NNs for each output table variable. To this end, three main NN structures are proposed based on the trade-off between increasing accuracy and decreasing the computational cost in data retrieval. A NN with a lower number of neurons and layers but a sufficiently small error is desired for each variable.

While the proposed structures are different for different variables, the training process is common. In all the NNs, the activation function in hidden layers is selected to be leaky rectified linear $LReLU(x) = \max(x, 0.001x)$ [54]. In the output layer, that function is linear. The NN weights are initialized randomly by the Xavier initialization algorithm [55] and updated via the Adaptive moment estimation (Adam) update rule [56] used in the back-propagation procedure. Adam is a well-known adaptive update rule, in which the learning rate for a weight at each iteration is determined by the running average of the magnitudes of recent gradients for that weight and the second moment of these gradients. The learning rate is initialized with 0.001.

A mini-batch, with a 30% of the data, training mode is also used, as it is helpful to avoid local-minima in the training process, and it more efficiently handles large data sets. The issue of overfitting can be observed even in simple regression problems, in which fitting a very high order polynomial leads to a smaller fitting error but a huge test error. To avoid overfitting and to improve the performance of the NN, we employed Tikhonov regularization during the training process.

The flamelet model assumes second-order ODEs for the species mass fractions and for the flame temperature. Other outputs of the flamelet model are essentially functions of species mass fractions and flame temperature. Thus, in developing NN-based models for those variables, flame temperature is also considered as an input. Accordingly, we have managed to significantly improve the accuracy of our NN-based models for $\Psi_1 = [\tilde{e}_f, \tilde{R}, \tilde{\lambda}, \tilde{\gamma}, \tilde{a}_\gamma]$. Including the flame temperature as an input along with the other flamelet inputs ($\Phi = [\tilde{Z}, B, \tilde{C}, \tilde{P}]$) not only helps to improve the accuracy but also ensures that the flamelet outputs are consistent when utilized in a CFD simulation by maintaining correct physical dependencies between different flame variables. A disadvantage of this approach is that the modeling error in $\tilde{T}_f$ can propagate in other variables as well.

Including flame temperature as an additional input improves accuracy in NN prediction. The highest accuracy improvement is for the linear expansion coefficient of heat capacity ratio (a_γ), as shown by the comparison in Fig. 3. The difference between CFD and flamelet temperatures, and consequently the difference between flamelet and flow internal energies, are very significant in the compressible regime. In our case, they are caused by the strong pressure gradient imposed on the flow field due to combustion instability. Therefore, the NN model ability to capture accurately a_γ behavior is crucial in this work. A NN developed on the original data set is shown in Fig. 3a. Fig. 3b shows the results in which

the training set is enhanced with values of a_γ at $Z = 0$, $Z = 1$ and $C = 0$, and flame temperature is added as an extra input to the model. Adding temperature as an extra input to the model helps the NN to learn the dynamic that was not observed in the original training data set. Significant improvement in the model prediction is observed for the interval of mixture fraction between 0.6 to 0.8; where the NN model faithfully captures the steep gradient dynamics when flame temperature is included as an extra input.

The NN designed for PVRR is the most expensive structure among all variables. Due to the very nonlinear dynamic of PVRR, finding an accurate NN model is a challenging task; this is discussed in more detail in Section 4.1.2. Our study did not indicate a considerable improvement in coupling PVRR inputs with $\tilde{T}_f$. The large structure for PVRR is selected after testing many other smaller structures which failed to capture its dynamic. The training error and testing error for the flame variables and PVRR are provided in Table 1 and further discussed in Section 4.1.

The structure of the NN proposed for each variable is provided in the second column of Table 1. In the third column, the computational cost of generating one output from each of the proposed NNs is given in terms the number of floating points operations (FLOP). Implementing these NNs inside CFD costs around 5815 FLOPs for calculating the outputs of the NN-based flamelet model at each point in time and space, which is the least NN-related computational cost that we could achieve among all of our several experiments, including our previous work [18]. As discussed in the literature, the computational cost issue related to the NN can be resolved by the utilization of GPU. However, in this work, CPU is used as the computational resource.

4. Results and analysis

The designed NNs are validated through different levels of testings using both offline and online data. Section 4.1 presents comparison between NN results trained from CFD data and the flamelet table itself to assess their performance. The objective of this activity is to identify the optimized NN structure. Note that such optimized NN should not be taken in the most absolute sense, but rather as the most optimized for the current configuration. The NNs developed from the first test are then implemented into the main CFD solver. CFD results between NN based and table based, which is where the training data are obtained, are compared. Finally, NNs simulation of triggered instability is performed. In this configuration, a 1030-K isothermal wall boundary condition is applied to dampen the instability of the dynamic equilibrium. Different perturbation waves are applied to the reactant flow rate, thus re-triggering the instability. The readers are referred to Nguyen et al. [35] for an extensive analysis the triggering instability phenomenon. Here, a setup with excitation through two periods of sinusoidal variation in mass flow rate is applied for the NN-based simulation. The main objective is to understand the potential of NNs for capturing correct behavior on data that they have not been trained on.

4.1. NN Validation using flamelet table

To analyze the performance of each NN, their outputs are compared with the corresponding outputs of the flamelet table, on the training set and on the whole table. To compare the set of the outputs, the overall relative error (e_o) defined in Eq. (5) is used:

$$e_o = \frac{\|\vec{d}^* - \vec{y}\|_2}{\|\vec{d}^*\|_2} \quad (5)$$

Here, $\vec{d}^*$ represents the outputs of the truth model (the flamelet table here), and $\vec{y}$ represents the outputs of the NN-based model. The training and testing errors are provided in Table 1, fourth and fifth

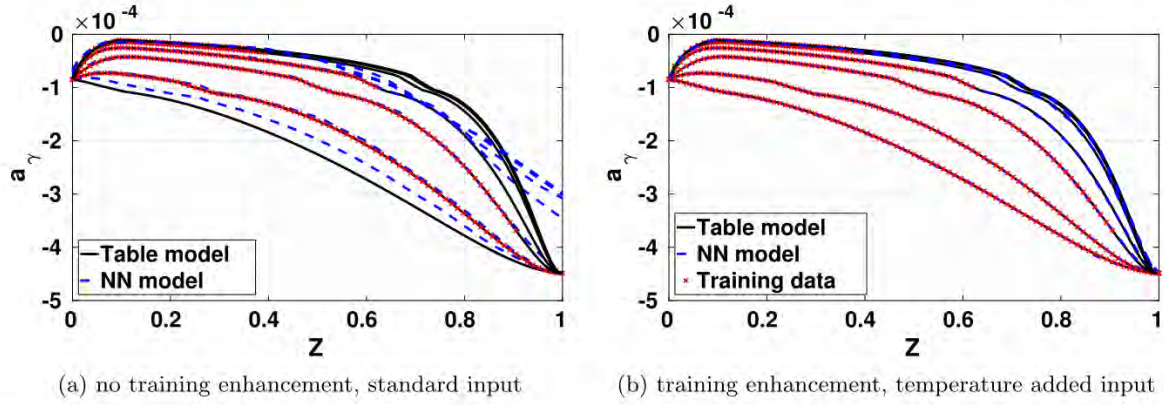


Fig. 3. Analysis on the effect of training data set enhancement and adding temperature to the input set on the performance of NN models for a_γ at $B=0$ when C varies.

Table 1
Selected structure for each NN for the flame variables.

Quantity	NN structure	FLOP	Training error (%)	Testing error(%)
$\tilde{T}_f$	4-15-10-15-1	375	0.59	4.83
$\tilde{e}_f$	5-15-10-15-1	390	0.0566	0.57
$\tilde{R}$	5-15-10-15-1	390	0.0526	0.65
$\tilde{\lambda}$	5-15-10-15-1	390	0.21	3.57
$\tilde{\gamma}$	5-15-10-15-1	390	0.0371	0.48
$\tilde{a}_\gamma$	5-15-10-15-1	390	0.22	1.41
$\tilde{\omega}_c$	4-15-20-25-35-25-20-15-5-1	3490	1.49	32.86

columns. e_o is essentially the root mean squared (rms) of the absolute error normalized by the rms of the target set. PVRR has the highest error in both cases. The variables in the Ψ_1 vector, which have flame temperature in their input set, are modeled with less than 0.25% in training and 4% error in test error. The flame temperature is modeled with an error of less than 0.6% in training and less than 5% in testing.

As discussed before, only parts of the flamelet library are included in the training set obtained from the CFD simulation. The distribution of the input values is not uniform, and the performance of the NN in the training stage and consequently testing is skewed by these distributions. For example, the frequency of occurrence of inputs in the laminar region or regions with lower turbulence is higher than that of points with higher turbulence levels. Therefore, it is to be expected that the performance of NN in the laminar zone will be better than in the rest of the table.

In Fig. 4, we compare the outputs from the NN for flame temperature, internal energy, gas constant, heat capacity ratio, its coefficient, and heat conductivity with the corresponding outputs from the flamelet table. Flame temperature is used as an extra input in the NN model for these variables (except itself). In each graph, a set of guidelines (dotted yellow line and dashed lines) are provided to measure the performance of the neural network in the training and testing stages. The dotted yellow line shows the 45-degree line, which is the loci of the desired data in a perfectly fitted model. The dashed guidelines reflect error bounds defined as a percentage of the maximum of the absolute value of each target variable, as shown in Fig. 4. The black crosses in Fig. 4 show the points from the testing stage.

4.1.1. Flame temperature

As mentioned above, flame temperature has a significant effect on the analysis of combustion. Therefore, a deeper analysis of the model's strengths and weaknesses could help in further improving the models. In the following, we compare the flamelet table data with the temperature calculated from both NN-based and the table-based models at different values of the parameter B . The ef-

fect of pressure on the errors in modeling flame temperature was insignificant; therefore, we only show the flamelets at a relatively high pressure point, 20 atm in Fig. 5. In each sub-figure, flame temperature is plotted as a function of mixture fraction for different values of progress variable (solid black curves). The maximum value of temperature has a monotonically increasing relationship with values of progress variable, i.e. when $\tilde{C}$ increases, maximum values of temperature increase, and curves converge together for higher $\tilde{C}$ values. The dark blue curves show the counterpart of each flamelet solution from NN-based models. On each curve, points used in the training set are shown with red cross markers.

The NN models for flame temperature are generated after reinforcing the training set with data from regions with high $\tilde{Z}$ values. In those regions, because there is no combustion, empirical evidence shows that $\tilde{T}_f$ depends linearly on $\tilde{Z}$. Essentially, there is a threshold in $\tilde{Z}$ value, which is a function of $\tilde{C}$, B , and $\tilde{P}$, above which this linear dependency sets-in. To determine the threshold values, we linearly interpolate $\tilde{T}_f$ values at specified $\tilde{Z}$ points where linear behavior is observed in the original data set. This way of reinforcing the training set helps to account for the lack of data in regions with high $\tilde{Z}$ values. The CFD simulations correspond to a fuel lean configuration, and therefore most of the collected data has lower $\tilde{Z}$ values. The lack of training points with high $\tilde{Z}$ values is correlated with deviations of NN-based models from the table-based models when $\tilde{Z}$ is near to one.

In Fig. 5a, the laminar flamelet model is shown. The availability of training data in the laminar zone is highest among different B values. It can be observed from Fig. 5 that where there is no training data, the NN-based curves deviate from the table curve. By increasing the turbulence level (parameter B), the availability of training points on the curve reduces, and the deviation of the NN-based curves increases Fig. 5b. Better performance can be observed in the lower mixture ratio side, where there is more data available.

4.1.2. Progress variable reaction rate

PVRR is a significant output of the flamelet model as it represents the combustion energy driving the transport equation for the

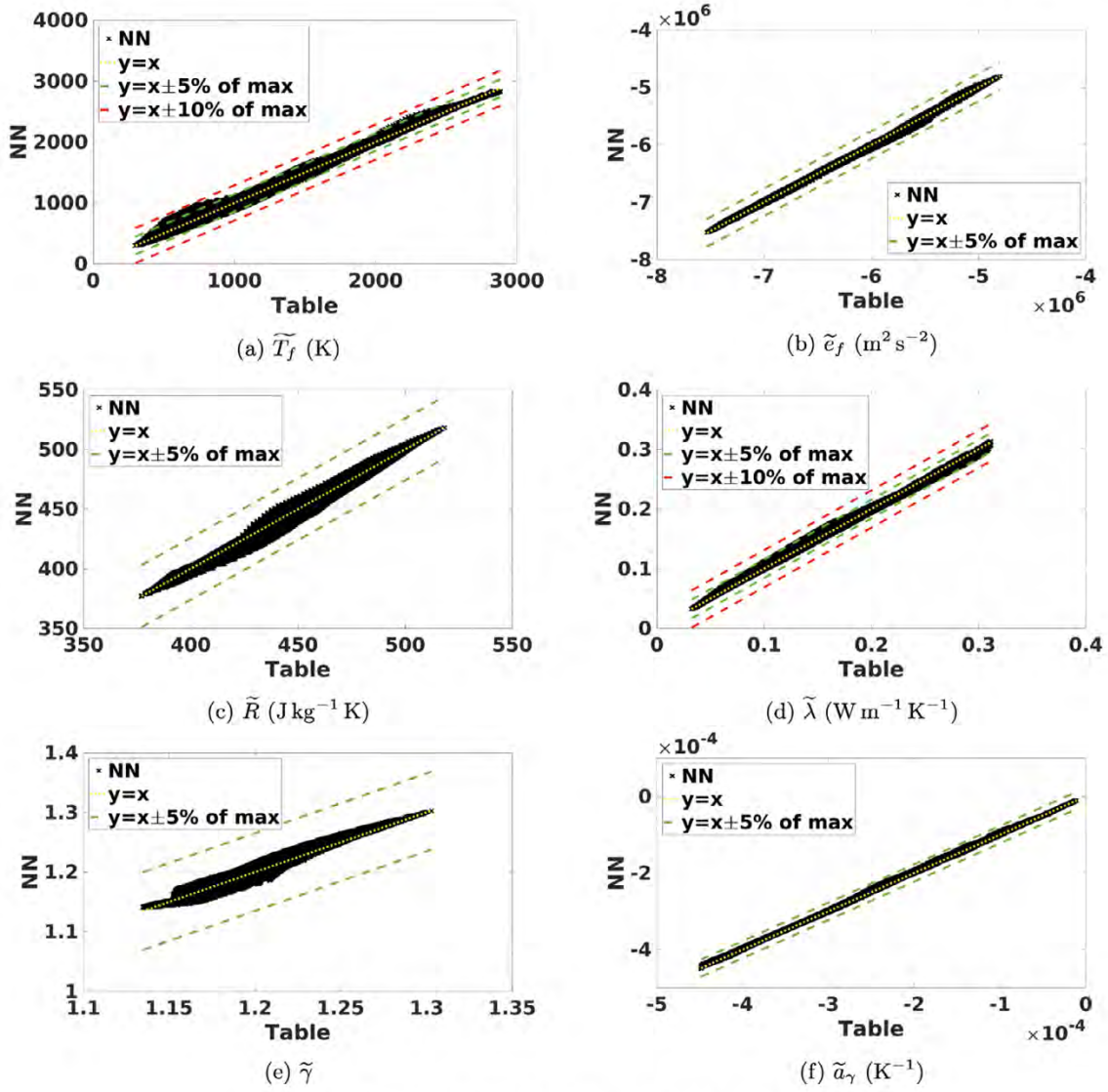
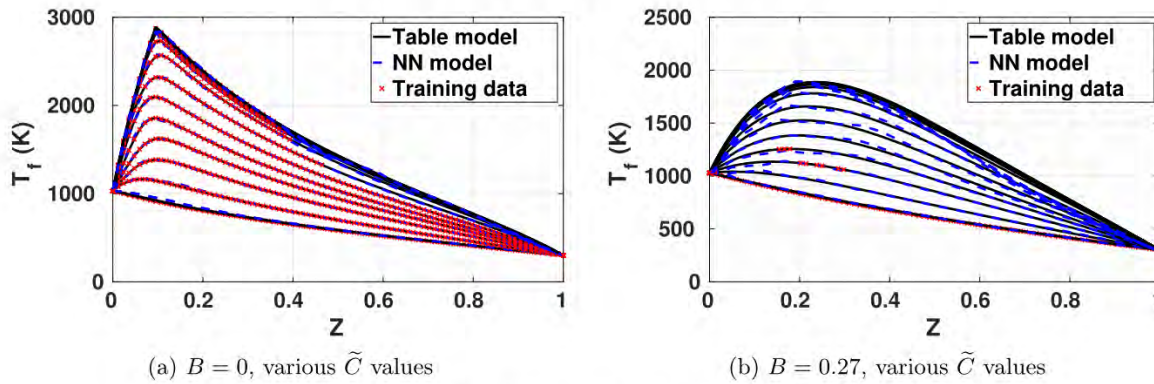


Fig. 4. Comparison of NN-based models and flamelet table data.

Fig. 5. Comparison of $\tilde{T}_f$ between the NN-based model and flamelet tables: dependence on B and $\tilde{C}$.

progress variable in the flamelet model. In this section, we investigate the performance of the NN-based model for PVRR. The magnitude of PVRR is drastically changed with pressure and, thus, it has multiple scales. This great range of magnitude affects the performance of the NN-based model. In the training process, we minimize the least squared-error in absolute manner; therefore, data

with a larger magnitude dominates the learning process, and the design becomes more affected by those points. The NN-based estimation of PVRR is compared with its table-based values in Fig. 6a. The black crosses show the test values. The testing points fall in the 5% guidelines, only for PVRR with higher magnitudes. The points with smaller values, however, have a higher error range and

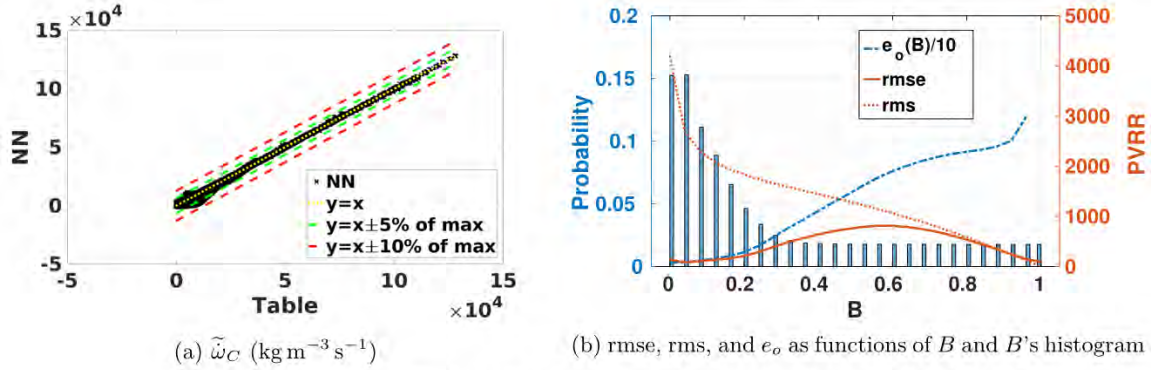
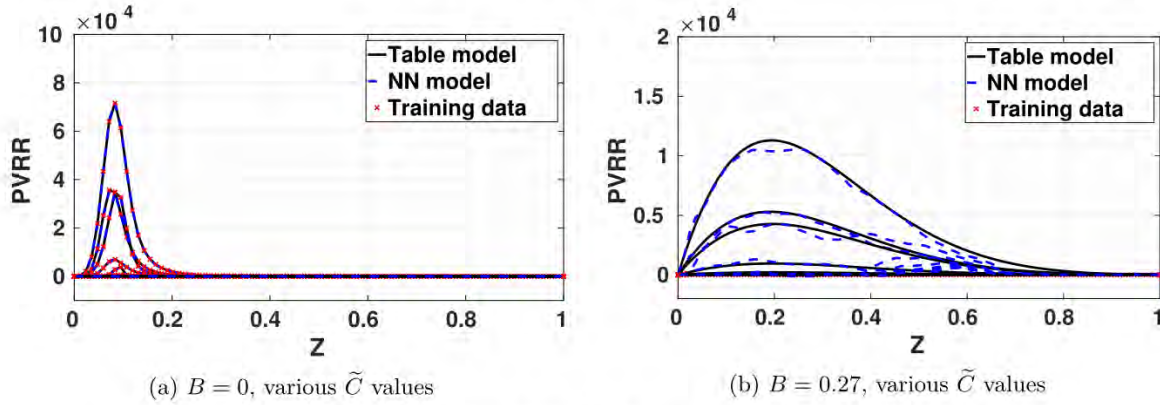


Fig. 6. PVRR NN performance analysis.

Fig. 7. Comparison of PVRR (kgm⁻³s⁻¹) between the NN-based model and flamelet tables: dependence on B and $\tilde{C}$.

fall in the 10% guidelines. In the analysis of combustion instability, the points associated with higher energy dominate the physics; so, better performance for the NN-based model for points with higher magnitude works in our favor. This result was achieved by reinforcing the training set with data from the dynamic equilibrium simulation, in which more points with higher pressure are available.

In the following, we investigate the flamelet solutions for PVRR in more detail. PVRR is highly affected by pressure. There is no data available with pressure values lower than 10 atm, and as a result, the averaged relative error is higher for the lower pressure range. Parameter B is also affecting the NN-based model performance significantly. The rmse and rms of PVRR as a function of parameter B is provided in Fig. 6b. The probability distribution of parameter B in the training set is also provided on the left axis of Fig. 6b. Around 60% of the training set has a B value lower or equal to 0.2. The one-tenth scaled relative error as a function of B is also provided on the left axis in Fig. 6b. For the laminar flame, where $B = 0$, the relative error is around 3%. Then it grows, as the probability distribution decreases in higher ranges of B values. The rms of PVRR also decreases with increasing the parameter B . The absolute error increases when the availability of data decreases and the distance of a point from B values with higher availability increases. When the rms becomes small, the rmse also decreases, while the relative error still goes higher.

In Fig. 7, we look into PVRR values of the flamelet table at 20 atm for different values of parameter B and progress variable. Different flamelet solutions of PVRR are provided with the black curves at different $\tilde{C}$ values in each plot. The behavior of PVRR changes drastically with the progress variable. Maximum values of PVRR occur at $\tilde{C}$ values around 0.15. The solid dark blue line shows the NN-based results. The training data are shown with a red cross

when read from the flamelet table. For the laminar flame ($B = 0$), there is more data available, and the NN-based model follows the flamelet solutions particularly well for lower $\tilde{Z}$ values, see Fig. 7b. The NN-based model starts to deviate when $\tilde{Z}$ goes to one, and there is not much data available due to fuel lean composition of the CFD-based data pool.

In Fig. 7, by increasing the B values, the availability of training data decreases, and performance degrades. The estimation maintained a decent level of accuracy up to $B = 0.27$ (see Fig. 7b) where the relative error is around 10%; yet, the results diverge more for higher B values. PVRR is the most challenging variable to model in the study of turbulent flame with unsteady pressure.

4.2. In-Situ test of NN-based models in CFD

To test the NN-based models further, we implement them into our CFD simulations by replacing the flamelet models. The configuration under study has a 14-cm oxidizer post length, which is characterized by a very high level of instability, according to [24]. Two simulations describing the dynamic equilibrium and triggering cases are analyzed. The results of the NN-based simulations are compared with the table-based ones to validate our NN-based models.

Since the NN models are trained on a set of data generated from a transient (TR) CFD simulation, as a first step, we implemented the model into the transient simulation. The pressure signal at two points in the oxidizer post and in the shear layer are compared for the NN-based and table-based simulations in Fig. 8. The NN-based simulation is more accurate where the pressure signal reaches the high amplitude limit cycle. The success of our NN-based model in this simulation is manifested by its ability to follow

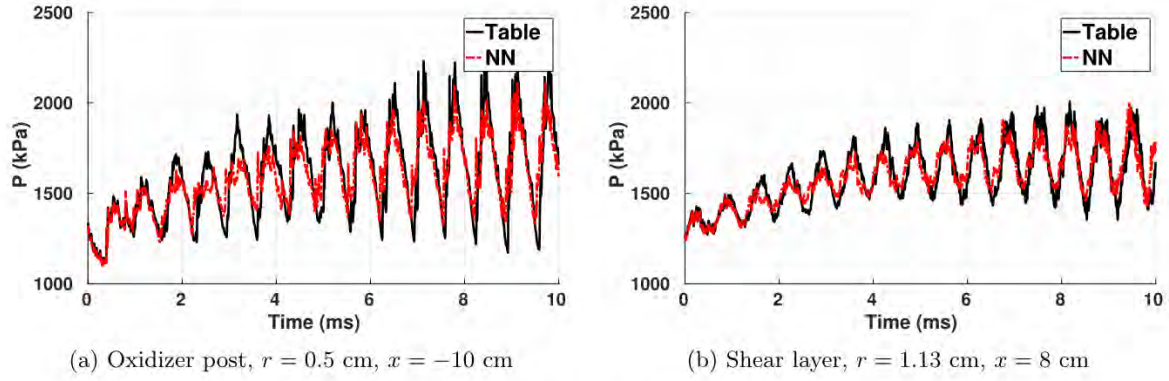
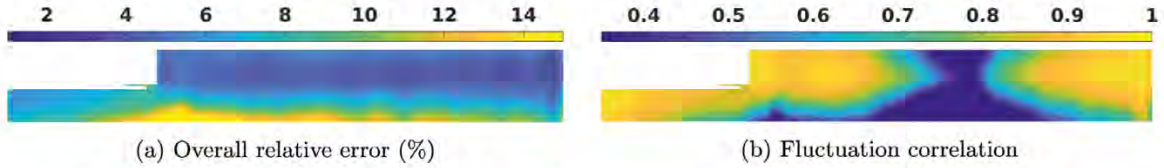


Fig. 8. TR: comparison of pressure time signals at representative points.

Fig. 9. DE: distribution of $e_o(\%)$ and correlation of pressure signals fluctuation between the NN- and table-based simulations.

the pressure growth from a low pressure point to a high amplitude limit cycle.

Another measure of performance of the simulation is how well the instability criterion is estimated. Coupling between the combustion heat release and the acoustic pressure wave is the most important factor for the combustion instability. Here, the correlation between PVRR fluctuations and pressure fluctuation is used as a measure of coupling between combustion energy and the acoustic wave. The analysis in [18] showed that the modified Rayleigh index (mRI), which is used here, resembles the same behavior as Rayleigh index. The time-averaged local mRI is defined in Eq. (6) over a time period (τ) which is typically few cycles; where p' , and $\dot{\omega}'_c$ are the local fluctuations in $\bar{P}$ and PVRR, respectively. Also, $\bar{P}$ and $\bar{\omega}_c$ are the global time averages of $\bar{P}$ and PVRR.

$$mRI = \frac{1}{\tau} \int_{t_0}^{t_0+\tau} \frac{\tilde{y} + 1}{\tilde{y}} \times \frac{p'}{\bar{P}} \times \frac{\dot{\omega}'_c}{\bar{\omega}_c} dt \quad (6)$$

Next, the performance of NN-based models are analyzed in the dynamic equilibrium and triggering cases.

4.2.1. Test on CFD: Dynamic equilibrium

First, we analyze the results from the dynamic equilibrium (DE) scenario, in which the simulation starts from an initial condition where instability has already set-in. In our analysis, we look at the overall relative error calculated at each spatial point by computing the norm of the difference of the pressure time waveforms from the NN-based and table-based CFD simulations. This error is shown in Fig. 9. In the combustor, most of the points have an e_o less than 5%. Higher errors occur on the centerline near the dump plane, where the numerical scheme is very complicated. Moreover, subtracting the mean pressure from each signal, we can also look into the correlation of the fluctuation of the pressure signals between the NN-based simulation and table-based one. This correlation is calculated using Pearson's formula [57] and is shown in Fig. 9b. The signals are highly correlated through the combustor except for regions in the vicinity of the pressure node, where the pressure fluctuation is very noisy.

Next, we look at the pressure time waveforms at two representative locations, one in the oxidizer post and another in the shear layer, see Fig. 10. In both locations, there is a great consistency between the table-based and NN-based simulations. The longitudinal

mode shapes of pressure at the centerline are plotted in Fig. 11. They represent the modulus of the Fourier spectrum first and second peaks of pressure signals at each grid point along the centerline. The phase of the first longitudinal mode is also compared at each grid point for the NN-based and table-based simulations in Fig. 11d. There is a great agreement in all of these graphs between NN-based and table-based simulations, with the exception of some inconsistencies in the vicinity of 20 cm location, which is a pressure node. The pressure waveform at the node can be considered as a noise signal, as the amplitude of the first harmonic is close to zero. The frequencies of the first and the second longitudinal modes across the combustor are around 1500 Hz and 3000 Hz, respectively.

The signal power of pressure fluctuations across the grid points of the combustor are compared between the NN-based and table-based simulations in Fig. 12b and Fig. 12a, respectively. The dark blue region in the combustor shows the vicinity of the pressure node where the oscillations have noisy behaviors. The main difference between the two simulations occurs in the middle of the oxidizer post, in which the NN-based simulation underestimates the rms. This is attributed to the inaccuracies in the PVRR model. In the oxidizer post, the PVRR should be zero or very close to zero, as there is no combustion occurring there. However, the training data was skewed toward higher values of PVRR, as they are important in the modeling of combustion instabilities. Generating an optimized training set for PVRR is a next step of this work.

Furthermore, the modified Rayleigh index is compared between the NN-based and table-based simulations in Fig. 12c and Fig. 12d, respectively. The high positive values in the left upper corner of the combustor show the driving effects of combustion on pressure instabilities. The two simulations are more consistent in the upper zone of the combustor. As it was discussed above and in [18], the behavior near the centerline is more complicated due to numerical considerations.

In Fig. 13, time-averaged values of flow temperature, PVRR, density, and axial velocity from the NN-based and the table-based simulations are compared. In all these variables, great consistency is observed between the two simulations. Mainly, PVRR shows differences on the centerline and axial velocity in the vicinity of the pressure node. In both of these locations, noisy behavior is observed due to their numerical and physical characteristics.

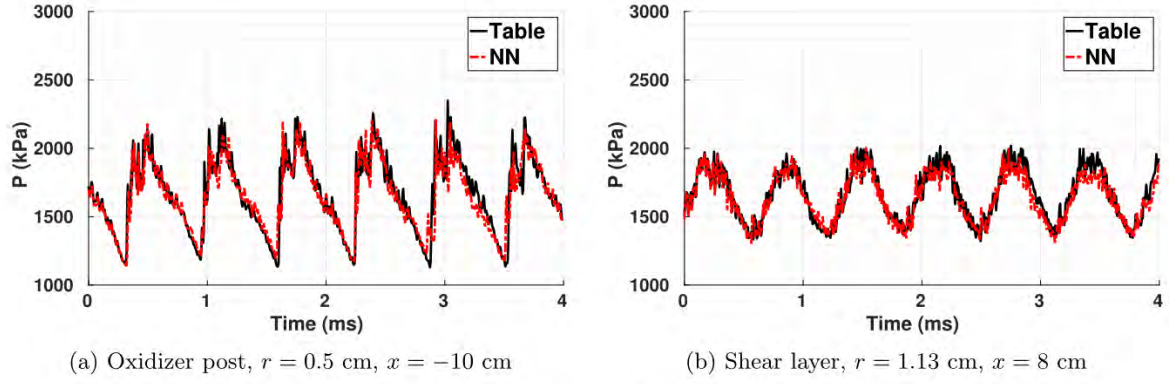


Fig. 10. DE: comparison of pressure time signals at representative points.

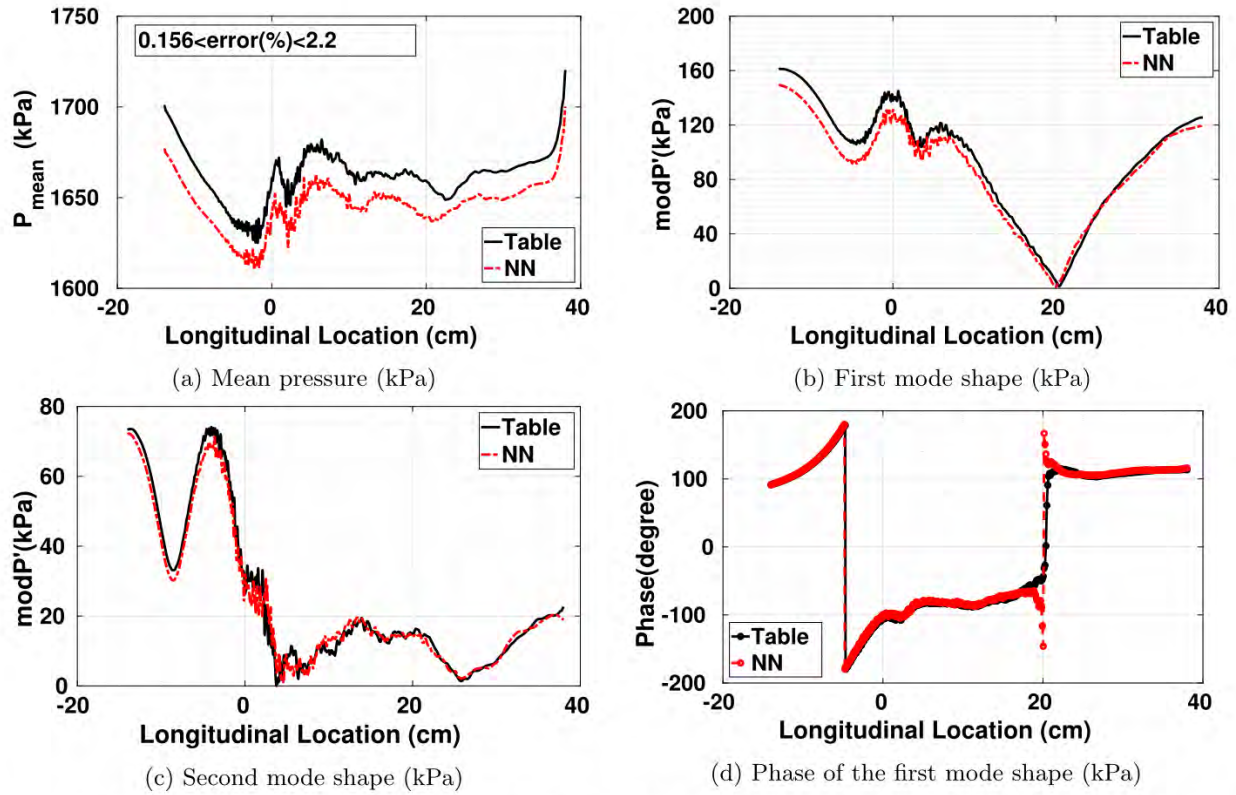
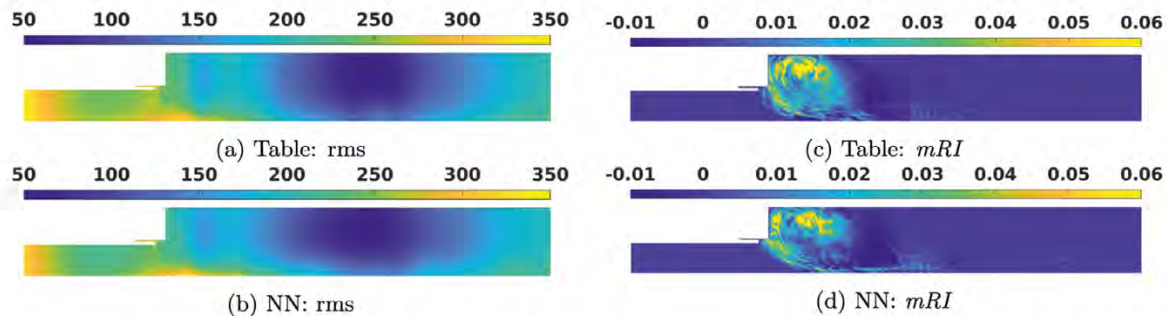


Fig. 11. DE: comparison of pressure mean, the first longitudinal mode and its phase, and the second longitudinal mode shapes between NN-based and table-based simulations along the centerline.

Fig. 12. DE: The rms of pressure signal fluctuations are compared between the simulations based on NN (12 b) and table(12 a). Also the mRI from the NN-based (12 d) and the table-based (12 c) simulations are compared.

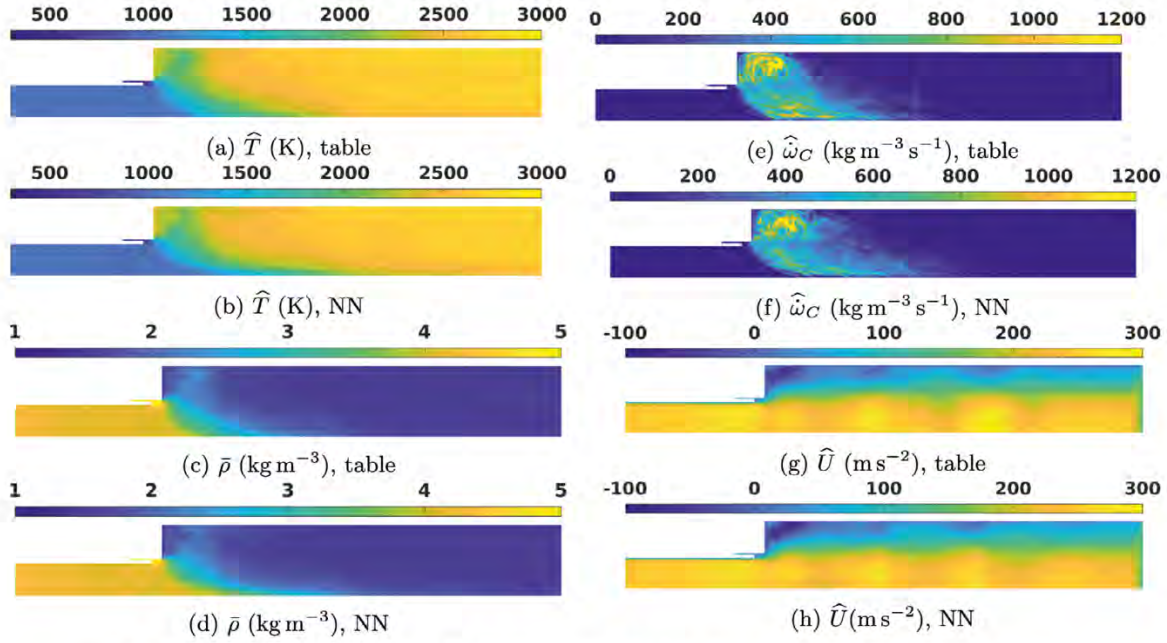


Fig. 13. DE: time-averaged temperature, PVRR, density, and axial velocity from the NN- and table-based simulations.

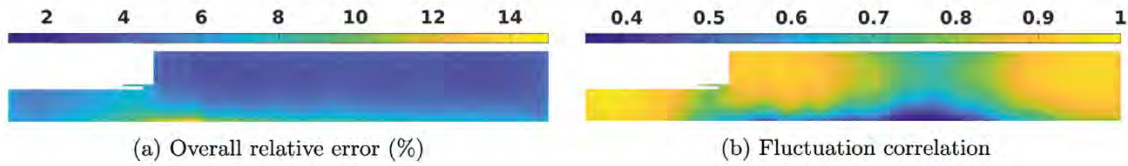


Fig. 14. TG: distribution of e_o (%) and pressure fluctuation signal correlation between the NN- and table-based simulations.

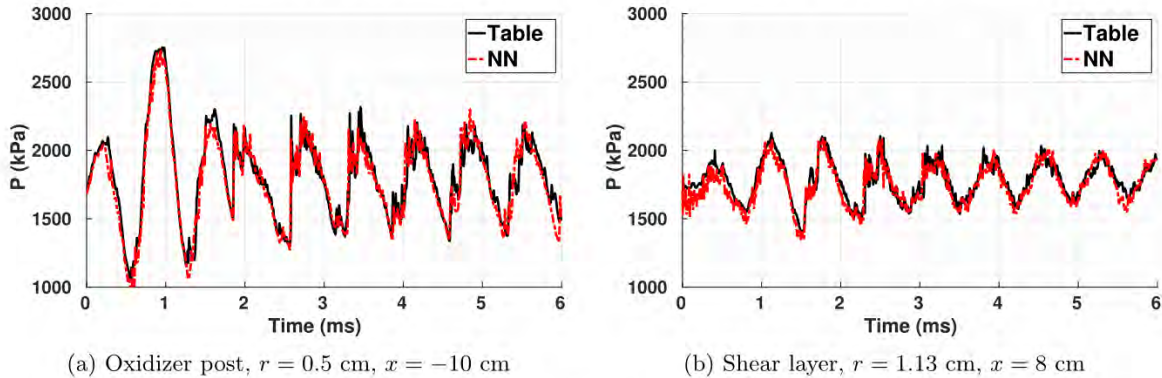


Fig. 15. TG: comparison of pressure time signals at representative points.

4.2.2. Test on CFD: Triggered oscillation

In the triggering (TG) scenario, heat loss is introduced by imposing an isothermal boundary condition on the chamber wall, and a sine wave perturbation on the propellant mass flow rate is applied for two periods. The top wall is modeled to be isothermal at 1030 K. The overall relative error between the pressure waveforms of the NN-based and table-based simulations is shown in Fig. 14a for most of the different grid points in the combustor to be less than 5%. We also look into the correlation of the pressure fluctuation signals between the NN-based and table-based simulations using the Pearson formula. The correlations are very high, except on the centerline in the vicinity of the pressure node, as shown in Fig. 14b.

Great consistency is observed in the pressure signal at the two representative locations (in the oxidizer post and in the shear

layer), Fig. 15. The pressure response to the perturbation in the mass flow rate can be observed in both simulations, with its effect on the response becoming damped after 2.5 ms.

The mean of pressure signal on the centerline, the amplitude and phase of the first harmonic of the Fourier spectrum, and the amplitude of the second longitudinal mode are plotted in Fig. 16. The mean pressure calculated from the NN-based simulation is within 2.2% of the table-based simulation. The amplitude of the first and second longitudinal modes are highly consistent between the two simulations. Differences exist in the inlet of the oxidizer post and near the nozzle, mostly in the second longitudinal mode. The phase graph of the NN-based simulation matches the one for the table-based simulation. The frequencies of the first and the second longitudinal modes across the combustor are around 1500 Hz and 3000 Hz, respectively.

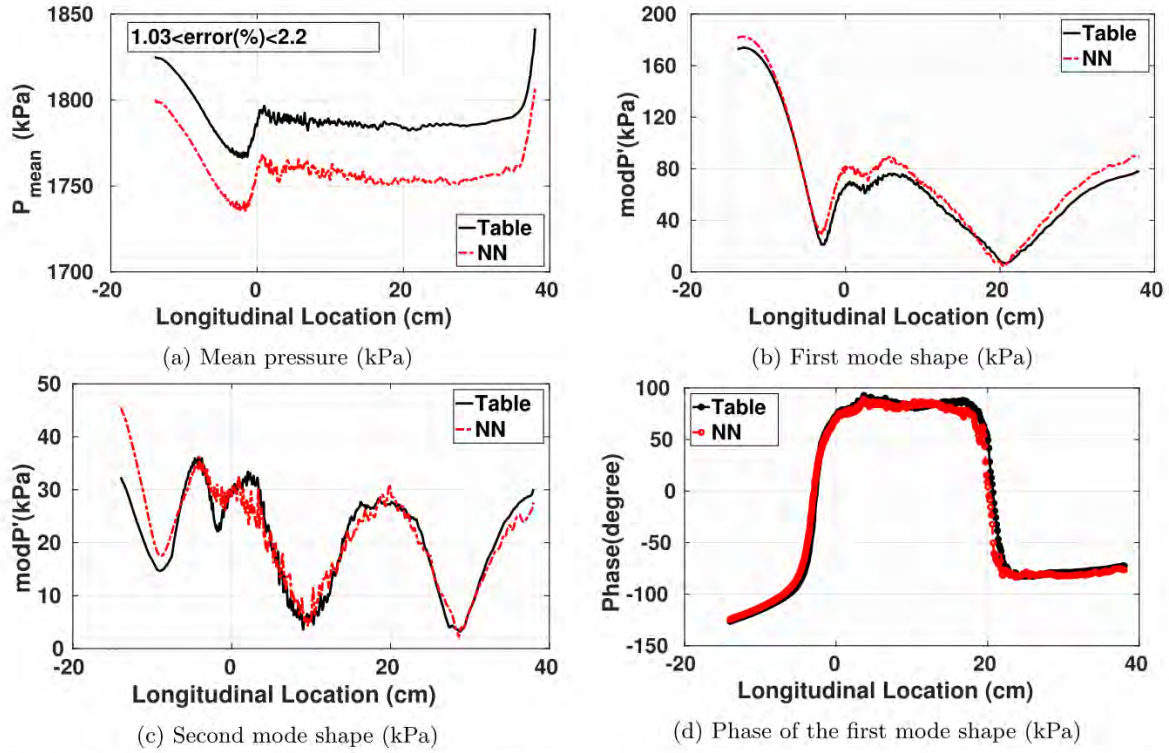


Fig. 16. TG: comparison of pressure mean, the first longitudinal mode and its phase, and the second longitudinal mode shapes between NN-based and table-based simulations along the centerline.

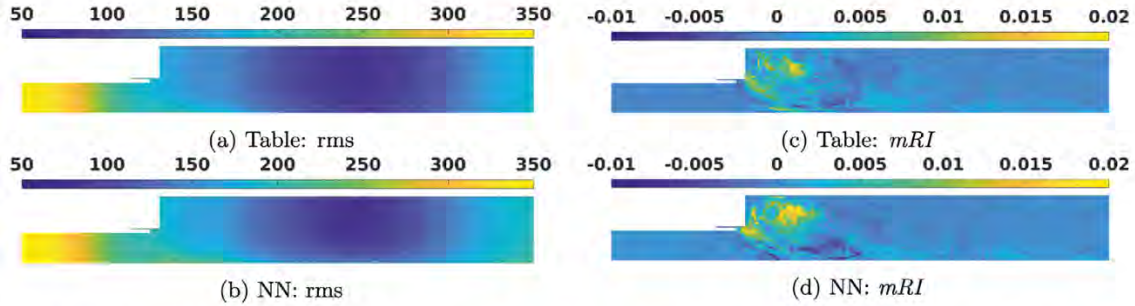


Fig. 17. TG: The rms of pressure signal fluctuations are compared between the simulations based on NN (17 b) and table (17 a). Also the mRI from the NN-based (17 d) and the table-based (17 c) simulations are compared.

Similar to DE scenario, the rms of pressure fluctuations across the grid points of the combustor are compared between the NN-based and table-based simulations in Fig. 17b and Fig. 17a, respectively.

The two graphs from the two simulations are highly consistent. Slight differences exist in the blue boundary in the combustion zone, indicating a slight overestimation of the pressure fluctuations in the NN-based simulation. This overestimation can also be observed through the mRI quantity that is compared between the NN-based and table-based simulations in Fig. 17d and Fig. 17c, respectively. The mRI shown in Fig. 17d indicates higher values leading to a higher instability level.

In Fig. 18, the snapshots of density are compared at the three time points of 1, 2, and 3 ms. The graphs are highly consistent between the two simulations. The first row in the figure shows the table-based simulation, and the second row shows the NN-based simulation. This consistency is also observed in the comparison of snapshots of axial velocity in Fig. 19, flow temperature in Fig. 20, and PVRR in Fig. 21, at the same time points. Although the detailed behavior is different at each snapshot, the overall characteristics are consistent between the two simulations. For example,

the location of the flame front, as shown in the graphs for PVRR, is similar between the two simulations.

4.2.3. Computational cost

In this work, we have not attempted script optimization and parallelization of the NN implementation in the CFD simulation. However, we can still compare the computational cost of the NN-based and table-based simulations lasting for one millisecond (200 snapshots) of simulation time in the dynamic equilibrium test. The average required CPU times per time step for the NN-based simulation is 39.2 times for that the table-based simulation. The computational cost of the table-based simulation is discussed in [24], where a 0.28 core-hour per millisecond was reported for an axisymmetric simulation with 6.26×10^4 grid points (the current work uses 1.375×10^5 grid points) based on a flamelet model for combustion of 27 species. The flamelet model requires around 1.2 GB of hard disk space, almost 118 times the required memory by the NN model, which is around 102 kB. As discussed before, given the very low required memory by NN-based models, GPU implementation is more feasible for the parallelization of the code and might be able to compensate for the higher required flops of the NN-based mod-

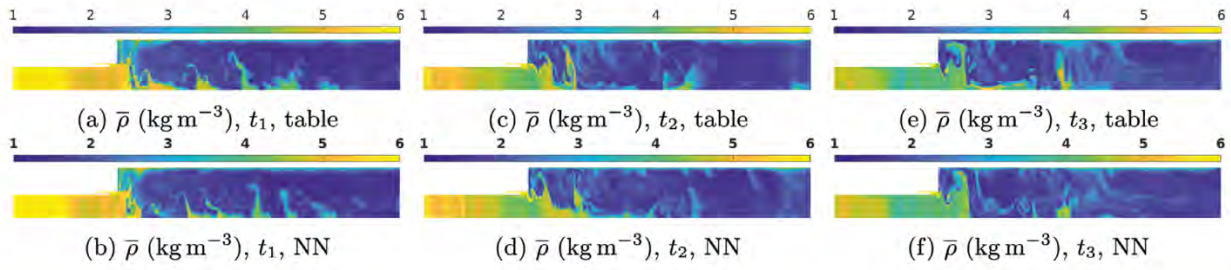


Fig. 18. TG: Density.

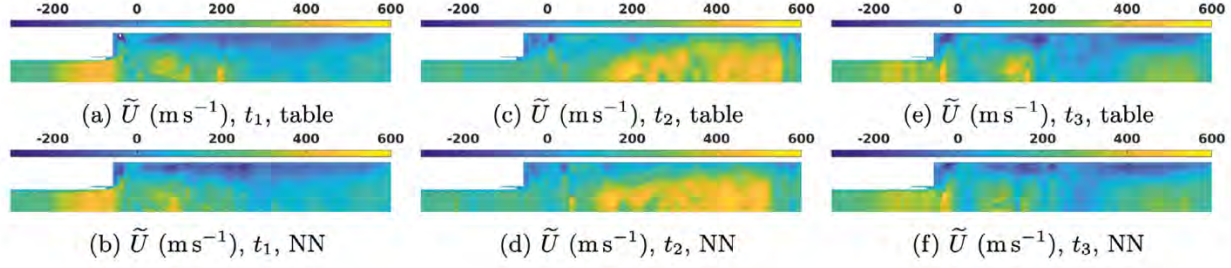


Fig. 19. TG: Axial velocity.

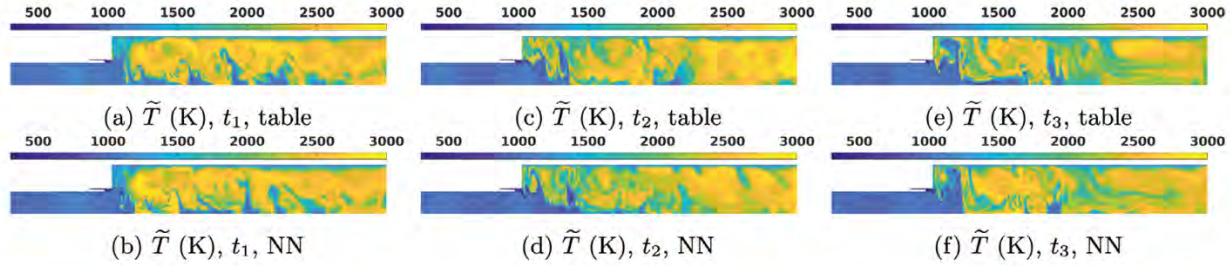


Fig. 20. TG: Temperature.

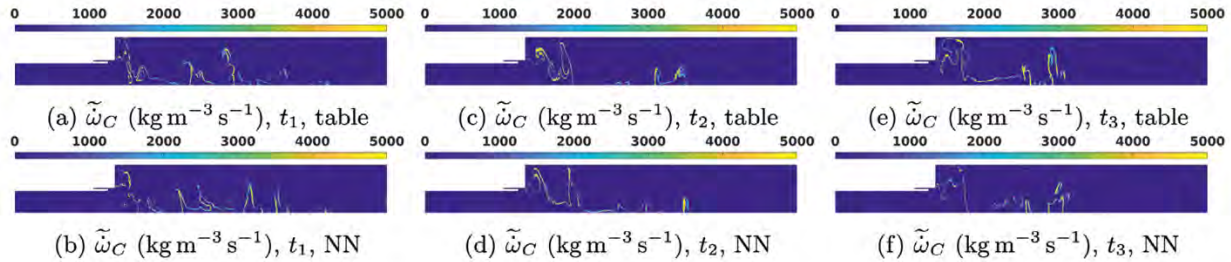


Fig. 21. TG: PVRR.

els. In 2010, one study showed that 16 to 137 times speed up in fluid mechanics related problems can be achieved when they are implemented on GPU [27].

5. Conclusions

NN-based models are proposed to represent the flamelet model outputs. The novel aspect is that the NN models are trained from data that are sampled from a CFD simulation of a transient scenario of a CVRC engine, in which pressure oscillations spontaneously develop from a low value to reach a high-amplitude limit cycle. Knowledge of the physics of the problem was leveraged to enhance the training data set, giving rise to a physics-aware NN-based model. We achieve this by adding more points implied by the physical constraints, such as boundary conditions of the flame variables in the flamelet space, to the training set. We also use an output of the flamelet model as an input to the other variables; which helps to improve each model's accuracy and consistency be-

tween the model outputs. Our method contributed to developing significantly better models that obey the physical constraints of the problem.

Relatively low cost, NN models are proposed with less than 0.6% training error. For PVRR, a very deep and more computationally expensive NN model is required for accurate modeling. The training error is around 1.5%, and the model fits great, especially for high values of PVRR, which are crucial for modeling combustion instability.

These NN-based models are validated first by testing them on the whole flamelet table and then by implementing them in CFD simulations of two different stability configurations of a highly unstable configuration with 14-cm oxidizer post, in addition to the transient case, and comparing them with the table-based simulations, which are the dynamic equilibrium and triggered instability cases of CVRC experiment. In both cases, great consistency is observed in different measures such as pressure, modified Rayleigh index, and temporal behavior of other quantities.

The model showed some weaknesses in modeling regions in which there is no combustion, i.e. the oxidizer post, due to the lack of sufficient training data collected through the CFD simulation.

Offline comparison of the NN models with the flamelet libraries confirms that the performance of a NN model is better in regions where more data is included in the training set. As the source simulation is a fuel lean setup, higher values of $\bar{Z}$ were lacking in the training set. Similarly, regions with higher turbulence levels of the table (high B values) have weaker performance because of the lack of data in the training set.

The goal of this work is to explore the possibilities of developing data-driven combustion models only from data generated from highly accurate numerical simulations or experiments. The significance is that each source of data observes only a subset of the actual model (which is assumed to be the flamelet library in this work). The information fusion power of NNs has been essentially tested in this work. Having a richer training set from multiple experiments allows having a more comprehensive NN model by providing better coverage of the actual dynamic behavior. Further investigation on selecting the right set of input and data can help in achieving better models.

While the training and validation activities in this work are still closely associated with the flamelet based method, the NN model developed with careful consideration of the flame characteristics simultaneously improve its fidelity and avoid some of the combustion model limitations. The success of the proposed approach paves the way for developing more descriptive by utilizing experiment and multiple sources of data. In future research, the framework presented in this work can be applied to high-quality data from sources other than the flamelet table, such as high fidelity LES and DNS, where the cost saving of using machine learning models can be highly advantageous.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Combustion Simulation of 82-Injector Rocket Engine

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A computational study of the nonlinear rocket-engine combustion instability is presented for an engine with 82 coaxial methane-oxygen injector ports, a choked nozzle, and a combustion chamber that models a Rocketdyne experiment. Computations use a three-dimensional unsteady $k - \omega$ shear-stress transport delayed detached-eddy simulation method. Four different one-step chemical kinetic rates are simulated on the resolved scale to determine the effect of the burning rate. Application of kinetic rates on the resolved scale give faster rates than expected with turbulent combustion where the final mixing and chemical reaction in the cascade occurs on the smallest scales; thus, reduction of the kinetic rate is examined here. When the normalized kinetic rate is 1, implying the nominal Westbrook-Dryer rate, only the longitudinal-mode instability is observed. As the kinetic rate decreases, less of the combustion occurs upstream near the longitudinal-mode pressure antinode, the longitudinal-mode instability becomes weak, and the first-tangential-mode instability emerges, which fits better with experiment. The proximity of the domain of major heat release to the longitudinal mode pressure antinode is found to be critical. Evidence is presented for the need for an improved combustion model that will provide a more accurate and lower burning rate.

Nomenclature

A_r	=	normalized chemical kinetic rate
c_p	=	specific heat at constant pressure, J/(kg · K)
D_c	=	diameter of combustor chamber, cm
D_t	=	diameter of nozzle throat, cm
$D_{k,j}$	=	mass diffusivity for species k in j direction, m ² /s
E	=	stagnation internal energy, J
e	=	stagnation specific internal energy, J/kg
H	=	stagnation internal enthalpy, J
HRR	=	heat-release rate, W
h	=	specific enthalpy, J/kg
h_s	=	stagnation specific enthalpy, J/kg
k	=	turbulent kinetic energy, m ² /s ²
$L_{chamber}$	=	length of combustion chamber
p	=	static pressure, bar
q_i	=	energy flux in i th direction, J/(m ² · s)
R	=	mixture specific gas constant, J/(kg · K)
R_{ad}	=	radius of chamber, cm
R_{throat}	=	radius of throat, cm
u_i	=	velocity components, m/s
$V_{k,i}$	=	correction velocity for species k in i th direction, m/s
T	=	temperature, K
t	=	time, s
W	=	total molecular weight, kg/mol
W_k	=	molecular weight of species k , kg/mol
X_k	=	mole fraction of species k
x_i	=	position, m
Y_k	=	mass fraction of species k
γ	=	ratio of specific heats
λ	=	total thermal diffusivity, m ² /s
λ_k	=	thermal diffusivity of species k , m ² /s
μ	=	total dynamic viscosity, kg/(m · s)
μ_k	=	dynamic viscosity of species k , kg/(m · s)
μ_t	=	turbulent eddy viscosity, kg/(m · s)

ν_t	=	turbulent kinematic viscosity, kg/(m · s)
ρ	=	mass density, kg/m ³
τ_{ij}	=	shear stress tensor, Pa
ω	=	specific rate of dissipation
ω_k	=	reaction rate of species k , kg/(m ³ · s)

I. Introduction

COMBUSTION instability in liquid-propellant rocket engines is a phenomenon involving coupling mechanisms between acoustic waves and flames that affect combustion dynamics and combustion instability [1–5]. The acoustic oscillations occur at natural resonant frequencies for the injection-combustor-nozzle configuration and have amplitudes that rise above the level of combustor noise related to vortex shedding. For the combustion instability, flames engage in the resonant interaction and provide oscillatory burning rates that reinforce the acoustic oscillations. Combustion instability has been studied for many decades [2–21] and is considered in all development programs for new rocket designs because it is an undesired and harmful phenomenon; the resulting large-amplitude pressure oscillation can modify the thrust vector and damage the engine through increased heat transfer to the walls and injector face. For liquid-propellant engines, the simulation with the largest number of injectors had 42 coaxial injectors [17]. In that study, Urbano et al. performed large-eddy simulation (LES) for a hydrogen-oxygen liquid-rocket engine with 42 coaxial injectors, addressing two experimental operating conditions investigated at the DLR, German Aerospace Center laboratory. The occurrence of transverse high-frequency combustion instabilities was predicted by superimposing a pressure disturbance with a first transverse modal distribution on the steady-state solution.

Jensen et al. [20] evaluated hydrocarbon fuels, such as methane, with liquid oxygen (LOX) considering combustion stability and performance behavior of a rocket engine with 82 injectors. The first mode of tangential combustion instability with frequency 5100 Hz was observed under some fuel/oxidizer ratio conditions. A previous computational study [21] modeled a rocket engine with 30 coaxial methane-oxygen injector ports, a choked nozzle, and a combustion chamber that is simplified from Jensen et al.'s [20] 82-injector experimental rocket engine. The 30 coaxial injectors were designated to provide a similar mass flux distribution in the radial and azimuthal directions as found for the experimental 82-injector design. The spontaneous longitudinal-mode and tangential-mode instabilities are observed. The strengths of the two instability modes alternate during the simulation time. The oscillation amplitudes of the two instability modes could be modified by pulsing the injector mass flux at certain pulsation frequencies.

In this study, a computational study for a rocket engine with an 82-injector combustor is performed and compared with Jensen et al.'s [20] experimental measurements to understand better the stability of the

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reacting flow in a multiple-injection rocket-engine combustor and to develop and validate the computational tool. To reduce the computational cost, the fuel and oxidizer injection geometry is simplified as a coaxial injector port without flare. The open-source computational fluid dynamics software OpenFOAM [22] is used for this study.

The analysis here is a substantial advancement in the complexity of liquid-propellant rocket engine analysis by LES. The three-dimensional flow system configured here includes the internal ports of 82 coaxial injectors, the main combustion chamber, and the transonic flow through the converging-diverging nozzle. The turbulent mixing of the 82 coaxial jets and the one-step methane-oxygen chemical reaction rate are resolved. The LES captures the combustion dynamics due to both the turbulence and the nonlinear acoustics known as combustion instability. In comparison with the previously most advanced configuration for a hydrogen-oxygen rocket engine [17], we have approximately double the number of their 42 coaxial injectors, and we use kinetics rather than the classical flame transfer function, which originated with the Crocco time-lag theory [2,4–8].

In Sec. II, the configuration, mathematical description, and the numerical method are presented. The results of the computations and the postprocessing of that data are given in Sec. III. Section IV contains the concluding remarks.

II. Numerical Method

A. Numerical Solver

In this study, OpenFOAM is used to solve the compressible Navier-Stokes equations, which can be expressed as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = \frac{\partial(\tau_{ij})}{\partial x_j} - \frac{\partial p}{\partial x_i} \quad (2)$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial((\rho E) + P)u_j}{\partial x_j} = \dot{\omega}_T - \frac{\partial q_i}{\partial x_i} + \frac{\partial(\sigma_{ij}u_i)}{\partial x_j} \quad (3)$$

where the viscous stress tensor τ_{ij} is given by

$$\tau_{ij} = \tau_{ij}^l + \tau_{ij}^p \quad (4)$$

$$\tau_{ij}^l = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (5)$$

$$\sigma_{ij} = \tau_{ij} - p \delta_{ij} \quad (6)$$

The detached-eddy simulation [23] model based on the $k-\omega$ shear-stress transport is used for turbulence closure.

The $\dot{\omega}_T$ represents the heat-release rate due to combustion, and q_i represents the energy flux and is given by

$$q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^{NS} h_k Y_k V_{k,i} \quad (7)$$

where $V_{k,i}$ represents the diffusion velocity and is defined as

$$V_{k,i} = -\frac{D_k}{X_k} \frac{\partial X_k}{\partial x_i} \quad (8)$$

The species transport equation is

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_{kj} \frac{W_k}{W} \frac{\partial X_k}{\partial x_j} \right) + \dot{\omega}_{k,c} \quad (9)$$

$k = 1, \dots, NS$

where W_k is the species molecular weight, W is the total molecular weight, D_k is the coefficient of species diffusion, and $\dot{\omega}_k$ is the generation of species due to chemical reaction. The Westbrook-Dryer one-step global reaction [24] for methane and oxygen is used to calculate the generation of species due to chemical reactions and the heat-release rate. No turbulent combustion closure is included. The reacting-mixtures model is used to calculate the properties of the mixtures. More details about the numerical models are given in Ref. [19].

The OpenFOAM 4.0 combustion simulation solver rhoReactingFoam with Pressure Implicit Pressure-Linked Equations (PIMPLE) is used for the compressible combustion simulation with chemical reaction. The Mach number in the combustion chamber is about 0.2. Most combustion are completed in the chamber. The flow is accelerated through the nozzle, and the maximum Mach number there is about 1.4. The differencing schemes used are second-order accurate in both space and time. The time discretization is second-order implicit backward differencing. Gaussian integration is used for the spatial discretization with linear interpolation from cell centers to cell faces for second-order derivatives. It is a standard Gaussian finite volume integration for the derivatives calculations, which is based on summing values on cell faces. The ideal-gas equation of state is used in this paper for simplicity. The specific heat c_p is calculated as a function of temperature from the JANNAF tables of thermodynamics.

B. Computational Mesh

An 82-injector rocket engine combustor is configured to mimic an experimental 82-injector rocket engine combustor [20] in this study. Figure 1 shows the 82-injector combustor geometry. P1–P6 mark six pressure probes around the combustion chamber wall. The experiment model [20] had a chamber length of 24 cm, and the combustion chamber diameter is 14.38 cm. In the experiment, 82-element coaxial injectors were used. In the computation model, the injector is simplified as a shorter length without outlet flare coaxial injector. The fuel and oxygen are injected with coaxial injectors. The D_{on} is 6.62 mm, and D_{fuel} is 7.505 mm. The length of the injector is 30 mm. The 6 deg flare outlet in the experimental geometry is not modeled in the simplified computational model, which might cause some discrepancy between the computation and experiment. Figure 2 shows the combustor geometry. In the simulation, the total mass flow rate and the mixture ratio match those in the experiments. Figure 3 shows the unstructured mesh for the 82-injector combustor. The ANSYS software is used for the mesh

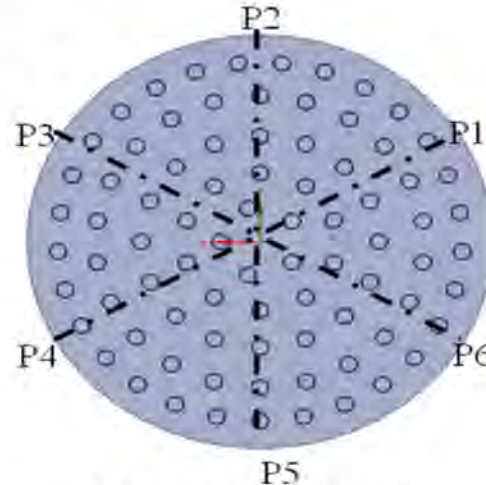


Fig. 1 Front view of the 82-injector plate.

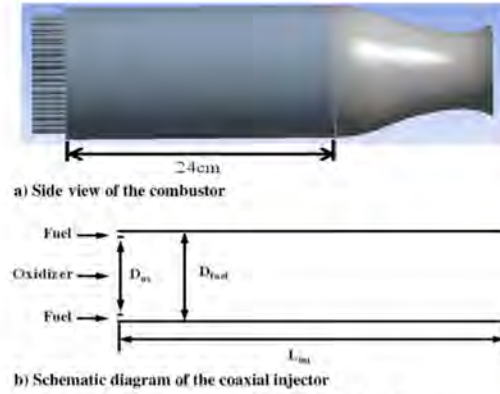


Fig. 2 Geometry of 82-injector combustor.



Fig. 3 Computational mesh.

generation. A grid independency was performed for a combustion chamber with 19-injector case in Ref. [19]. The results show that overall grid independent solutions were achieved on both coarse and fine meshes. In this paper, a fine mesh including about 16.5 million nodes and 50 million elements and a coarse mesh including 8.2 million nodes and 21 million elements are generated for the 82-injector combustion chamber grid independent study.

C. Boundary Conditions

Along the wall, the no-slip boundary condition is used. The normal pressure gradient on the wall is zero. Adiabatic walls with no surface

Table 1 Imposed flow conditions

XXXX	Case 19
Mixture ratio	2.53
Velocity ratio	11.0
Momentum ratio	4.31
$\dot{m}_{fuel}$, lb/s	24.23
$\dot{m}_{O_2}$, lb/s	61.74
T_{fuel} , F	20.7
T_{ox} , F	-244
ρ_{fuel} (lb/ft ³)	8.1
ρ_{ox} (lb/ft ³)	64.7
V_{fuel} (ft/s)	708
V_{ox} (ft/s)	64

Table 2 Experimental observations

XXXX	Case 19
Instability Mode	Tangential 1T
Frequency, Hz	5100
Chamber pressure, bar	130

Table 3 Combustion chamber characteristic frequencies

Mode	Frequency, Hz
1L	1875
2L	3751
3L	5625
1T	5100
2T	8462
1R	10626

chemistry are assumed. In the injector ports, the mean mass fluxes for methane and oxygen are fixed to yield the steady-state mass flow rate at the sonic point for the convergent nozzle. The wave-transmissive boundary condition is used at the exhaust nozzle outlet boundary because of the supersonic nozzle flow. This boundary condition ensures that no backward propagating waves enter the system to avoid occurrences of shocks or backflow in the combustion. The flow condition is chosen to represent a case with unstable tangential modes based on the experiments. The imposed flow conditions are listed in Table 1. The experimental observations at the conditions are listed in Table 2. The combustion chamber characteristic frequencies are listed in the Table 3. Only the 1T instability was found in the test case 19.

III. Computational Results

The simulations only consider the gas phases of the methane and oxidizer and use the ideal-gas equations of state, which might introduce some errors for the description of the cold propellant flow at the very high pressures. The computational simulation results are shown in Table 4. The computational results on the fine and coarse meshes show that overall grid-independent solutions were achieved. Similar combustion chamber pressure level, pressure oscillation frequencies, and instability behaviors were captured on both coarse and fine meshes. However, unlike the Rocketdyne results [20] and 30-injector combustor simulation results [21], only the first longitudinal instability mode with frequency 2403 Hz is observed for the 82-injector combustor when the chemical kinetic rate is 1, normalized by the value given by the Westbrook–Dryer model, [24]. The 30-injector combustor studied in Ref. [21] is simplified from the experimental 82-injector combustor in Ref. [20]. The mixing of the 82-injector combustor is faster than the 30-injector combustor, which enhances

Table 4 Parameters of the computation cases

Injector	Ar	L _c , cm	P _c , bar	Longitudinal mode	f _L	Tangential mode	f _T
82	1.0	24	130	1L	2403	—	—
82	1.0	24	131	1L	2433	—	—
(coarse)							
82	0.5	24	125	1L	1918	1T	4657
82	0.375	24	126	1L	1753	1T	4383
82	0.25	24	122	—	—	—	—
30	1.0	24	125	1L	2063	1T	4550

the combustion rates, moves the combustion upstream in the chamber, and results in only the first longitudinal instability mode appearing for the 82-injector combustor. Three other combustion simulations are tested for the 82-injector combustor with different chemical reaction rates. When the chemical reaction rate is decreased to 0.5, the first tangential instability mode appears, but the first longitudinal instability mode still dominates the pressure oscillation. When the chemical reaction rate is decreased to 0.375, the first tangential instability mode strength grows and dominates the pressure oscillation with frequency 4383 Hz. The smaller reaction rate slows down the combustion in the chamber, which permits the tangential instability to grow. With a further decrease of the combustion reaction rate to 0.25, the flow inside the combustion chamber becomes stable.

The 30-injector simulation involves slower mixing rates than the 82-injector simulation because the distance between adjacent injectors and the sizes of injector ports are larger. The burning rates of the 82-injector simulation and the 30-injector simulation can be aligned

closer by artificially reducing the chemical kinetic rate for the 82-injector simulation. This adjustment aligns better the region of major heat-release rate with respect to the pressure antinode of the longitudinal mode. Specifically, the reduced chemical kinetic rate moves the heat-release action farther downstream from the injector plate, weakening the probability of a longitudinal mode without any weakening of the tangential mode.

A. 82-Injector and 30-Injector Combustors

Simulation results are listed in Table 4. The simulations start from an initially quiescent flow at 3000 K and an equilibrium chamber pressure at 200 bar. The higher chamber temperature helps to shorten the ignition process and reduce the computational time without the use of an explicit ignition model in the simulation.

Figure 4 shows the pressure oscillation at six equally distributed probes around the combustor chamber wall at 1 cm downstream from the injection plate for the 82-injector and 30-injector combustors. The

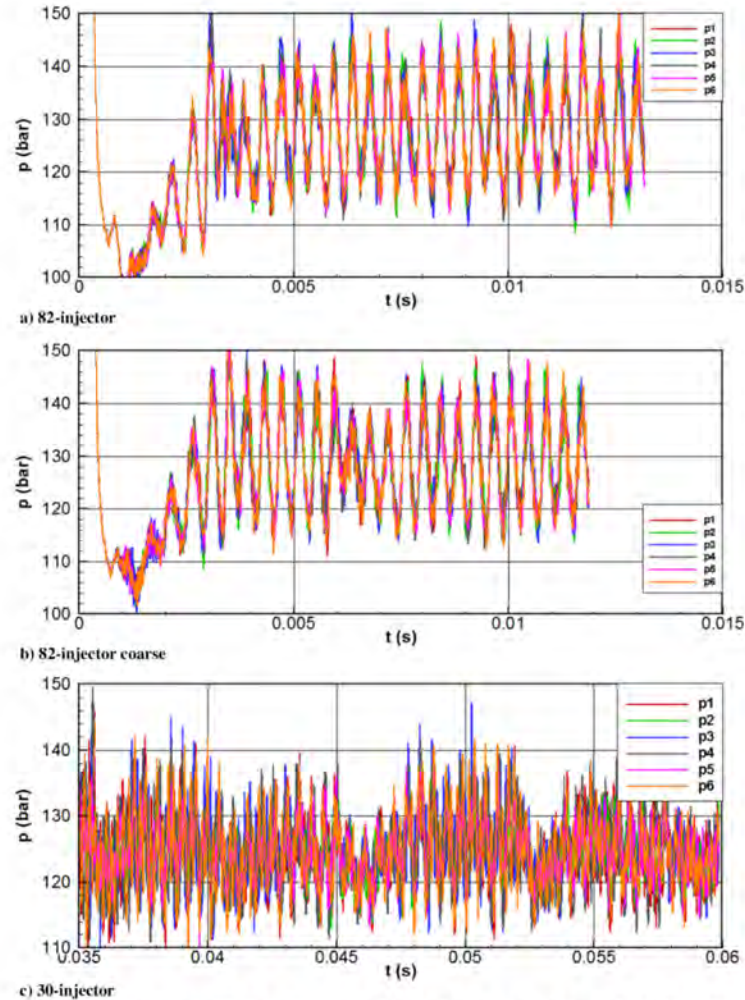


Fig. 4 Pressure history at p1–p6 on the combustion-chamber wall for reaction rate $Ar = 1$. ($z = 1$ cm).

30-injector combustor is simplified from the 82-injector combustion [21]. The pressure oscillations at the six probes are almost completely in phase for the 82-injector case, while those for the 30-injector case appear to show different phases, indicating a pure longitudinal mode for the 82-injector results, while the 30-injector contains mixed modes. Figure 5 shows the FFT analysis of the pressure oscillation at probe 1. The pressure oscillation spectra on the fine and coarse mesh are similar. Both fine and coarse mesh capture the first longitudinal instability mode with 2403 and 2433 Hz, respectively, which confirm the grid independent results are achieved. To contrast the differences, Fig. 5b reproduces the results for the 30-injector study from Ref. [21]. Two dominant frequencies, 2063 and 4550 Hz, are observed for the 30-injector combustor. The 2063 Hz pressure oscillation corresponds to the first longitudinal mode of combustion instability. The 4550 Hz pressure oscillation indicates the first tangential mode. We demonstrate in this study that the discrepancy of the combustion simulation results is caused by the different mixing rates and the reaction rates between the 82-injector and 30-injector combustors.

The higher frequencies for the 82-injector combustion chamber imply a higher speed of sound at the higher temperature, and faster and more complete combustion. This is to be expected because of the shorter mixing lengths and thereby faster mixing rates resulting from

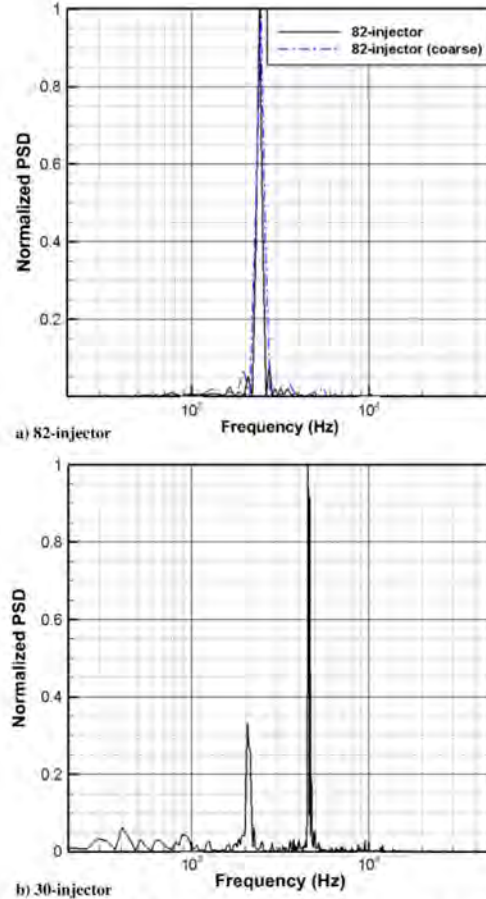


Fig. 5 FFT of the pressure history at probe p1 on the combustion-chamber wall for reaction rate $Ar = 1$. ($z = 1$ cm).

the smaller size of injector ports and smaller distances between adjacent injectors.

B. Chemical Kinetic Rate Effects

Now, we consider the combustion modeling with the different normalized chemical kinetic reaction rates of 0.5, 0.375, and 0.25, respectively. Figure 6 shows the pressure oscillations around the combustor chamber wall at 1 cm downstream from the injection plate for the three cases. The FFT analysis of the pressure oscillations is presented in Fig. 7. When the normalized chemical kinetic reaction rate is 0.5, the first tangential instability mode appears, but the first longitudinal instability mode still dominates the pressure oscillation. When the normalized chemical kinetic reaction rate decreases to 0.375, the first tangential instability mode strength grows and dominates the pressure oscillation with frequency 4383 Hz. With the normalized chemical kinetic reaction rate reaching to 0.25, the flow inside the combustion chamber gradually becomes stable.

Figures 8–14 present the fuel CH_4 mass fraction at seven different cross-sections for the 30-injector and the 82-injector combustors with different reaction rates. Figures 15–21 show the product H_2O mass fraction at the same seven different cross-sections. The heat-release rate at meridian plane (1,0,0) for the different cases are presented in Fig. 22. For the 82-injector, when the normalized chemical kinetic rate is 1, the combustion mostly happens near the injector plane. The fuel CH_4 is consumed fast. The high heat-release rate near the pressure antinode favors the development of the longitudinal mode inside the combustion chamber. So, only the longitudinal mode is observed. When the normalized chemical kinetic rate decreases, the combustion region moves downstream. As the normalized chemical kinetic rate reaches 0.375, the combustion region moves away from the longitudinal mode pressure antinode point. This move of heating zone favors the tangential mode inside the combustion chamber. The tangential instability mode dominated the pressure oscillation inside the combustion chamber for this case. When the normalized chemical kinetic rate is 0.375 for the 82-injector combustor, the burning rate behavior of the fuel and oxidizer is similar to that of the 30-injector combustor. Thus, the locations of heat release are similar. So, the instability behaviors are similar for the two cases. The distance of high heat-release rate zone from the pressure antinode of the longitudinal mode is critical. Figure 23 presents the instantaneous contours of the flame index on the chamber meridian planes for the chemical kinetic rate 0.375 case. The flame index is defined as the heat-release rate per unit volume masked by the sign of the dot product of the gradient of the oxygen mass fraction and the gradient of the fuel mass fraction, in other words,

$$FI = HRR \cdot \text{sign}(\nabla(CH_4) \cdot \nabla(O_2)) \quad (10)$$

where HRR is heat-release rate per unit volume. If the index is positive, fuel and oxygen diffuse in the same direction, indicating a premixed flame. If the dot product is negative, the oxygen and fuel diffuse in opposing directions, indicating a diffusion flame. In Fig. 23, the dark red indicates premixed flames, and the dark blue indicates diffusion flames. Premixed flames dominate near the injectors for the case when the chemical kinetic rate is 0.375, which favors the tangential instability.

IV. Conclusions

A computational study of the nonlinear rocket-engine combustion instability is presented for an engine with 82 coaxial methane-oxygen injector ports, a choked nozzle, and a combustion chamber. The analysis is a substantial advancement in the complexity of liquid-propellant rocket engine analysis by large-eddy simulation because of the larger number of coaxial injectors and the use of chemical kinetics rather than a flame transfer function. Use of kinetic rates on the resolved scale gives faster rates than expected with turbulent combustion where the final mixing and chemical reaction in the cascade occurs on the smallest scales; thus, reduction of the kinetic rate is examined here. When the normalized kinetic rate is 1.0, the full

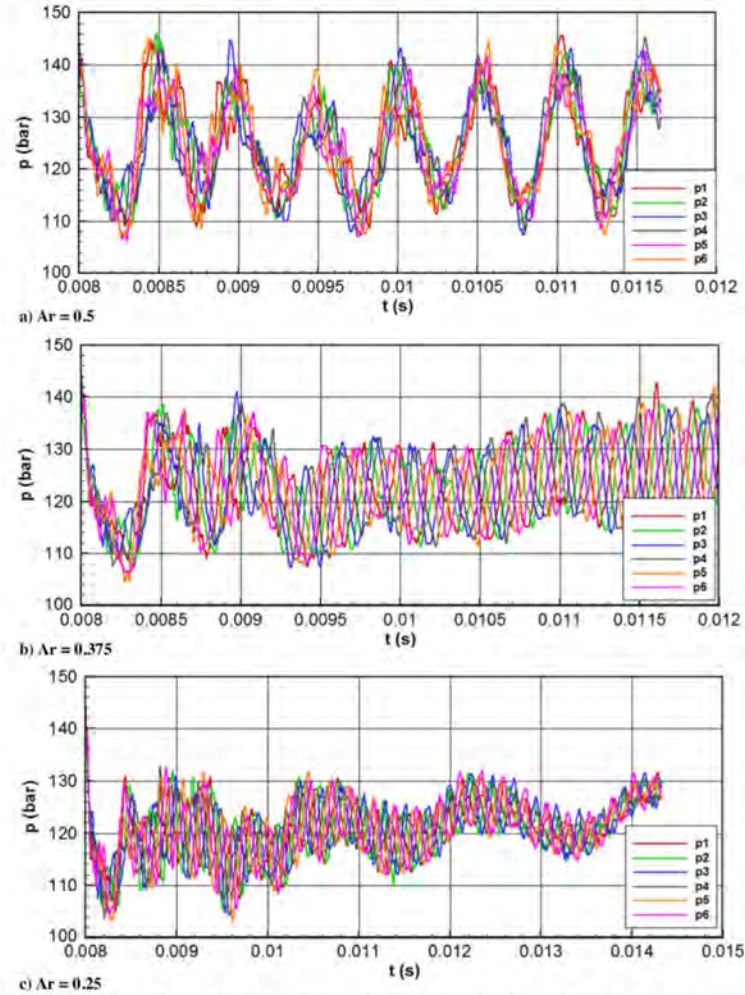


Fig. 6 Pressure history at p1-p6 on the combustion-chamber wall. ($z = 1$ cm).

and correct Westbrook–Dryer rate is given; the normalized rates 1.0, 0.5, 0.375, and 0.25 are used in the combustion simulation. When the normalized chemical kinetic rate is 1.0, only the first-longitudinal-mode instability is observed. With reduction of that rate to 0.5, the first-tangential instability mode appears, but the first-longitudinal instability mode still dominates the pressure oscillation. With further reduction of the normalized chemical kinetic rate to 0.375, the first-tangential instability mode strength grows and dominates the pressure oscillation with frequency 4383 Hz. For the normalized chemical kinetic rate equal to 0.25, the flow inside the combustion chamber gradually becomes stable. The different chemical kinetic rates change both the heat-release rate and the location of the heat release, which results in different pressure-oscillation behavior in the combustion chamber. A faster burning rate places more of the heat release at the upstream end of the combustion chamber and thereby closer to the pressure antinode for the longitudinal mode. Thus, it favors the longitudinal instability.

The Rocketdyne experiment [20] indicated the tangential mode was dominant. Agreement with the 82-injector experiment was better with the 30-injector simulation [21] at the same pressure,

mass flux, and mixture ratio where the larger mixing lengths reduced the burning rate and moved the heat release farther downstream. This disagreement with experiment for the full chemical rate applied at the resolved scale is not surprising because combustion process actually occurs primarily in the final stage of the turbulent cascade at the smallest scales. We have unpublished evidence [25] in other multi-injector rocket-engine analyses that subgrid modeling with a flamelet-theory approach reduces the burning rate and moves heat release farther downstream in comparison to chemical kinetics applied on the resolved scale. There can be other issues as well related to disagreement with experiment: 1) the Westbrook–Dryer scheme was designed for premixed flames rather than the mixtures of premixed and nonpremixed flames found in a rocket chamber, 2) detailed kinetics might present a slower global rate, 3) mixing rates at high pressure might not be simulated as well as needed, and/or 4) injector-port simulation is not exact, which can modify mixing rates.

Nevertheless, the simulation does present an explanation for some of the instabilities found in the Rocketdyne experiment [20]. Furthermore, the relation of the dominant mode of instability to details in

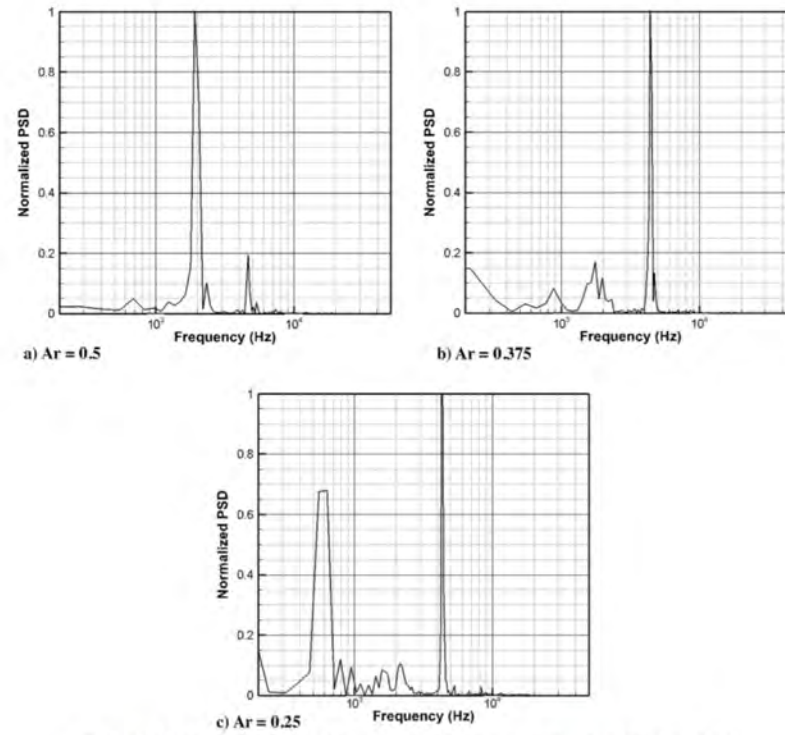


Fig. 7 FFT of the pressure history at probe p1 on the combustion-chamber wall. ($z = 1$ cm).

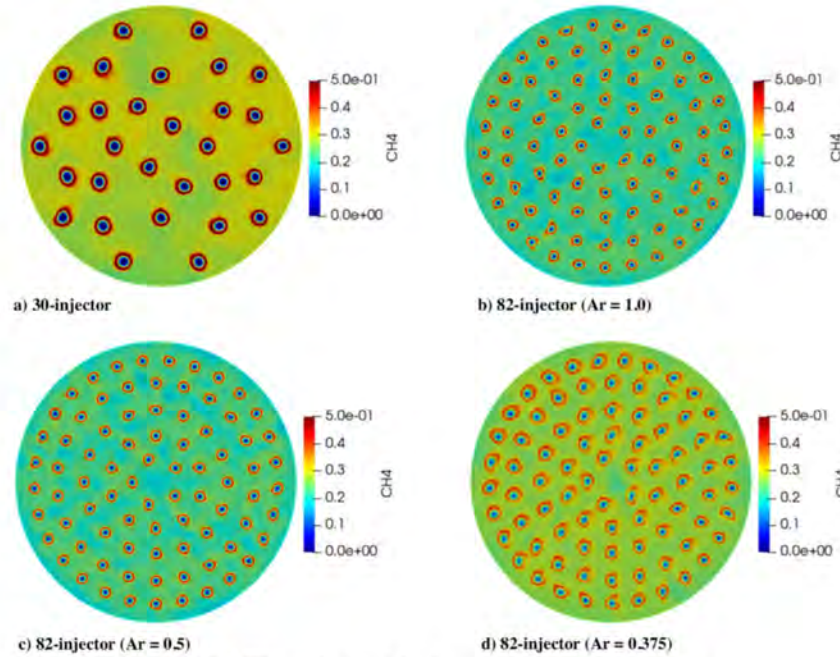


Fig. 8 Fuel CH_4 mass fraction at chamber cross-sectional plane. ($z = 1.0$ cm).

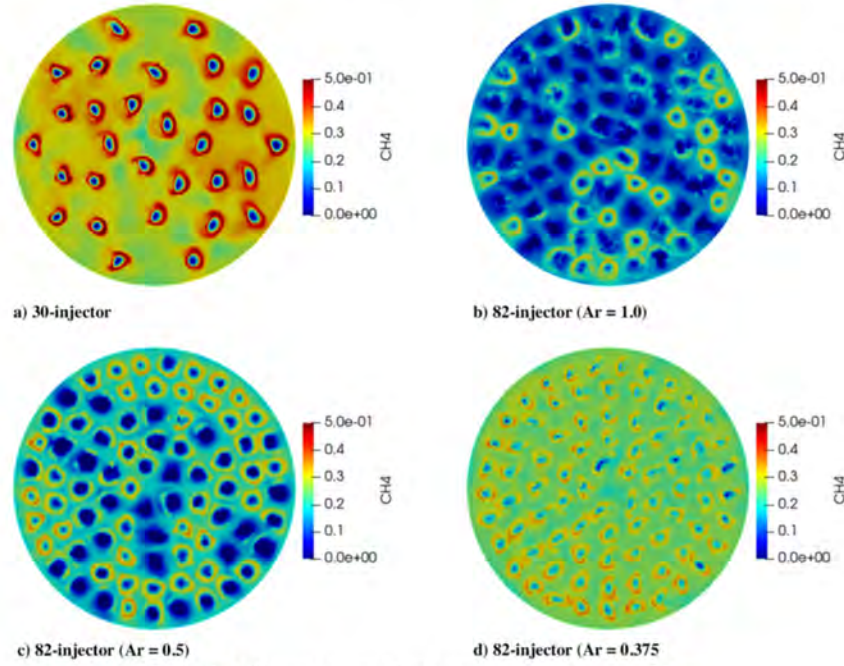


Fig. 9 Fuel CH_4 mass fraction at chamber cross-sectional plane. ($z = 3.0$ cm).

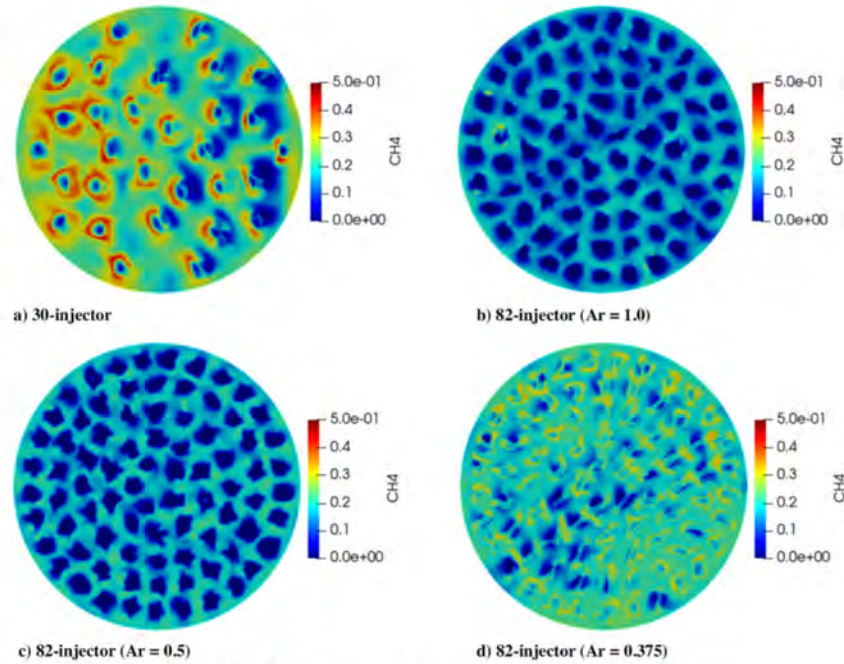
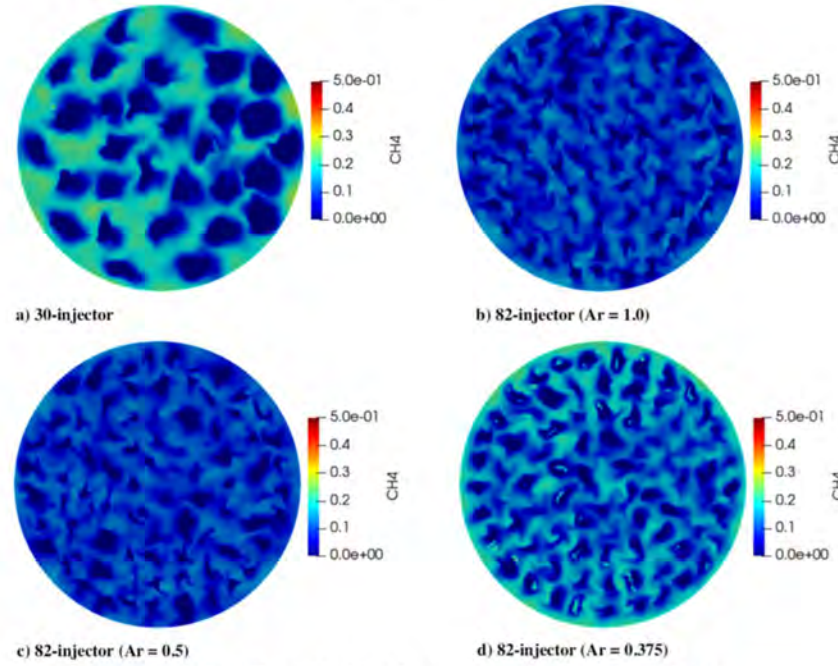
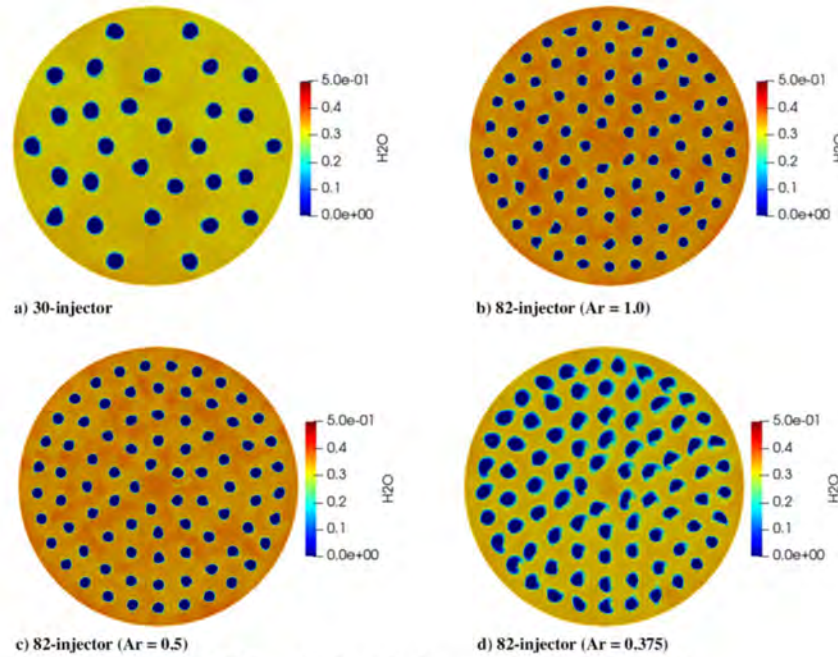


Fig. 10 Fuel CH_4 mass fraction at chamber cross-sectional plane. ($z = 5.0$ cm).

Fig. 11 Fuel CH_4 mass fraction at chamber cross-sectional plane. ($z = 10.0$ cm).Fig. 12 H_2O mass fraction at chamber cross-sectional plane. ($z = 1.0$ cm).

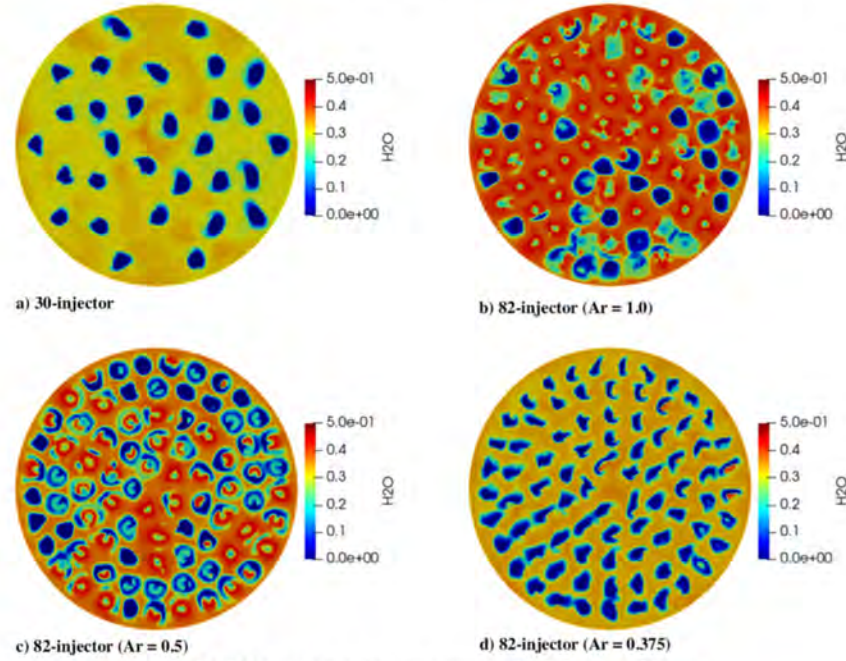


Fig. 13 H₂O mass fraction at chamber cross-sectional plane. ($z = 3.0$ cm).

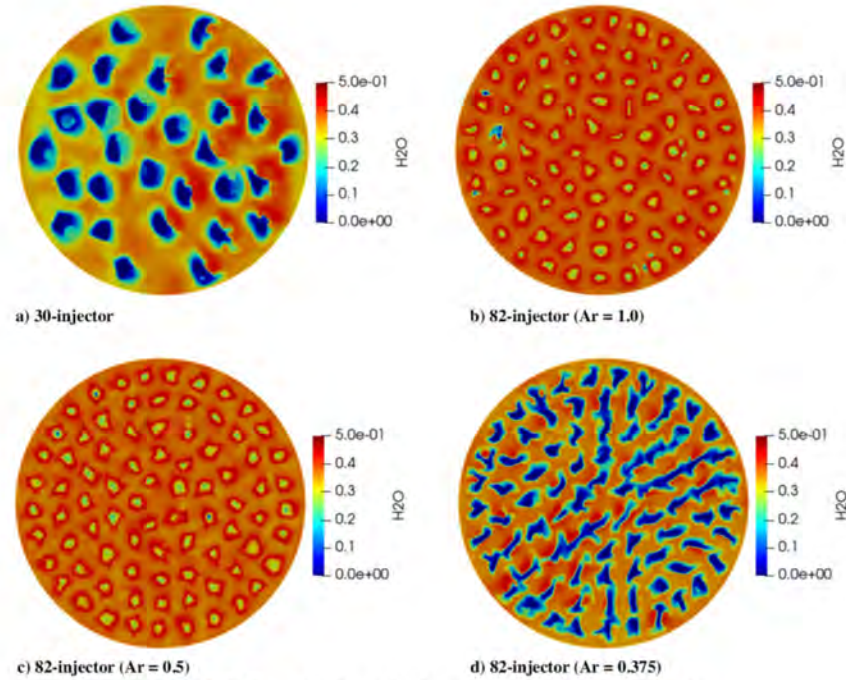


Fig. 14 H₂O mass fraction at chamber cross-sectional plane. ($z = 5.0$ cm).

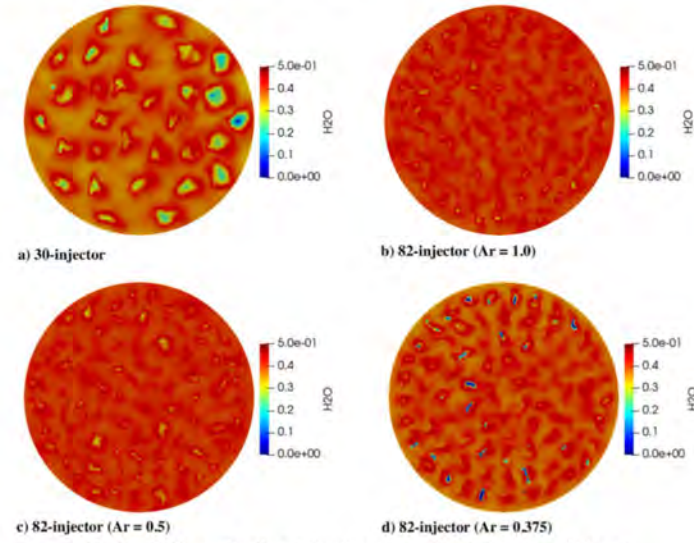
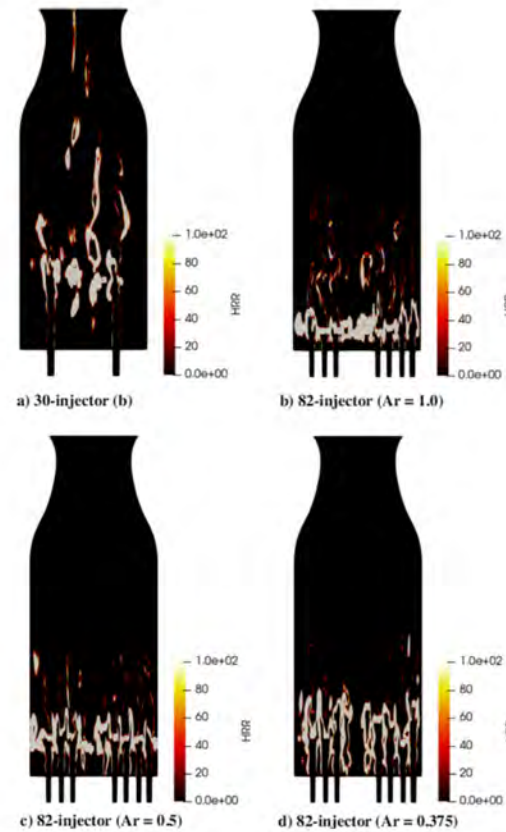
Fig. 15 H₂O mass fraction at chamber cross-sectional plane. ($z = 10.0$ cm).

Fig. 16 Heat-release rate at meridian plane (1,0,0).

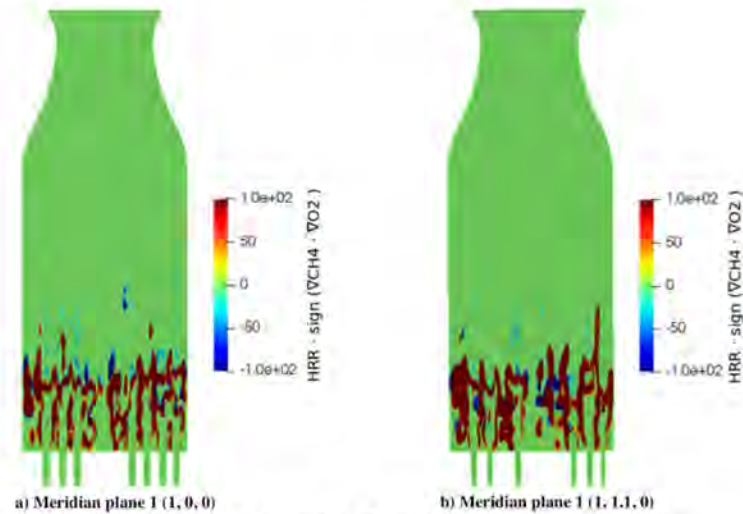


Fig. 17 Instantaneous flame index on the chamber meridian planes ($Ar = 0.375$).

the distribution of the heat-release rate has been demonstrated. The simulation demonstrates that the ability exists to address more practical rocket engine combustors with a large number of injectors.

The poor fit of a simple combustion model in providing agreement in the instability-mode prediction indicates the need for an improved combustion model. The success of the flamelet model in matching experimental results for a single-injector rocket engine [10–12,16] suggests that it should be applied to the multi-injector engine. Preliminary work in that direction with a ten-injector engine [25] indicates that the flamelet model gives the desired lower burning rate and favors the transverse mode accordingly.

Acknowledgments

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Y. Ju
Associate Editor

Addendum III

Triggered Tangential Combustion Instability of a Multi-injector Rocket Engine Using the Flamelet Progress Variable Model

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Abstract

The triggered tangential combustion instability is investigated numerically for a 19-injector rocket engine using the flamelet progress variable (FPV) model. The turbulent combustion is simulated using a newly developed C++ code based on OpenFOAM 4.1. Flamelet tables are generated for methane/oxygen combustion at the background pressure of 200 bar using a 12-species chemical mechanism. A power law is employed to rescale the reaction rate for the progress variable according to pressure. The tangential traveling wave pulsation always triggers a major instability of the same type of wave despite different pulsing amplitudes. However, the magnitude of the triggered instability grows with the pulsing amplitude. The tangential standing wave pulsing doesn't change the wave type in the responding instability as well. The dominant frequency of the triggered instability is slightly higher than the pulsing frequency for both types of pulsation. The major pressure fluctuation is driven by the unsteady heat release rate and is also strongly coupled with the fluctuation of the progress-variable reaction rate. Compared to the one-step kinetics(OSK) model, the lower fuel burning rate in the FPV approach results in a cooler combustion chamber, a lower mean pressure, and a weaker sustained instability mode.

1. Introduction

Combustion instability is an acoustical phenomenon in which an unstable pressure oscillation is excited and sustained by combustion. In most high-power propulsion systems that propel rockets and airplanes, the high-energy release rate reinforces acoustical oscillations with very high amplitudes. Such oscillations can affect thrust in an undesirable way and sometimes lead to engine destruction.

In recent years, there is an increasing need for three-dimensional high-fidelity numerical study of combustion instability in multi-injector rocket engines. Compared to the single-injector configuration [1, 2], the combustion instability mechanism is more complex in a multi-injector combustion chamber because of the possible interactions among injectors and interactions with the complicated feed system and upstream

manifold. Systematic experimental investigations of combustion instability for such configurations are quite expensive and technically difficult. Compared to experimental measurement, numerical simulations based on high-fidelity turbulence modeling and detailed chemical reaction mechanisms are able to provide more details about the flow physics as well as the combustion dynamics and hence gain a deeper insight into the combustion instability mechanisms. Among various instability modes, the transverse acoustic modes with large amplitude were observed in experiments under certain conditions [3, 4, 5]. Urbano et al. [6, 7] carried out combustion simulations using an inhouse code for a complete small-scale rocket engine with 42 coaxial injectors and a nozzle outlet. Large eddy simulation (LES) was employed and a four-species H_2/O_2 reacting mechanism was considered. Combustion instability was studied with emphasis on the interaction between transverse and radial modes. Under the experimental condition which leads to self-sustained oscillations, computational results showed that tangential instability can be triggered when the system is perturbed by superimposing a large-amplitude pressure disturbance with a first transverse modal distribution. Hwang et al. [8] employed their OpenFOAM-based code to study the combustion instability for the same multi-injector rocket engine. The same turbulence model and combustion model were used. However, a chemical mechanism with 8 species and 12 reaction steps was adopted. The same type of pressure perturbation was superimposed under the experimentally unstable condition and a pressure disturbance greater than a threshold value was needed to trigger the limit-cycle tangential oscillations. Guo et al. [9] investigated the transverse combustion instability of a 91-injector rocket engine using the standard $k - \epsilon$ two-equation turbulence model and the eddy-dissipation combustion model. A single-step global chemical reaction mechanism was adopted to model the chemical reaction process of the Dodecane/oxygen combustion. Self-excited high-frequency combustion instability of first-order tangential (1T) mode was observed. Two different kinds of 1T patterns, standing wave mode and traveling wave mode, were captured for two different oxygen-to-fuel ratios. Xiong et al. [10, 11] presented a computational study of the nonlinear combustion instability of a similar methane-oxygen configuration, which has a choked nozzle and a combustion chamber fed by 19 or 30 coaxial injector ports. Detailed time-resolved information about the combustion instability was provided using a three-dimensional unsteady $k - \omega$ shear-stress transport delayed detached-eddy simulation. The global one-step reaction was adopted for methane/oxygen combustion. The triggered instability modes were explored for the tangential traveling wave and the tangential standing wave pulsing in the injector mass flux. It was shown that an oscillating combustion-chamber flow can be triggered to a new mode with a larger disturbance amplitude.

While high-fidelity turbulence modeling was commonly adopted, many studies employed quite simple

chemical mechanisms that involve very few species and reaction steps. The widely used combustion models in previous studies were the laminar closure model (LCM) and the steady laminar flamelet (SLF) model. For the LCM model, it is difficult to incorporate any realistic detailed-reaction mechanism involving many species and reactions due to the huge computational cost. Additionally, the stiffness arising from the nonlinearity of species reaction source terms and the wide range of chemical time scales makes the system very difficult to solve [1]. The SLF model is favorable in efficiently adopting realistic chemical mechanism [12, 13]. However, scalar dissipation rate is used to parameterize the flamelet tables and each scalar dissipation rate could be related to multiple solutions. Therefore, despite the high computational efficiency, the SLF model only explores a part of the flamelet solutions so that the selected solutions are single-valued functions of the scalar dissipation rate. To incorporate complex chemical kinetics efficiently while exploring all the flamelet solutions, Pierce and Moin [14] introduced the flamelet progress variable (FPV) approach. The scalar dissipation rate is replaced by the reaction progress variable, which is defined as the total mass fraction of selected major species in a chemical mechanism, to reparameterize the flamelet tables. This transition makes the flamelet solutions well-defined functions of all parameters including the progress variable. The baseline FPV approach was primarily applied in simulations of incompressible combustion. In recent years, the use of the FPV approach was extended to the computations of compressible combustion by considering the kinetic energy in the energy balance regime [15, 16]. Nguyen et al. [2] examined the capability of the FPV model in simulating combustion instability in the continuously variable resonance chamber of a single-injector rocket engine. The numerical results for pressure oscillation frequencies and amplitudes showed good agreement with the experiment data.

In the current research, our goal is to perform a three-dimensional high-fidelity turbulent combustion simulation of a 19-injector rocket engine and study the triggered tangential combustion instability using the efficient compressible FPV approach and detailed chemical reaction mechanism. In this report, we present the primary computational results of the work.

2. The Flamelet Progress Variable Approach

2.1. The Governing Equations

For a mixture of multi-species, the Favre-averaged Navier-Stokes equations are written in the following conservative form as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_j}{\partial x_j} = 0 \quad (1)$$

3

$$\frac{\partial \bar{\rho} \tilde{v}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_i \tilde{v}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial (\tau_{i,j} + \tau_{i,j}^R)}{\partial x_j} \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{h}_a}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_j \tilde{h}_a}{\partial x_j} + \frac{\partial \bar{\rho} \tilde{K}}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_j \tilde{K}}{\partial x_j} - \frac{\partial \tilde{p}}{\partial t} = \frac{\partial [\tilde{v}_i (\tau_{i,j} + \tau_{i,j}^R)]}{\partial x_j} + \frac{\partial}{\partial x_j} \left[\left(\frac{\lambda}{c_p} + \frac{\mu_t}{Pr_t} \right) \frac{\partial \tilde{h}_a}{\partial x_j} \right] \quad (3)$$

where $\bar{\rho}$ is the mean density, $\tilde{v}_j$ is the mean velocity vector and $\bar{p}$ is the mean pressure. In the energy equation, $\tilde{h}_a$ is the mean total(or absolute) enthalpy, which is the summation of the mean sensible enthalpy $\tilde{h}_s$ and the mean enthalpy of formation $\tilde{h}_c$, and $\tilde{K} = \frac{1}{2} (\sum_{j=1}^n \tilde{v}_j \tilde{v}_j)$ is the mean kinetic energy. λ and C_p are the heat conductivity coefficient and the specific heat at constant pressure. Pr_t is turbulent Prandtl number. $\tau_{i,j}$ and $\tau_{i,j}^R$ are the molecular and turbulent viscous stress tensors and expressed as $\tau_{i,j} = \mu (\frac{\partial \tilde{v}_i}{\partial x_j} + \frac{\partial \tilde{v}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{v}_k}{\partial x_k} \delta_{i,j})$ and $\tau_{i,j}^R = \mu_t (\frac{\partial \tilde{v}_i}{\partial x_j} + \frac{\partial \tilde{v}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{v}_k}{\partial x_k} \delta_{i,j})$ with μ and μ_t being the molecular and turbulent viscosity.

2.2. The Turbulent Combustion Model

In computations of turbulent combustion based on the Reynolds-Averaged Navier-Stokes (RANS) methods, such as those in this report, only the mean quantities are transported. Hence, the laminar flamelet solutions need to be convoluted with assumed probability density functions of the independent scalars, including mean mixture fraction $\tilde{Z}$ and the mean variance of mixture fraction $\widetilde{Z''^2}$. The convolution generates flamelet libraries of mean quantities which can be accessed efficiently during the computational fluid dynamics (CFD). In the progress-variable variant of the flamelet model (FPV), the flamelet tables are also parameterized by a mean reaction progress variable $\tilde{C}$. In this report, the progress variable is defined as the total mass fraction of four major species, which are CO_2 , H_2O , H_2 and CO . Hence, a mean thermal and chemical quantity $\tilde{\psi}_i$, such as composition and temperature, is given by

$$\tilde{\psi}_i(\tilde{Z}, \widetilde{Z''^2}, \tilde{C}) = \int_0^1 \int_0^1 \psi_i(Z, C) \tilde{P}(Z, Z''^2, C) dZ dC \quad (4)$$

where $\tilde{P}$ is the PDF function for $\tilde{\psi}_i$. The PDF for the progress variable is frequently assumed to be the Dirac δ function; thus, (4) is reduced to

$$\tilde{\psi}_i(\tilde{Z}, \widetilde{Z''^2}, \tilde{C}) = \int_0^1 \int_0^1 \psi_i(Z, \tilde{C}) \tilde{P}(Z, Z''^2) dZ \quad (5)$$

Finally, the β PDF is assumed for $\tilde{P}$, which gives

$$\tilde{P}(Z, Z''^2) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1}}{\Gamma(\alpha)\Gamma(\beta)}\Gamma(\alpha+\beta) \quad (6)$$

where Γ is the gamma function. α and β are shape functions which are defined as $\alpha = Z\gamma$ and $\beta = (1-Z)\gamma$ with $\gamma = [Z(1-Z)/Z''^2] - 1 \geq 0$.

For compressible combustion, the tables should be generated at different background pressures and pressure should be included as an input to access the tables. Pecnik et al. [15] showed that the composition of the reacting mixture is not sensitive to the background pressure and only the reaction rate changes dramatically. This fact justifies the method of using tables under one background pressure (usually the averaged pressure) and rescaling the reaction rate for other pressures. In this report, we adopt this approach to simplify preparation of the tables and the table lookup process.

At each time step in the CFD computation, the transport equations for scalars $\tilde{Z}$, $\widetilde{Z''^2}$ and $\tilde{C}$ are solved. When the Lewis number is equal to one, these equations are given as

$$\frac{\partial \tilde{\rho} \tilde{Z}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{v}_j \tilde{Z}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right) \frac{\partial \tilde{Z}}{\partial x_j} \right] \quad (7)$$

$$\frac{\partial \tilde{\rho} \widetilde{Z''^2}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{v}_j \widetilde{Z''^2}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right) \frac{\partial \widetilde{Z''^2}}{\partial x_j} \right] + 2 \frac{\mu_t}{Sc_t} \frac{\partial \tilde{Z}}{\partial x_j} \frac{\partial \tilde{Z}}{\partial x_j} - \tilde{\rho} \tilde{\chi} \quad (8)$$

$$\frac{\partial \tilde{\rho} \tilde{C}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{v}_j \tilde{C}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right) \frac{\partial \tilde{C}}{\partial x_j} \right] + \tilde{\omega}_C \quad (9)$$

where $\tilde{\chi}$ is the Favre-averaged scalar dissipation rate. By comparing the integral scalar time scale and the turbulent flow time scale, $\tilde{\chi}$ is frequently expressed as $\tilde{\chi} = C_\chi \frac{\tilde{\epsilon}}{\tilde{k}} \widetilde{Z''^2}$ with $\tilde{k}$ and $\tilde{\epsilon}$ being the mean turbulent kinetic energy and mean turbulent dissipation. A constant value of 2.0 is often used for C_χ . The laminar and turbulent Schmidt number Sc and Sc_t are 1.0 and 0.7, respectively. The source term $\tilde{\omega}_C$ in equation (9) is the reaction rate for the progress variable.

2.3. The laminar flame calculator

Here, the laminar flamelet solutions are generated using FlameMaster, an open source C++ program package for zero-dimensional combustion and one-dimensional laminar flame calculations [17]. The code can be used for steady and unsteady computations of premixed as well as non-premixed flames. For the

methane/oxygen combustion that we consider, we use the module of the code that solves the steady flamelet equations in the mixture fraction space by assuming counterflow configuration. To run the code, a chemical mechanism and corresponding thermo and transport data are needed. The background pressure, composition and temperature on both the fuel and oxidizer sides are required. For each given stoichiometric scalar dissipation rate (χ_{st}), the code generates a flame solution in form of distributions of temperature, composition, reaction rates and heat release rate in the mixture fraction space. Hence, the laminar flamelet solutions are already parameterized by the scalar dissipation rate and the mixture fraction.

Since chamber pressure in the current study is around 200 bar, a chemical mechanism suitable for high-pressure combustion is desired. We adopt a skeletal model of 12 species, which is generated by selecting relevant species and reaction pathways from version y of a 119-species Foundation Fuel Chemistry Model (FFCM-y) [18, 19]. The FFCM models were recently developed with uncertainty minimization against up-to-date experimental data for the combustion of small hydrocarbon fuels. The models were tested for fuels, such as methane, over the pressure range of 10-100 atm. The 12 species in the skeletal model are H_2 , H , O_2 , O , OH , HO_2 , H_2O , CH_3 , CH_4 , CO , CO_2 , and CH_2O . Reaction rate constants in the model are optimized for the same pressure range, using the FFCM-y computation results as the optimization targets. The 12-species skeletal model is called FFCMy-12 mechanism in this report and it is fed into the FlameMaster code for calculation of laminar flames.

2.4. Numerical Solver

To numerically simulate combustion using the FPV approach, a C++ code is developed based on OpenFOAM 4.1. There is a similar open-source code called flameletFoam [20]. However, it only provides the original version of the flamelet model. The progress variable approach is not available. Moreover, tabulated temperature is directly used without any correction, which makes the code applicable only to incompressible combustions. Last but not least, since the code is based on the outdated 2.4 version of OpenFOAM, the selection of a turbulence model is quite limited. For example, the hybrid RANS/LES based on the SST $k - \omega$ model is not available. In the newly developed code, transport equations (7), (8) and (9) are solved for $\tilde{Z}$, $\tilde{Z}''^2$ and $\tilde{C}$. These quantities are then accessed to retrieve composition, $\tilde{\omega}_C$ and h_c from the tables. Since $\tilde{\omega}_C$ is tabulated only for background pressure of 200 bar (denoted by 0), it is rescaled using the power law (10) and (11) for other values of pressure as follows:

$$\tilde{\omega}_C = \tilde{\omega}_{C_0} \frac{\tilde{p}^\alpha}{\tilde{p}_0^\alpha} \quad (10)$$

and

$$\alpha = (3.0882Z'' + 0.0101)Z^2 + (-3.7851Z'' + 0.9567)Z + (0.6638Z'' + 1.4589) \quad (11)$$

Here, the energy equation is solved for h_a . After that, sensible enthalpy h_s is obtained by subtracting h_c from h_a . Temperature is then calculated from sensible enthalpy h_s using the Joint Army Navy NASA Air Force (JANAF) polynomials and tables of thermodynamics [21].

Here, the hybrid RANS/LES based on the SST $k - \omega$ model is selected for both the FPV approach and the one-step-kinetics(OSK) method. The latter only considers the one-step global chemical reaction and uses the canonical OpenFOAM code called rhoReactingFoam [10]. As temperature for each individual species is higher than its critical point of gas, all species are in the gaseous phase. Hence, the ideal-gas state equation is employed. The reacting-mixtures model is adopted to calculate the properties of the mixture. Since compressibility is considered in the combustion simulation, a density-based thermodynamics package is used. The differencing schemes are second-order accurate in both space and time. Implicit backward differencing is selected for time discretization. For spatial discretization, Gaussian integration is chosen. Second-order derivatives are approximated using linear interpolation from cell centers to cell faces.

3. Results and Discussions

3.1. Combustion simulation without pulsing

In this calculation, turbulent combustion is numerically simulated in a chamber with a convergent-divergent nozzle and nineteen coaxial fuel/oxidizer injectors [10]. The three-dimensional unstructured mesh with 3.364189×10^6 grid cells is shown in Figure 1(a). The combustion chamber has a diameter of 43 cm and a length of 33 cm. The oxidizer, which is pure oxygen, is injected into the center of each coaxial port. The fuel, which is pure methane, is injected into the outside annulus. The mass fluxes for the fuel and oxidizer are 16 kg/s and 64 kg/s, respectively. The diameter of the fuel injector is 1.61 cm and that of the oxidizer is 1.42 cm. The temperature at both the fuel and oxidizer injector inlets is 400 K. The simulations start from an initially quiescent flow at 3229 K and an equilibrium chamber pressure at 200 bar. The higher chamber temperature shortens the ignition process and reduces the computational time as no explicit ignition model is included in the current simulation.

To monitor time histories of pressure and other quantities for the study of combustion instability, probes are placed 1 mm away from the chamber wall and equally distributed in the circumferential direction as shown in Figure 1(b). For the case without any pulsing, Figure 2 shows the pressure time histories on the

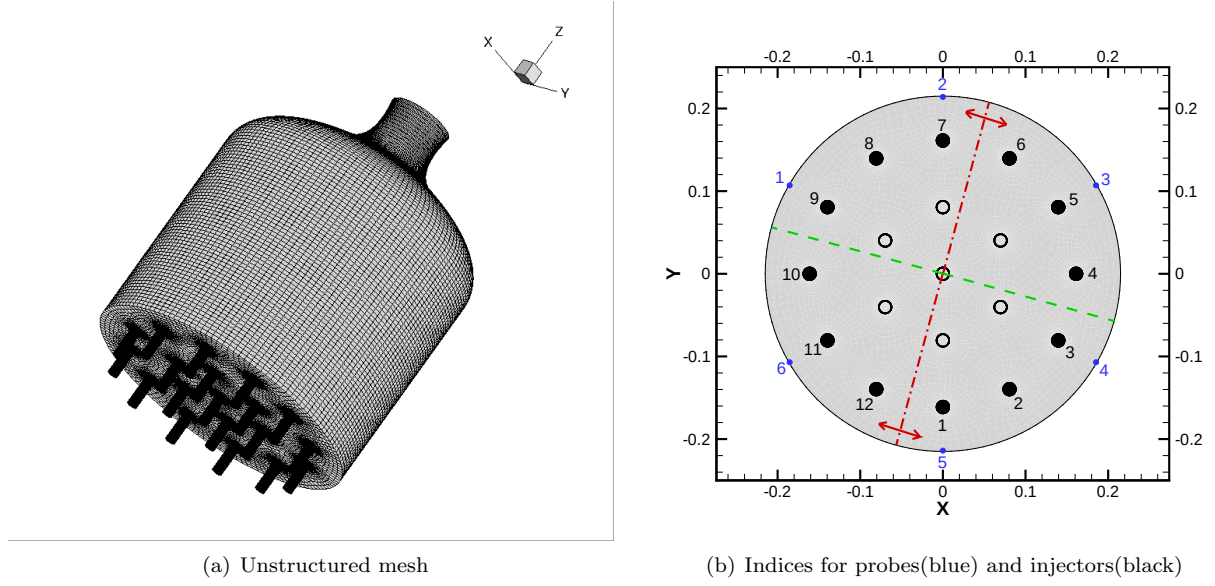


Figure 1: Illustration of 19-injector combustion chamber

near-wall probes at 1 cm downstream of the injector plate using the FPV model. The FPV approach predicts a chamber pressure nearly 10 bar lower than the OSK prediction[10]. By theoretical estimation, the flame temperature in the equilibrium of the 12-species mechanism (used in the FPV approach) is around 3800 K while that of the 4-species one-step global reaction rises to 5000 K. This indicates the flames simulated by the FPV approach is cooler in the combustion chamber, which is consistent with a calculated lower pressure. A weak longitudinal mode is predicted by the OSK method for this case. In the current FPV approach, the mass flow rate at the nozzle outlet already becomes balanced with that at the injector inlets(80 kg/s) after 30 ms as shown in Figure 3. However, no instability-related modes are found even after 43 ms, suggesting stable combustion.

3.2. Combustion instability triggered by tangential traveling wave pulsing

To trigger the tangential traveling wave (TTW) instability modes for the 19-injector combustion chamber, the following pulsing is performed on the mass flow rate at the 12 near-wall injector ports, which are shown with black-filled circles in Figure 1(b):

$$\dot{m} = \epsilon \dot{m}_0 \sin[2\pi f(t - t_0) + \phi] + \dot{m}_0 \quad (12)$$

where $\dot{m}_0$ is 0.8425 kg/s for the fuel and 3.37 kg/s for the oxidizer. The pulsing begins at $t_0 = 0.02223$ s with a frequency of $f = 1500$ Hz and lasts for three cycles. ϕ is the circumferential phase angle of a

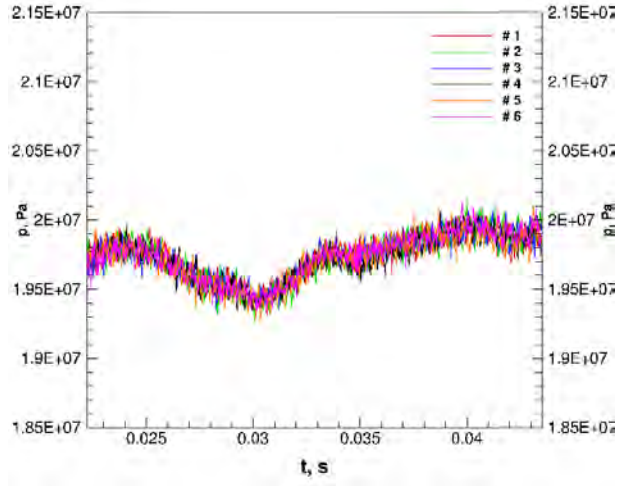


Figure 2: Pressure time history on near-wall probes at $z = 1$ cm using the FPV model for the case without pulsation

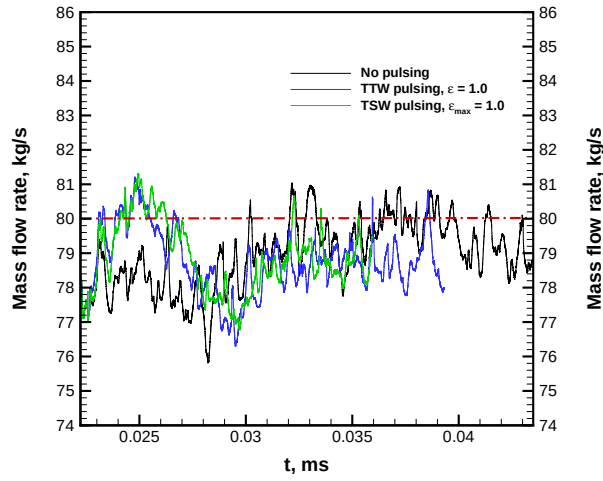


Figure 3: Time history of mass flow rate at nozzle outlet using the FPV model

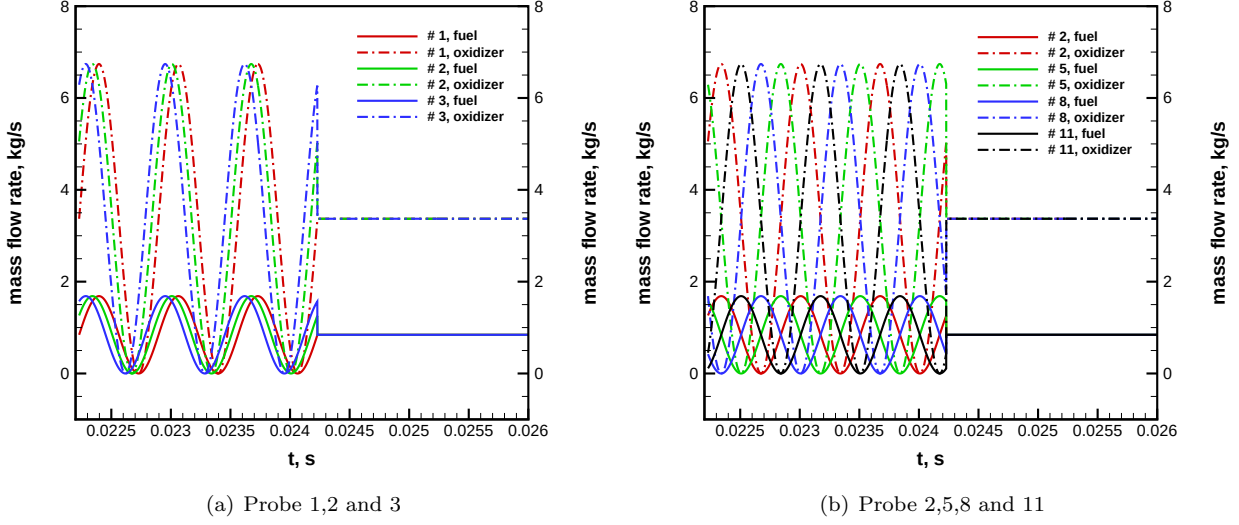


Figure 4: Mass flow rate at the injector ports for the TTW pulsing case where $\epsilon = 1.0$

near-wall injector. It is measured from injector 1 and increases in the counter-clockwise direction. ϵ controls the magnitude of the pulsing and varies between 0 and 1. The pulsing at the fuel port is in phase with that at the oxidizer port. The traveling wave pattern with $\epsilon = 1.0$ is shown in Figure 4 for a group of injectors that are 30 degrees apart and a group of injectors that are 90 degrees apart.

In order to investigate the responses for different external pulsing, four different pulsing mass-flux magnitudes are chosen and they are $\epsilon = 0.25$, $\epsilon = 0.5$, $\epsilon = 0.75$, and $\epsilon = 1.0$. Figure 5 shows the pressure time histories on the near-wall probes at 1 cm downstream of the injector plate for these cases. The filtered pressure at all probes experiences a remarkable increase during pulsing, then drops after the pulsing ends and finally becomes almost plateaued. This is consistent with the time history of mass flow rate at the nozzle outlet as shown in Figure 3 for the case where $\epsilon = 1.0$. As another direct response to the pulsing, the pressure fluctuation has a larger magnitude for a higher ϵ value, suggesting stronger combustion instability.

To identify the dominant mode of the final sustained pressure fluctuation, Fourier analysis is performed for the case where $\epsilon = 1.0$. The pressure time history at each probe in the most recent 2 ms is shown in Figure 6(a). Its spectrum reveals that the dominant frequency is slightly larger than 1500 Hz (the pulsing frequency). Reconstructed time history using the 1500 Hz mode only is shown in Figure 6(c), which clearly suggests a tangential traveling wave mode with a peak-to-peak variation of around 4 bar.

Figure 7 and 8 show the instantaneous pressure contours in the $x = 0$ meridian plane and the $z = 1$ cm cross-sectional plane of the combustion chamber during one cycle for the case where $\epsilon = 1.0$. Since they

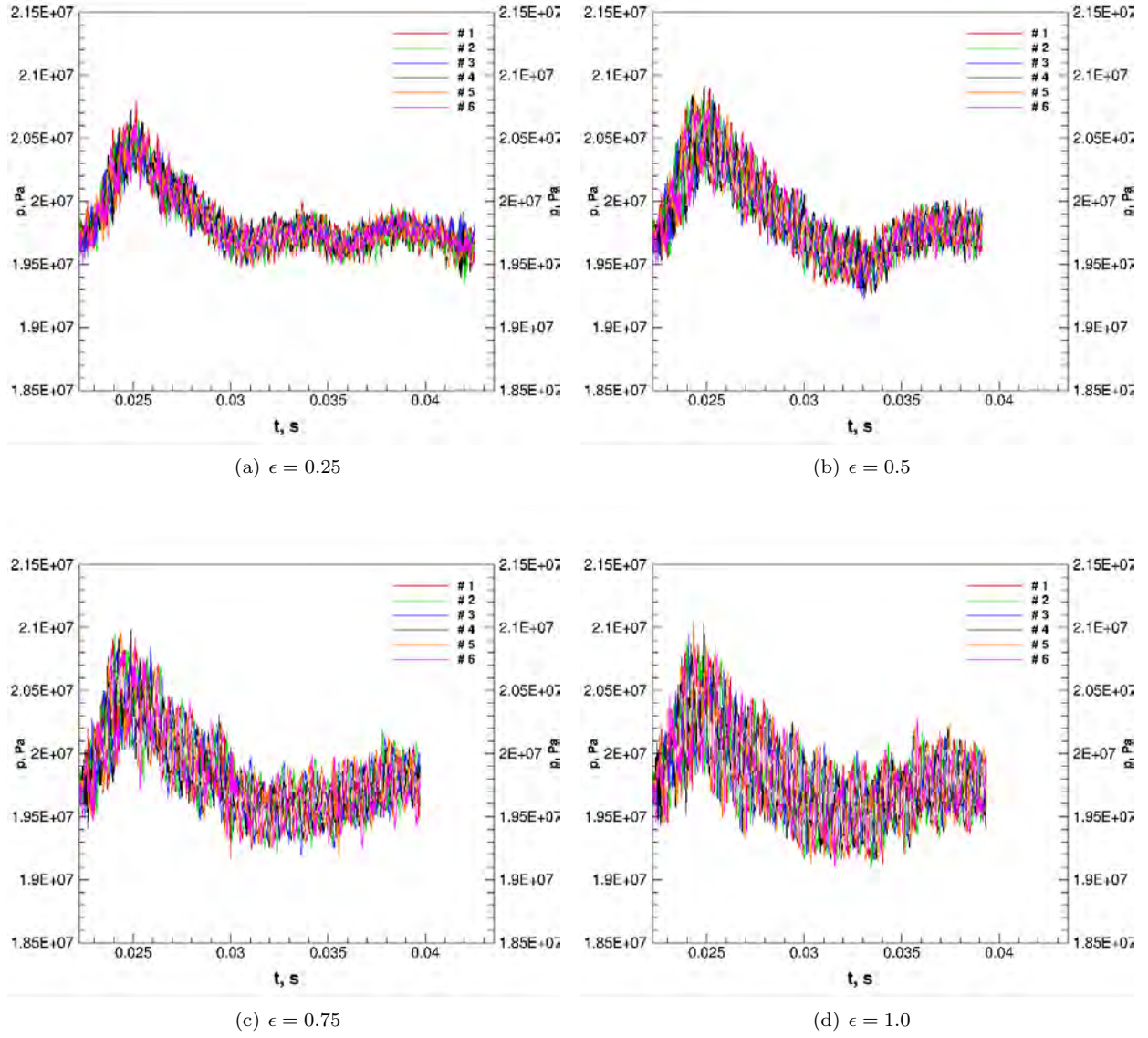


Figure 5: Pressure time history on near-wall probes at $z = 1$ cm using the FPV model for the TTW pulsing cases

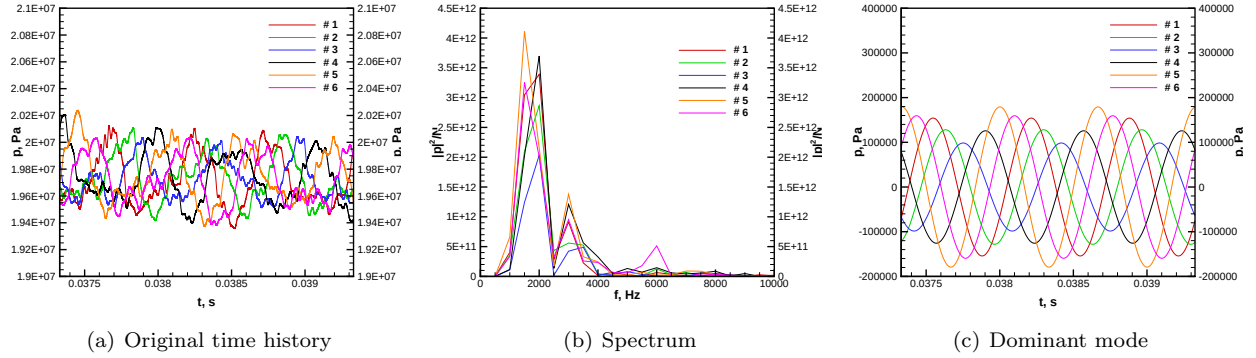


Figure 6: Mode analysis of pressure on near-wall probes at $z = 1$ cm using the FPV model for the TTW pulsing case where $\epsilon = 1.0$

are reconstructed for the 1500 Hz mode only, the major instability wave pattern in the entire combustion chamber is illustrated.

At $\frac{1}{4}$ period, the pressure reaches the positive maximum on the combustion-chamber left side and the negative maximum on the right. The fluctuation gradually decreases from the chamber wall to the center of the chamber, which is frequently seen for the fluid tangential mode. Observed in the circumferential direction, the nodal points of the near-wall fluctuation are found on the top and at the bottom. The pressure fluctuation in the injectors is out of phase with the pressure fluctuation inside the combustion chamber. At $\frac{1}{2}$ period, the pressure wave rotates about 90 degrees in the clockwise direction around the combustion chamber. At $\frac{3}{4}$ period, the pressure distribution in both the combustion chamber and injector is opposite in sign to that at $\frac{1}{4}$ period. At a full period, the pressure becomes opposite in sign as compared to its values at $\frac{1}{2}$ period. During one cycle, the diameter connecting the two near-wall nodal points rotates around the combustion chamber, indicating a tangential traveling wave instability.

Figure 9 shows the time-averaged fuel mass fraction, the heat release rate, the reaction rate for the progress variable, and the temperature in the $x = 0$ cm meridian plane of $\epsilon = 1.0$ case with the time duration covering 2 oscillation periods. Compared to the OSK prediction [10], the fuel burning rate is lower in the FPV approach as the fuel jets travel a longer distance in the combustion chamber. This is reasonable because the OSK method assumes a fast reaction. The reaction simulated by the FPV approach in the upstream half of the combustion chamber is remarkably weaker compared to the OSK prediction. It is consistent with the cooler combustion chamber, the lower mean pressure, and the weaker sustained instability mode.

A frequently used indicator of combustion instability is the Rayleigh index, which is a correlation used

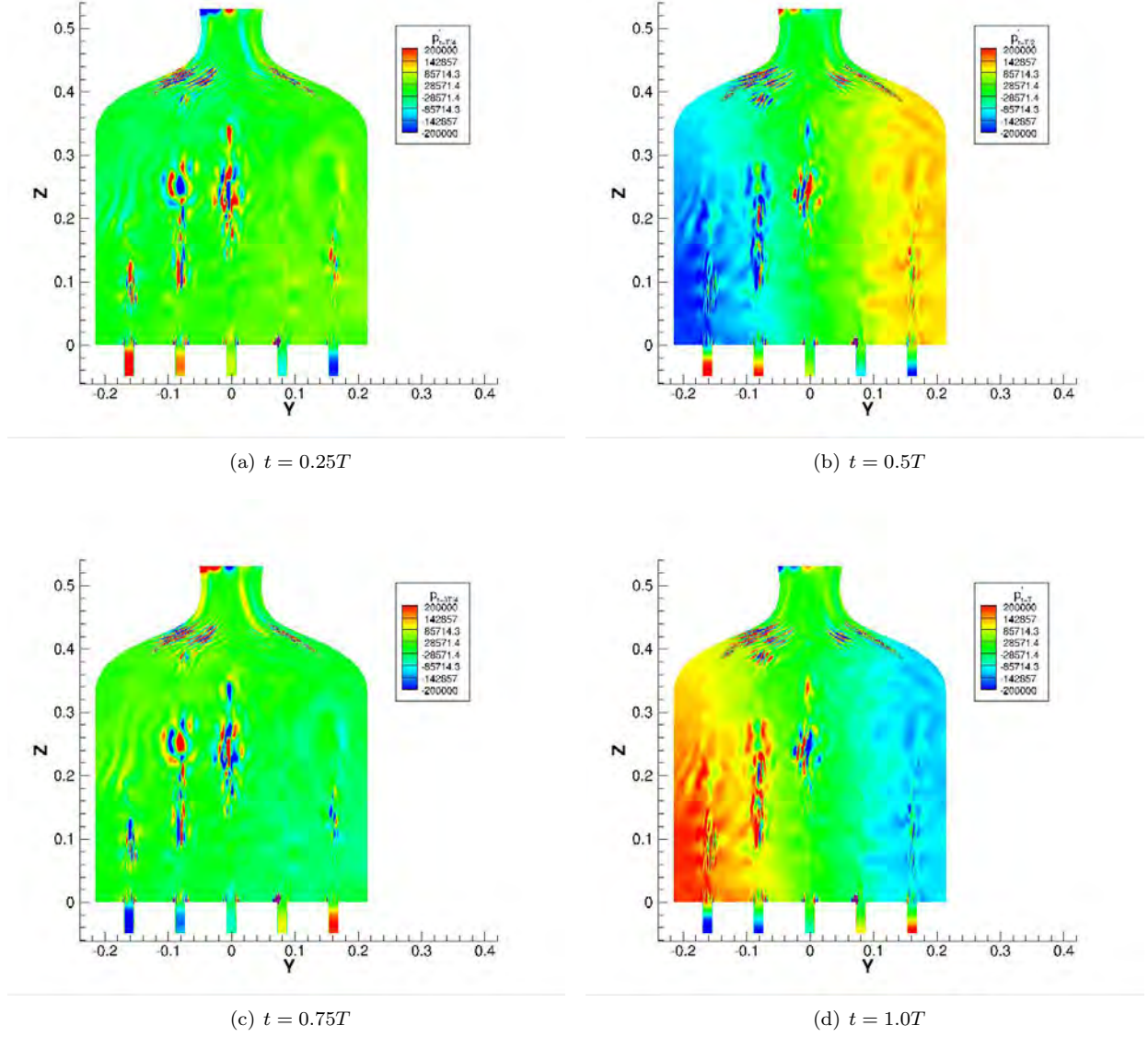
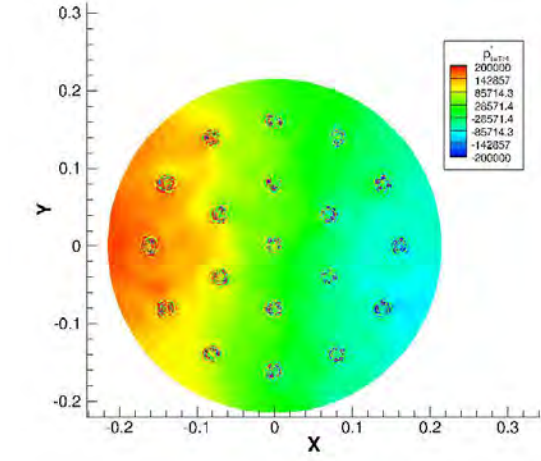
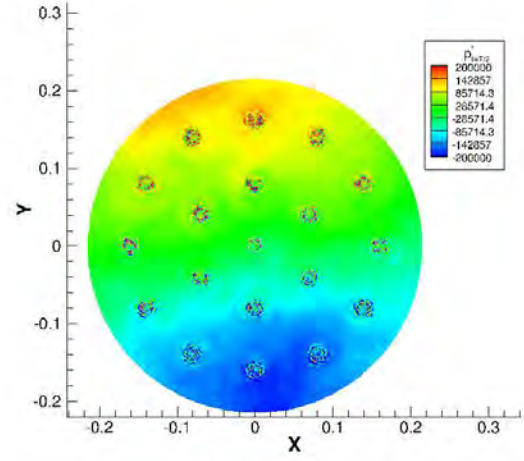


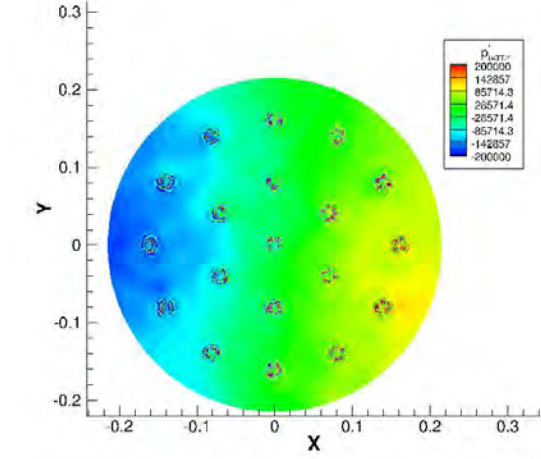
Figure 7: Instantaneous pressure of the dominant mode on the chamber $x = 0$ cm plane using the FPV model for the TTW pulsing case where $\epsilon = 1.0$



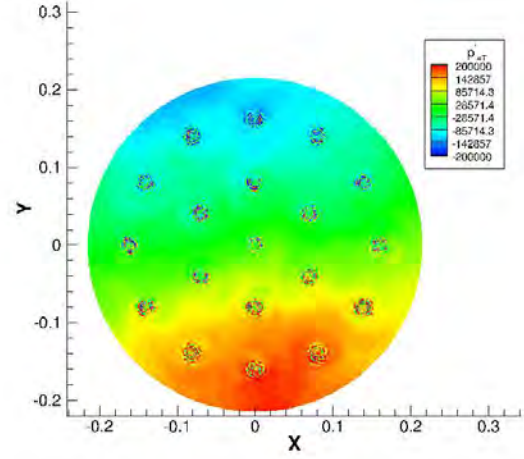
(a) $t = 0.25T$



(b) $t = 0.5T$

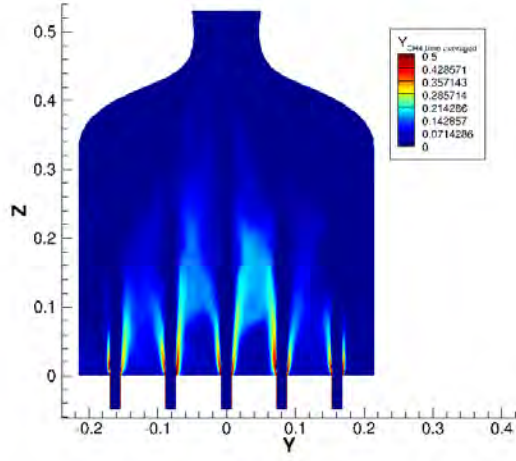


(c) $t = 0.75T$

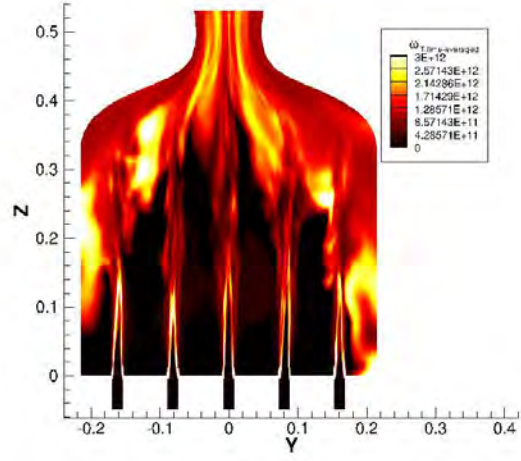


(d) $t = 1.0T$

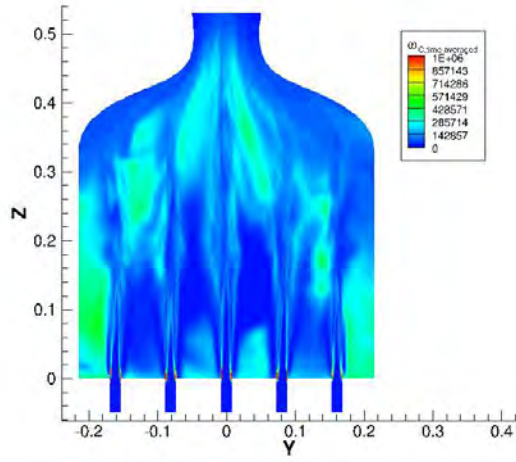
Figure 8: Instantaneous pressure of the dominant mode on the chamber $z = 1$ cm plane using the FPV model for the TTW pulsing case where $\epsilon = 1.0$



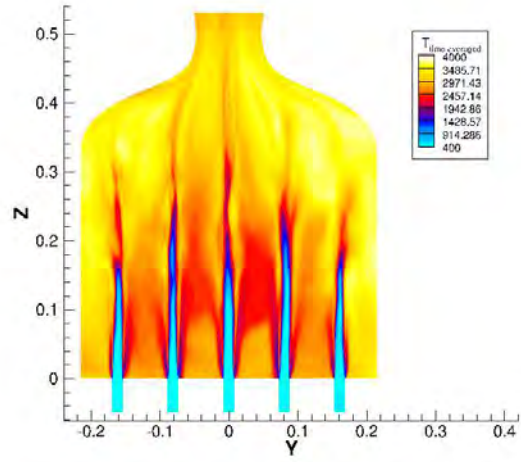
(a) Y_{CH_4}



(b) Heat release rate



(c) progress-variable reaction rate



(d) Temperature

Figure 9: Time-averaging on the chamber $x = 0$ cm plane using the FPV model for the TTW pulsing case where $\epsilon = 1.0$

to determine locally the correlation between the pressure oscillations and the unsteady heat release rate. If the pressure oscillates in phase with the heat release rate, the flow is more likely to be unstable. The out-of-phase oscillations often suggest a stable case. The time-averaged local Rayleigh index (RI) is defined as follows

$$RI = \frac{1}{\tau p_a} \int_{t_0}^{t_0+\tau} \frac{\gamma - 1}{\gamma} p' \dot{\omega}'_T dt \quad (13)$$

where τ is the period of the instability, p' is the local pressure oscillation, p_a is the local time-averaged pressure, γ here is the specific heat ratio, and $\dot{\omega}'_T$ is the local oscillation of heat release rate. The most recent 2 ms of the simulation is used for the time-averaging.

Figure 10 shows the Rayleigh index in the $x = 0$ meridian plane and three cross-sectional plane of the combustion chamber for the TTW case where $\epsilon = 1.0$. Positive large values of the Rayleigh index are found in the surrounding region of the fuel/oxidizer jets where the strong reaction occurs. The spinning tangential instability wave travels around the chamber and makes the large positive Rayleigh index region extends all through the chamber. The maximum positive Rayleigh index region appears in the outer regions near the chamber wall, in particular on the $z = 14$ cm plane as shown in Figure 10(c). This indicates that, in the near-wall region, the pressure fluctuation is strongly driven by the unsteady heat release rate. This mechanism is critical in sustaining the TTW instability.

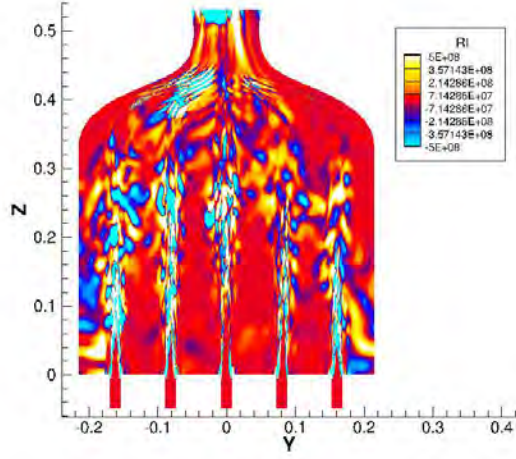
In the current FPV approach, the tabulated heat release rate is not introduced in the energy equation as a source term. For this reason, it might be also helpful to calculate the correlation of pressure fluctuation and unsteady reaction rate for the progress variable when studying the coupling between acoustic waves and flames. A local index for that correlation can be defined as:

$$IPRRC = \frac{1}{\tau p_a} \int_{t_0}^{t_0+\tau} p' \dot{\omega}'_C dt \quad (14)$$

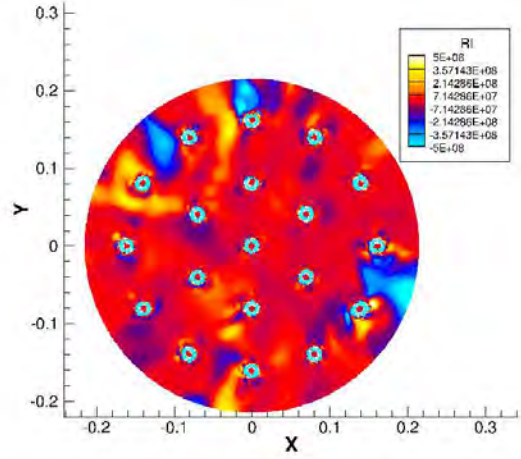
where τ is the period of the instability, p' is the local pressure oscillation, p_a is the local time-averaged pressure, and $\dot{\omega}'_C$ is the local oscillation of progress-variable reaction rate. The most recent 2 ms of the simulation is used for the time-averaging as well.

Figure 11 shows IPRRC in the $x = 0$ meridian plane and three cross-sectional plane of the combustion chamber for the TTW case where $\epsilon = 1.0$. The features including the locations of large positive values are similar to those of the Rayleigh index contours.

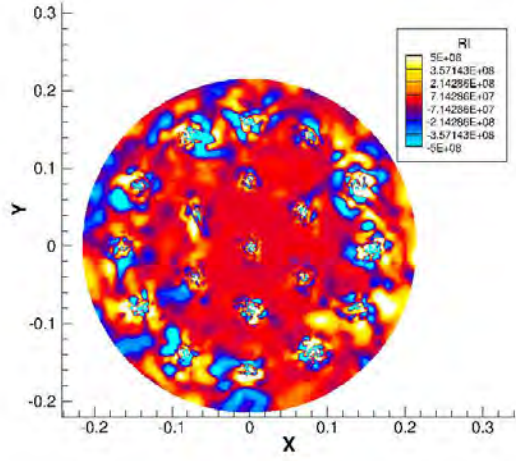
Figure 12 shows the time histories of the volume-averaged pressure and the progress-variable reaction



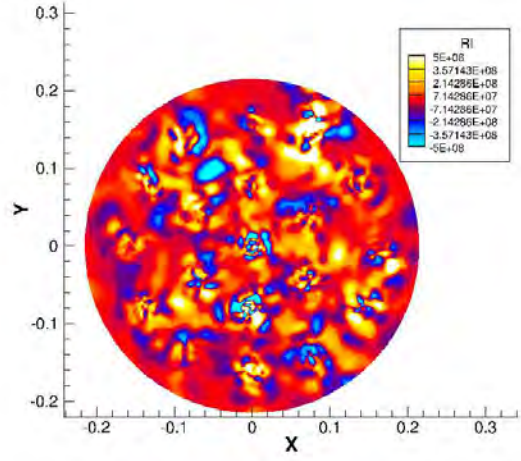
(a) $x = 0$ cm plane



(b) $z = 1$ cm plane

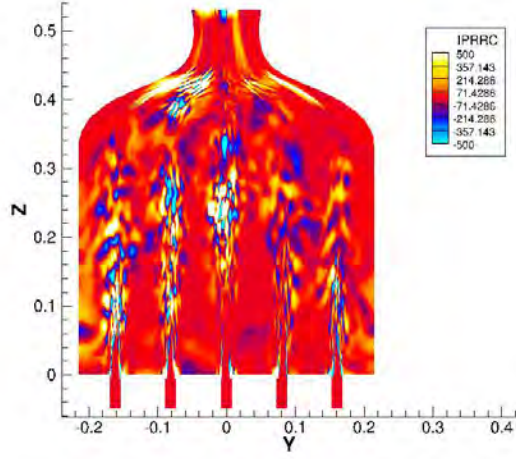


(c) $z = 14$ cm plane

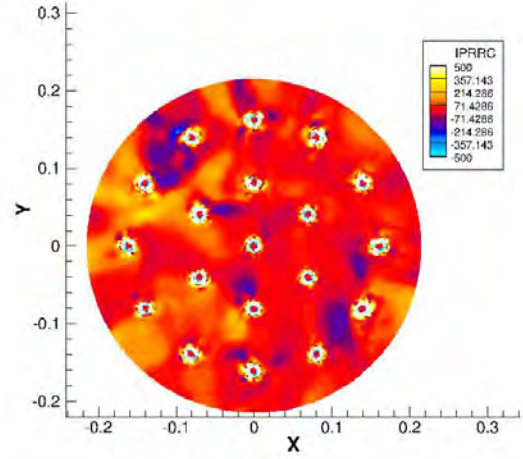


(d) $z = 28$ cm plane

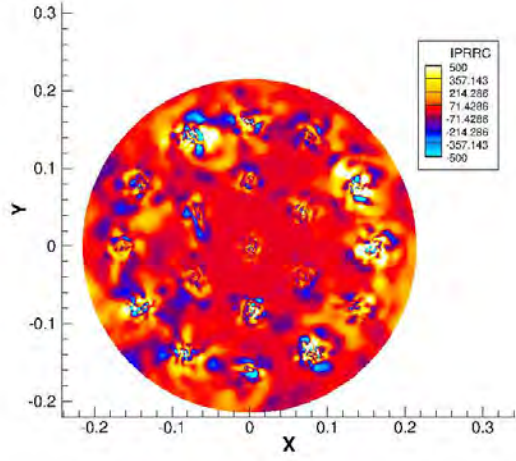
Figure 10: Time-averaged Rayleigh Index using the FPV model for the TTW pulsing case where $\epsilon = 1.0$



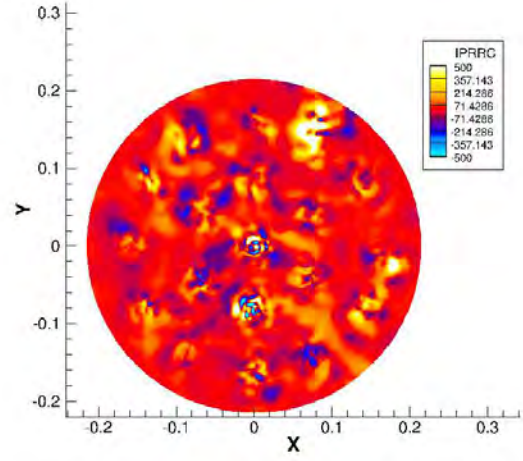
(a) $x = 0$ cm plane



(b) $z = 1$ cm plane



(c) $z = 14$ cm plane



(d) $z = 28$ cm plane

Figure 11: Time-averaged IPRRC using the FPV model for the TTW pulsing case where $\epsilon = 1.0$

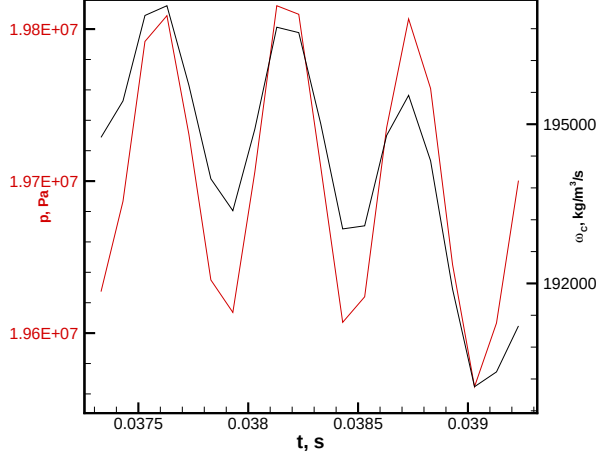


Figure 12: Volume-averaged pressure and progress-variable reaction using the FPV model for the TTW pulsing case where $\epsilon = 1.0$

rate for the case where $\epsilon = 1.0$. The volume selected for averaging contains half of the combustion chamber on one side of the $x = 0$ meridian plane. The injectors and the nozzle are not considered in the calculation. The progress-variable reaction rate is completely in phase with the pressure oscillation, which results in strong tangential instability.

3.3. Combustion instability triggered by tangential standing wave pulsing

The triggered instability response to the tangential traveling wave (TSW) pulsing is also studied for the 19-injector combustion chamber. The pulsing is still performed on the mass flow rate at the 12 near-wall injector ports but using a different strategy as follows:

$$\dot{m} = \epsilon(\phi)\dot{m}_0 \sin[2\pi f(t - t_0)] + \dot{m}_0 \quad (15)$$

where most of the parameters remain the same as in the TTW pulsing cases. However, the magnitude of the pulsing changes with the azimuthal position so that ϵ becomes a function of the circumferential phase angle ϕ . The 12 injectors are divided into two groups by the meridian plane(plane of antisymmetry) represented using the red dash-dot line as shown in Figure 1(b). A standing wave is excited in the transverse direction by pulsing the two groups with the pulses 180 degrees out of phase. The pulsing amplitude for each injector is proportional to ϕ measured from the plane of antisymmetry. It reaches a maximum near the plane of symmetry for the standing wave (represented by the green dash line in Figure 1(b)) and minimum close to the plane of antisymmetry. The standing wave pattern with $\epsilon_{max} = 1.0$ is shown in Figure 13 for a group

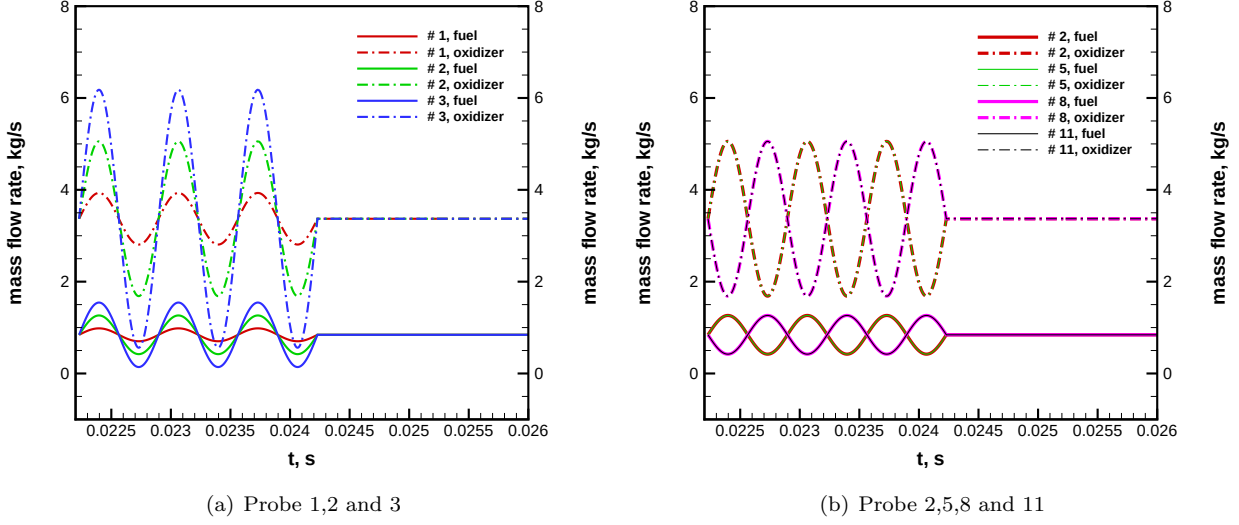


Figure 13: Mass flow rate at the injector ports for the TSW pulsing case

of injectors that are 30 degrees apart and a group of injectors that are 90 degrees apart.

To study the response to the TSW pulsing, only one case is considered where the maximum ϵ is one. Figure 14 shows the pressure time histories on the near-wall probes at 1 cm downstream of the injector plate for these cases. Similar to the TTW cases, the filtered pressure at all probes in the current TSW case experiences a remarkable increase during pulsing, then decreases after the pulsing ends and finally turns to be plateaued. This is consistent with the time history of mass flow rate at the nozzle outlet as shown in Figure 3. Compared to the TTW case with $\epsilon = 1.0$, the pressure fluctuates with a smaller amplitude here. This is because ϵ in the current TSW case changes on different injectors. Although the maximum ϵ is one, the averaged pulsing magnitude over the 12 injectors falls less than one. Hence, the overall pulsing in the current TSW case is weaker than in the TTW case where $\epsilon = 1.0$ and a weaker instability is triggered in the current case.

To identify the dominant mode of the final sustained pressure fluctuation, Fourier analysis is performed. The pressure time history at each probe in the most recent 2 ms is shown in Figure 15(a). The dominant frequency is also slightly larger than 1500 Hz (the pulsing frequency). However, compared to the TTW case with $\epsilon = 1.0$, the amplitude of the dominant mode is significantly reduced in the current case. Reconstructed time history using the 1500 Hz mode only is shown in Figure 15(c). The pressure fluctuations at any pair of probes that are 180 degrees apart are about 180 degrees out of phase. Pressure at probes 1 and 4 fluctuates with the largest amplitude as the pair of probes are close to the plane of symmetry for the TSW pulsing.

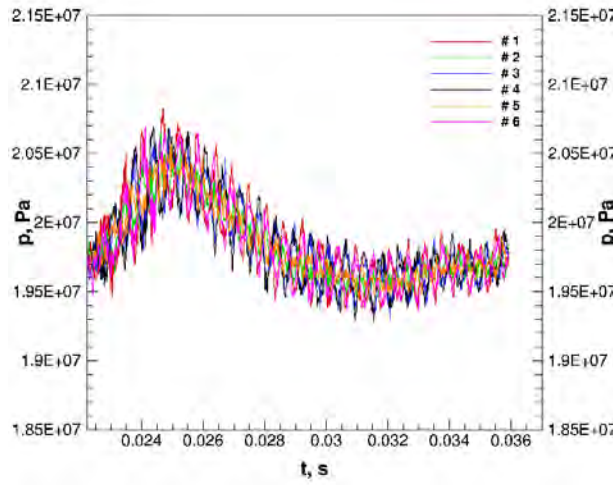


Figure 14: Pressure time history on near-wall probes at $z = 1$ cm using the FPV model for the TSW pulsing case

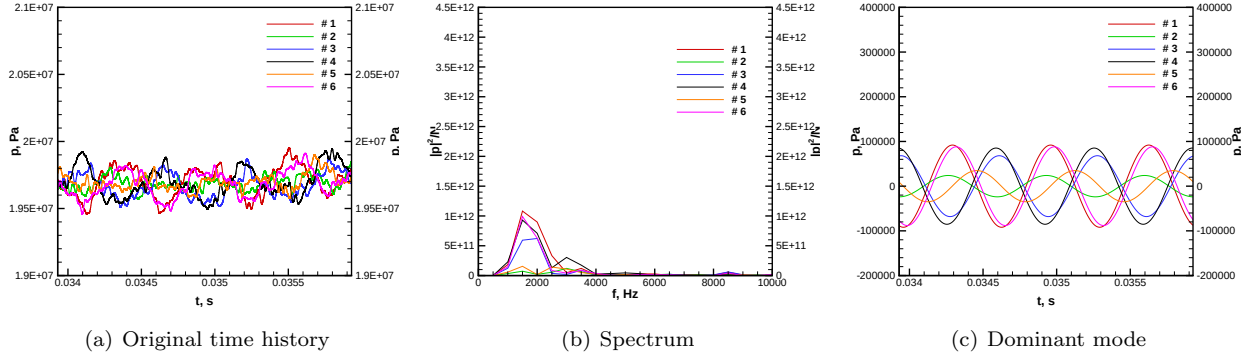


Figure 15: Mode analysis of pressure on near-wall probes at $z = 1$ cm using the FPV model for the TSW pulsing case

Probes 3 and 6 are located farther from the plane of symmetry and the pressure fluctuation at them has a smaller magnitude. Pressure at probes 2 and 5 fluctuates with a substantially reduced amplitude as the two probes are very close to the plane of antisymmetry for the TSW pulsing. All these features clearly suggest a tangential standing wave mode with a maximum peak-to-peak variation of around 2 bar.

Figure 16 and Figure 17 show the the instantaneous pressure contours in the $y = 0$ meridian plane and the $z = 1$ cm cross-sectional plane of the combustion chamber during one cycle of the TSW pulsing. Since they are reconstructed using the 1500 Hz mode only, the major instability wave pattern in the entire combustion chamber is illustrated. The wave pattern is standard for TSW instability. Moreover, the diameter connecting the nodal points for the instability wave doesn't rotate and always overlaps with the plane of antisymmetry for the TSW pulsing. The antinodal points of the instability fluctuation occur at the azimuthal positions

where the pulsing magnitude reaches a positive/negative maximum.

Figure 18 shows the Rayleigh index in the $x = 0$ meridian plane and three cross-sectional planes of the combustion chamber for the current case. Positive large values of the Rayleigh index are found in the surrounding region of the fuel/oxidizer jets where the strong reaction occurs. The standing tangential instability wave resonates in the chamber and makes the relatively large positive Rayleigh index region extend all through the chamber. Figure 18(c) shows that the maximum positive Rayleigh index mainly occurs near the antinodes of the TSW pulsing and hence the mechanism helps to sustain the TSW instability.

Figure 19 shows IPRRC in the $x = 0$ meridian plane and three cross-sectional plane of the combustion chamber for the current TSW case. The features including the locations of large positive values are similar to those of the Rayleigh index contours.

Figure 20 shows the time histories of the volume-averaged pressure and the progress-variable reaction rate. The volume of averaging contains only half of the combustion chamber on one side of the $x = 0$ meridian plane. The fluctuation of progress-variable reaction rate is completely in phase with the pressure oscillation. This is another proof that the acoustic waves and the flames are strongly coupled in the current TSW instability.

4. Conclusion

The triggered tangential combustion instability is computationally studied through the flamelet progress variable (FPV) approach for a nineteen-injector rocket engine. The governing equations for the FPV approach are solved by a newly developed C++ code which is based on OpenFOAM 4.1. The Flamemaster code is used to generate the flamelet tables for methane/oxygen combustion at a background pressure of 200 bar. A 12-species kinetics is adopted to represent the chemical reactions. To consider the pressure effect on the reaction rate for the progress variable while saving the computational cost of retrieving data from the tables, the reaction rate is rescaled using a power law.

Two different pulsation schemes are used in the present work to study the triggered tangential combustion instability. One is the traveling wave pulsation and the other is the standing wave pulsation. For the former scheme, four different pulsing amplitudes are considered to investigate the instability response. The first tangential traveling wave mode is found dominant regardless of the pulsing amplitude. However, the magnitude of the dominant instability mode grows as the pulsing amplitude increases. The dominant frequency at large pulsing amplitude is found slightly higher than the frequency of pulsation. The current results using the FPV approach are qualitatively similar to the OSK simulations. However, the FPV

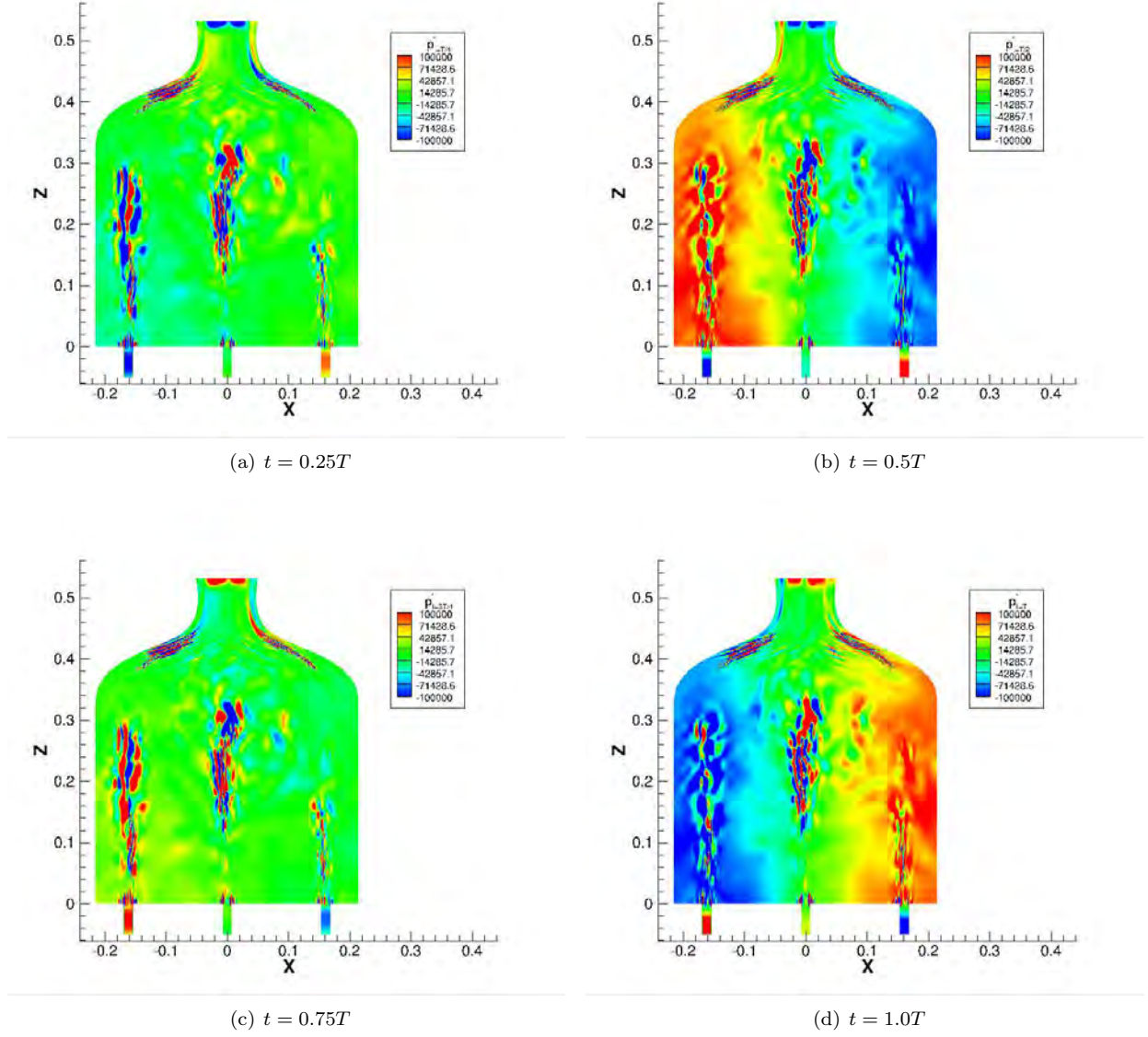
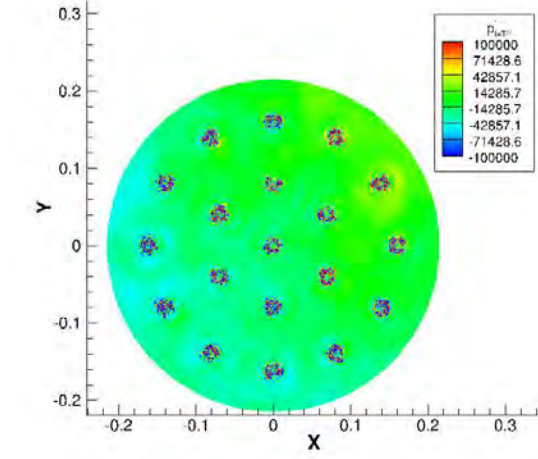
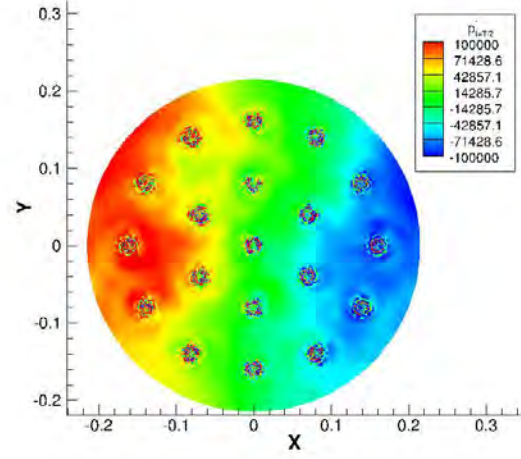


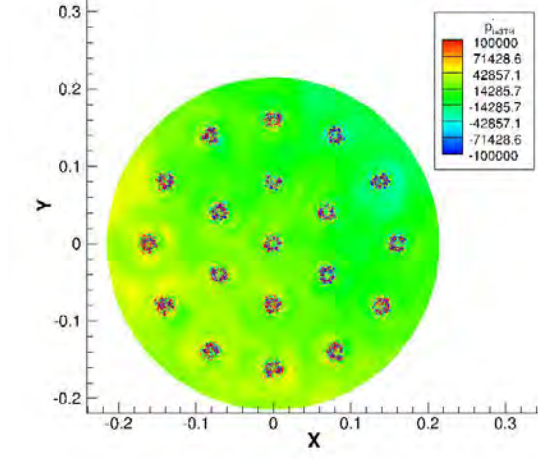
Figure 16: Instantaneous pressure of the dominant mode on the chamber $y = 0$ cm plane using the FPV model for the TSW pulsing case



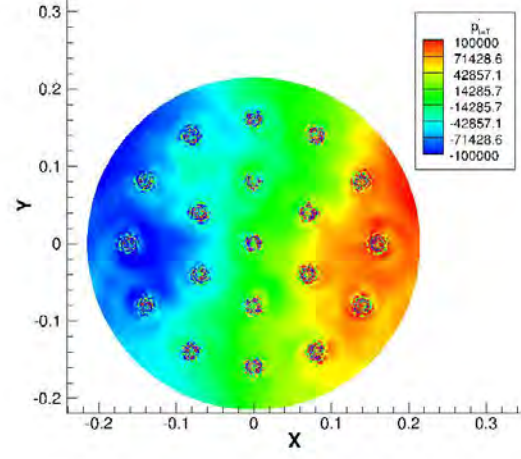
(a) $t = 0.25T$



(b) $t = 0.5T$

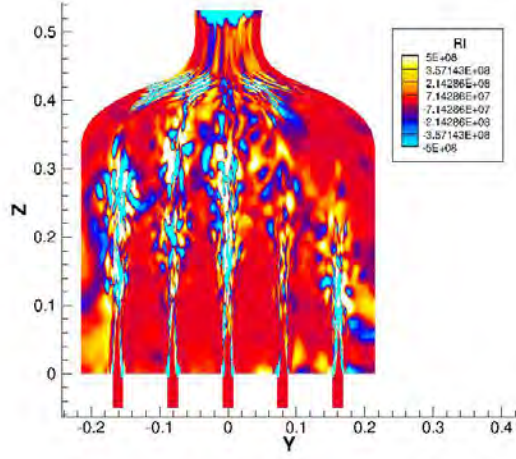


(c) $t = 0.75T$

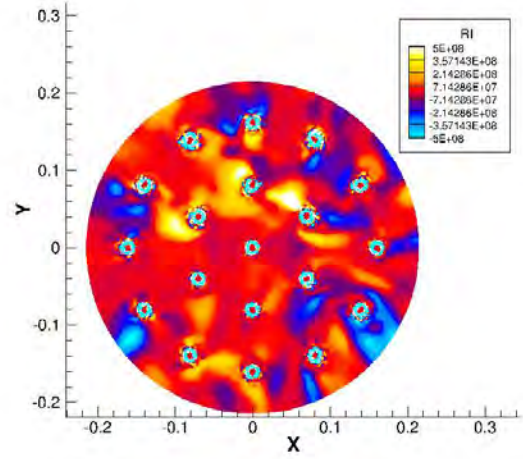


(d) $t = 1.0T$

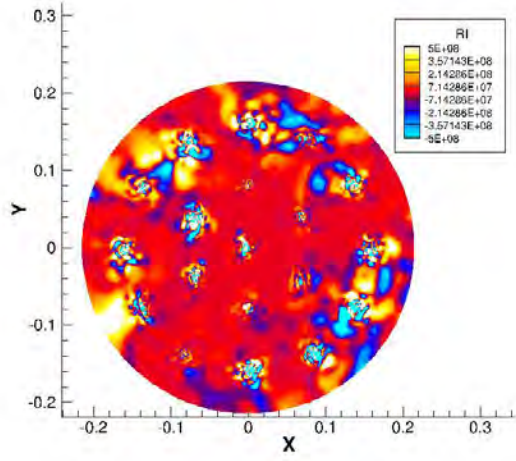
Figure 17: Instantaneous pressure of the dominant mode on the chamber $z = 1$ cm plane using the FPV model for the TSW pulsing case



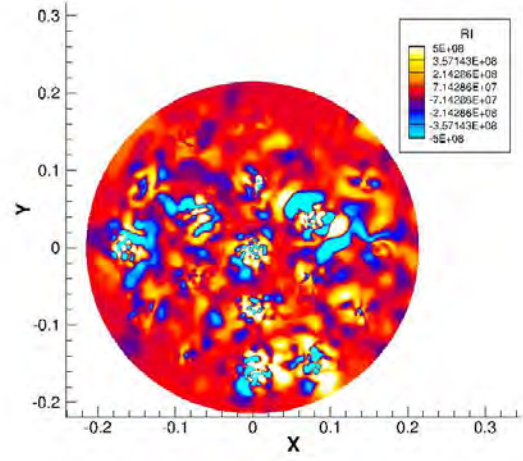
(a) $x = 0$ cm plane



(b) $z = 1$ cm plane

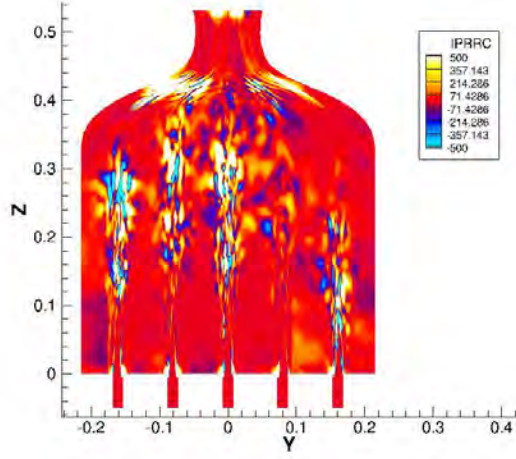


(c) $z = 14$ cm plane

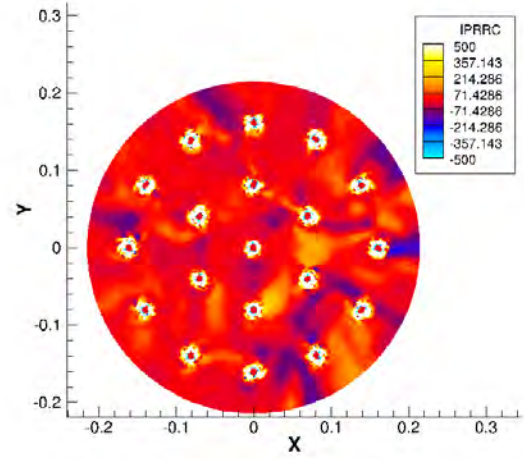


(d) $z = 28$ cm plane

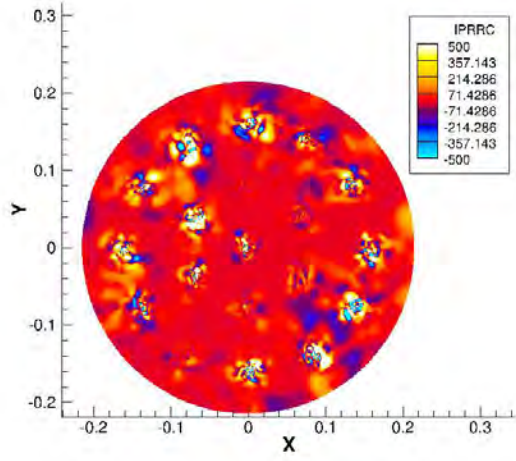
Figure 18: Time-averaged Rayleigh Index using the FPV model for the TSW pulsing case



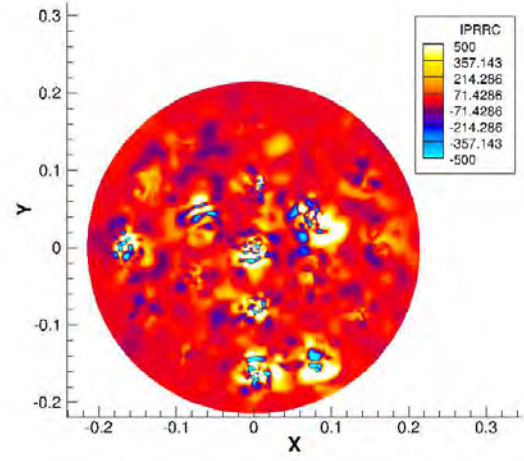
(a) $x = 0$ cm plane



(b) $z = 1$ cm plane



(c) $z = 14$ cm plane



(d) $z = 28$ cm plane

Figure 19: Time-averaged IPRRC using the FPV model for the TSW pulsing case

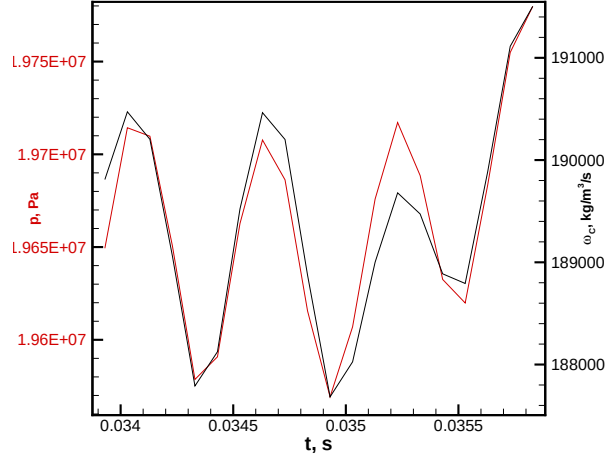


Figure 20: Volume-averaged pressure and progress-variable reaction using the FPV model for the TSW pulsing case

approach predicts a much lower magnitude of the triggered instability. Moreover, the longitudinal mode is not triggered with the weakest tangential traveling wave pulsing in the current FPV predictions. Further research is needed to uncover the mechanism that causes this difference. Analysis of the Rayleigh index and the interaction between the pressure fluctuation and the fluctuation of the progress-variable reaction rate confirms that the triggered instability mode is driven by the unsteady heat release rate or the unsteady progress-variable reaction rate. Compared to the OSK prediction, the lower fuel burning rate results in a cooler combustion chamber, a lower mean pressure, and a weaker sustained instability mode in the FPV approach.

With the FPV approach, the latest computational results show that a tangential traveling wave mode is not triggered through the tangential standing wave pulsation. The tangential standing wave is found dominant in the triggered instability. The mechanism that causes this difference will be studied in the future. The frequency of the major instability wave is also found slightly higher than the frequency of pulsation. Evaluation of the Rayleigh index and the interaction between the pressure fluctuation and the fluctuation of the progress-variable reaction rate indicate that the triggered instability mode is driven by the unsteady heat release rate or the unsteady progress-variable reaction rate.

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Addendum IV

Three-dimensional, Rotational Flamelet Closure Model with Two-way Coupling

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JFM Keywords:	Combustion < Reacting Flows, Turbulent reacting flows < Reacting Flows
Abstract:	A new flamelet model is developed for sub-grid modeling and coupled with the resolved flow for turbulent combustion. The model differs from current models in critical ways. (i) Non-premixed flames, premixed flames, or multi-branched flame structures are determined rather than prescribed. (ii) The effects of shear strain and vorticity are determined. (iii) The strain rates and vorticity applied at the sub-grid level are directly determined from the resolved-scale strain rates and vorticity without a contrived progress variable. (iv) The flamelet model is three-dimensional. (v) The effect of variable density is addressed. Solutions to the multicomponent Navier-Stokes equations governing the flamelet model are obtained. By coordinate transformation, a similar solution is found for the model, through a system of ordinary differential equations. Vorticity creates a centrifugal force on the sub-grid counterflow that modifies the molecular transport rates and burning rate. Sample computations of the rotational flamelet model without coupling to the resolved flow are presented first to demonstrate the importance of the new features. Scaling laws are presented for relating strain rates and vorticity at the sub-grid level to quantities at the resolved-flow level for coupling with large-eddy simulations or Reynolds-averaged flows. The time-averaged behavior of a simple turbulent flow is resolved with coupling to the rotational flamelet model. Specifically, a two-dimensional, multicomponent, time-averaged planar shear layer with variable density and energy release is employed using a mixing-length description for the eddy viscosity. Needs for future study are identified.

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Three-dimensional, Rotational Flamelet Closure Model with Two-way Coupling

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April 5, 2022

Abstract

A new flamelet model is developed to be used for sub-grid modeling and coupled with the resolved flow description for turbulent combustion. The model differs from current models in several critical ways. (i) Non-premixed flames, premixed flames, or multi-branched flame structures are determined rather than prescribed. (ii) The effects of shear strain and vorticity on the flames are determined. (iii) The strain rates and vorticity applied at the sub-grid level are directly determined from the resolved-scale strain rates and vorticity without the use of a contrived progress variable. (iv) The flamelet model is three-dimensional without need for assuming axisymmetry or planar geometry. (v) The effect of variable density is addressed in the flamelet model. Solutions to the Navier-Stokes equations and the associated scalar equations governing the flamelet model are obtained without the boundary-layer approximation. By appropriate coordinate transformation, a similar solution is found for the rotational flamelet model, reducing it to system of ordinary differential equations (ODEs). Vorticity is shown to create a centrifugal force on the sub-grid counterflow that modifies the molecular transport rates and burning rate. Sample computations of the rotational flamelet model without coupling to the resolved flow are presented first to demonstrate the importance of the new features of the model. Scaling laws are presented for relating strain rates and vorticity at the sub-grid level to those quantities at the resolved-flow level for coupling with large-eddy simulations or the

time-averaged mean-flow level for Reynolds-averaged flows. The time-averaged behavior of a simple turbulent flow is resolved with coupling to the rotational flamelet model. Specifically, a two-dimensional, multicomponent, time-averaged planar shear layer with variable density and energy release is employed using a mixing-length description for the eddy viscosity. Needs for future study are identified.

1 Introduction

Combustion in high mass-flux chambers is the practical and major method for energy conversion for mechanical power and heating. Inherently, the high mass-flow rate leads to turbulent flow. Thereby, many length and time scales appear in the physics making serious challenges for both computational and experimental analyses. For computations where the smallest scales typically cannot be resolved, the method of large-eddy simulations (LES) is employed wherein the smaller scales are filtered via integration over a window size commensurate with the computational mesh size that allows affordable computations. Consequently, the essential, rate-controlling, physical and chemical processes that occur on shorter scales than the filter size must be modelled. Those sub-grid models must be properly coupled to the resolved LES flow field.

Current flamelet models that are used for LES or Reynolds-averaged Navier-Stokes (RANS) methods have some advantages. Typically, the flamelet equations are a system of ordinary differential equations (ODEs) that can be solved offline with solutions available in tabular form or through neural networks (NN). The flamelet models can handle multi-species, multi-step oxidation kinetics without requiring small time steps during the solution of the resolved-scale fluid dynamics. Thus, for several reasons, savings of computational resources can be huge compared to direct numerical simulation. We aim here to retain these very attractive features while removing some less desirable features. Already, some progress has been made in extending the fundamental flamelet theory beyond its long-term limitation of a single-flame structure, two-dimensional (or axisymmetric) configuration, and use of the uniform-density assumption. However, those advances still must be applied to LES or RANS. In addition, the flamelet theory must be advanced to consider shear strain and vorticity at the small scale of the flamelet; these are the vital forgotten physics in current flamelet modelling. Furthermore, the strain

rates in the flamelet model are far from properly connected to the strain rates at the resolved scale. Attempts at corrections of these weaknesses are made here.

The focus here is on the types of turbulent flames found in the shear-driven flows of practical combustors. Thereby, we address flamelets as originally described by Williams (1975), namely “highly sheared small diffusion flamelets” and “forming a turbulent flame brush which appears on the average to fill” the flow domain. Our discussion will not cover some interesting work on corrugated or wrinkled flames. The goals in this paper are to improve the flamelet model by including several important physical effects that are commonly neglected in present models and to identify other issues, related to the coupling between the sub-grid-scale physics and the resolved-scale (or time-averaged) physics, that require further study.

1.1 Existing Flamelet Theory

There is need to understand the laminar mixing and combustion that commonly occur within the smallest turbulent eddies. These laminar flamelet sub-domains experience significant strain of all types: shear, tensile, and compressive. Some important works exist here but typically for either counterflows with only normal strain or simple vortex structures in two-dimensions or axisymmetry and often with a constant-density approximation. See Linan (1974), Marble (1985), Karagozian and Marble (1986), Cetegen and Sirignano (1988), Cetegen and Sirignano (1990), Peters (2000), and Pierce and Moin (2004). Linan and Peters focused on the counterflow configuration. Williams (1975) first established the concept of laminar flamelets in the turbulent diffusion flame structure. Karagozian and Marble examined a three-dimensional flow with radial inward velocity, axial jetting, and a vortex centered on the axis. The flame sheet wrapped around the axis due to the vorticity. An interesting review of the early flamelet theory is given by Williams (2000). Generally, flamelet studies have focused on either premixed or nonpremixed flames; a unifying approach to premixed, nonpremixed, and multi-branched flames has not been developed. That unifying approach is taken here.

Most flamelet studies have not directly considered vorticity interaction with the flamelet. See, for example, Linan (1974); Peters (2000); Williams (2000); Pierce and Moin (2004). Mueller (2020) presented the flamelet model in a somewhat different mathematical framework but without the addition

of new physical description. Williams (1975) first recognized the advantage of separating rotation (due to vorticity) and stretching by transformation to a rotating, non-Newtonian reference frame. He did not however examine the momentum consequences in the new reference frame which will be examined later here. The other works that have examined vortex-flame interaction have not separated the effects of stretching and rotation. See Marble (1985); Karagozian and Marble (1986); Cetegen and Sirignano (1988, 1990); Meneveau and Poinso (1991).

Again, with the above-mentioned emphasis on turbulent flames in shear-driven flows as defined by Williams (1975), some interesting work on corrugated or wrinkled premixed laminar flames is not detailed here. The reader is guided to Swaminathan and Grout (2006), Steinberg and Driscoll (2009), Chakraborty and Swaminathan (2007), and Mura and Champion (2009) for examples of those studies.

The two-dimensional planar or axisymmetric counterflow configuration has become a foundation for flamelet model. Local conversion to a coordinate system based on the principal strain-rate directions can provide the counterflow configuration in a general flow. Furthermore, the quasi-steady counterflow can be analyzed by ordinary differential equations because the dependence on the transverse coordinate is either constant or linear, depending on the variable. Pierce and Moin modified the nonpremixed-flamelet counterflow configuration by fixing domain size and forcing flux to zero at the boundaries. Flamelet theory as a closure model for turbulent combustion is typically based on the tracking of two variables: a normalized conserved scalar and the strain rate. The latter is generally given indirectly through a progress variable. Mixture fraction is traditionally used for the conserved scalar.

The flamelet model has become a popular sub-grid model for gaseous-fueled combustors. Some development is also underway for the use of flamelets in spray combustion but here we will focus on the former type. The flamelet model for LES developed by Pierce and Moin (2004) was a substantial advancement through the introduction of the flamelet progress variable (FPV). Their approach has also been used by Ihme et al. (2009), Nguyen et al. (2018); Nguyen and Sirignano (2018, 2019), and others. Other works are based on the use of the original form developed by Peters (2000). Pierce and Moin extended that work in two ways. Firstly, the inclusion of both the upper and middle branches of the curve of flame temperature vs. scalar dissipation rate allowed better representation of the unsteady details in turbulent combustion

such as extinction and re-ignition. Secondly, they created a progress variable as a function (of the scalar dissipation rate) which is governed by a PDE (added to the LES equations) with a chemical-rate source term determined through the flamelet model. Nguyen and Sirignano (2018) found that the inclusion of both branches for flame stability resulted in better agreement with experiment. Note that Nguyen and Sirignano (2018) addressed rocket combustion instability which places a greater demand on the flamelet model than most other applications. In addition to the velocity fluctuations due to turbulence, it becomes necessary to address very large fluctuations in both velocity, pressure, and temperature due to the nonlinear acoustics.

There are concerns with the existing model. While there is clear utility for the FPV approach, there are concurrently clear signs of incompleteness in the flamelet model and contradiction between the tenets of the model and the LES results produced with the model. A few examples of problems that require resolution are provided here. Firstly, the design of the flamelet model uses a counterflow configuration where only normal strain is imposed on the flame region by the ambient flow. Yet, the LES results show that the flame is embedded in a flow field with substantial shear strain rate, i.e., a flow with vorticity. Secondly, the current models assume that the inflowing streams in the counterflow are irrotational; yet, we know that the smaller scales in turbulent combustion are highly rotational. Thirdly, the classical flamelet model is two-dimensional (or axisymmetric) whereas it has been used in flows that are clearly three-dimensional. The model considers only a single-branched diffusion flame while its coupled use in LES commonly predicts multi-branched flames in qualitative agreement with experimental evidence. A fourth issue involves the quasi-steady assumption for the flamelet model that is used in a highly unsteady LES flow with a broadband noise.

These models are built around the postulate that the flamelets are always nonpremixed (i.e., diffusion) flames or premixed flames. However, evidence of both nonpremixed and premixed flames has been found in LES and experimental results. In fact, they can co-exist in a multi-branched structure. Nguyen et al. (2018) and Nguyen and Sirignano (2018, 2019) employed the Pierce and Moin (2004) flamelet approach in the simulation of a single-injector rocket engine. They showed the importance of flamelets subject to high strain rates. However, contradictions occurred in that both premixed flames and nonpremixed flames appeared in the predictions. In fact, they report multi-branched flames; in particular, the combination is often seen of a fuel-lean premixed-flame branch with a branch consisting of a merged

diffusion flame and fuel-rich premixed flame.

Note that the mixture fraction has been used widely as an independent variable to display non-premixed flamelet scalar variations; this cannot be useful for premixed flames. Sirignano (2021a) has shown that any conserved scalar can serve well as an independent variable to present scalar results for nonpremixed and multi-branched flamelets.

Experiments and asymptotic analysis by Hamins et al. (1985) showed that a partially premixed fuel-lean flame and a diffusion flame can co-exist in a counterflow with opposing streams of heptane vapor and methane-oxygen-nitrogen mixture. Thus, a need exists for flamelet theory to address both premixed and non-premixed flames. Recently, Rajamanickam et al. (2019) provided an interesting three-dimensional triple-flame analysis, describing the effect of imposed normal strain on a multibranched flame. While it did not consider shear strain, it was a helpful step followed by the work of Sirignano (2021c) where both shear strain and normal strain were considered.

The classical counterflow treatment by Linan (1974); Peters (2000) has two opposing streams, fuel or fuel plus a chemically inert gas and oxidizer or oxidizer plus an inert gas. They considered uniform density. That critical assumption was relaxed by Sirignano (2019) for reacting flows and heated flows. Sirignano (2021a,c) with one-step kinetics and López-Cámara et al. (2020) with detailed kinetics address that single diffusion-flame case. In addition, situations are addressed where the inflowing streams from y_∞ and $y_{-\infty}$ may consist of a combustible mixture of fuel and oxidizer, thereby allowing another flame or two besides the simple diffusion flame to co-exist. Sirignano (2021a) provides a counterflow analysis with three-dimensional strain and shows the possibility for a variety of flame configurations to exist depending on the compositions of the inflowing streams: (i) three flames including fuel-lean partially premixed, nonpremixed (i.e., diffusion-controlled), and fuel-rich partially premixed; (ii) nonpremixed and fuel-rich partially premixed; (iii) fuel-lean partially premixed and nonpremixed; (iv) nonpremixed; and (v) premixed. López-Cámara et al. (2020) extended the counterflow analysis to consider detailed kinetics for methane-oxygen detailed chemical kinetics and confirmed that combinations of premixed and non-premixed flames could exist in a multi-flame counterflow.

1.2 Relative Orientations of Principal Strain Axes, Vorticity, and Scalar Gradients

Both normal strain rate and shear strain rate are important. There is a strong need to study mixing and combustion in three-dimensional flows with both imposed normal strain and shear strain and therein imposed vorticity with global circulation. Shear strain can, in general, be decomposed into a normal strain and a rotation (whose rate is half of the vorticity magnitude). For example, a rectangular shape that is changed by shear strain can be viewed as a combination of deformation to a parallelogram caused by normal strain perpendicular to the diagonal and rotation of the diagonal caused by vorticity. The behavior due to the strain and rotation becomes especially important on the smallest scales of turbulence where mixing and chemical reaction occur. The magnitudes of strain rate and vorticity increase as the eddy size (or wavelength) decreases in the turbulence energy cascade process. The Kolmogorov scale size is determined by the dissipation rate of turbulence kinetic energy and dynamic viscosity and is the smallest turbulence length scale. The final molecular mixing and chemical reaction in the combustion process occur on a still smaller scale, where there will be an axis (or direction) of principal compressive normal strain and an orthogonal axis for principal tensile strain; the third orthogonal axis could be either tensile or compressive. These axes would rotate under shear strain (or equivalently vorticity). Similarly, the direction of the scalar gradient rotates under shear. A useful flamelet model must have a statistically accurate representation of the relative orientations on this smallest scale of the vorticity vector, scalar gradients, and the directions of the three principal axes for strain rate. Several studies exist that are helpful in understanding this important alignment issue.

Generally and always for incompressible flow, one principal strain rate γ locally will be compressive (corresponding to inflow in a counterflow configuration), another principal strain rate α will be tensile (also named extensional and corresponding to outflow), and the third can be either extensional or compressive and will have an intermediate strain rate β of lower magnitude than the other like strain rate. Specifically, $\alpha > \beta > \gamma$, $\alpha > 0$, $\gamma < 0$, and, for incompressible flow, $\alpha + \beta + \gamma = 0$. If the intermediate strain rate $\beta < 0$, there is inflow from two directions with outflow in one direction; a contracting jet flow occurs locally. Conversely, with $\beta > 0$, there is outflow in two directions and inflow in one direction; a counterflow or, in other words,

the head-on collision of two opposed jets occurs. Betchov (1956) has shown that, for homogeneous, isotropic turbulence in an incompressible flow, the situation with $\beta > 0$ and resulting counterflow is the most important for production of vorticity and the turbulence energy cascade to smaller scales.

Several interesting findings result from direct numerical simulations (DNS) for incompressible flows. Both Ashurst et al. (1987) and Nomura and Elghobashi (1992) compared a case of homogeneous sheared turbulence with a case of isotropic turbulence. They report that the vorticity alignment with the intermediate strain direction is most probable in both cases but especially in the case with shear. Furthermore, the intermediate strain rate is most likely to be extensive (positive) implying a counterflow configuration. Dresselhaus and Tabor (1991) uses a kinematic approach to study the stretching of material and vorticity in a fluid flow and predict the tendency towards alignment of the intermediate strain direction with the vorticity. If the vorticity had strong alignment with the major compressive or major tensile strain direction, the magnitude of helicity, the dot product of velocity $\vec{u}$ and vorticity $\vec{\omega}$, would be large. Kerr (1987) reports that large values of helicity are not found in the turbulence cascade process. Ashurst et al. (1987) note further that the positive intermediate strain rate has a significantly smaller magnitude than either of the other two principal strain rates. Furthermore, the time for alignment of the vorticity with that intermediate direction is short compared to the eddy-turnover time.

Nomura and Elghobashi (1993) studied reacting flow and show that in regions of exothermic reaction and variable density, alignment of the vorticity with the most tensile strain direction can occur. Still though as the strain rates increase, the intermediate direction becomes more favored for alignment with vorticity; that direction is also preferred in regions where mixing occurs without substantial divergence of the velocity due to chemical reaction.

We may also expect that a material interface most probably aligns to be normal to the direction of the compressive normal strain. That is, the scalar gradient and the direction of compressive strain are aligned. See Ashurst et al. (1987); Nomura and Elghobashi (1992, 1993) and Boratav et al. (1996, 1998). Authors agree that the most common intermittent vortex structures in regions of high strain rate are sheets or ribbons rather than tubes.

An important issue for flamelet modelling is the relative magnitudes of the vorticity and the rates of principal normal strain. For homogeneous, incompressible turbulence, Betchov (1956) showed that, for the average across all length scales, these quantities are of the same order of magnitude. Of

course, the smallest scales contribute more to the average since the velocity derivatives are larger on those scales. Also, for shear flows, we expect that the turbulence at the smaller scales will be isotropic and behave more like the homogeneous flow. In our analysis for variable-density, reacting shear flows, we assume the same order-of-magnitude similarity between vorticity and the rates of principal normal strain applies for the smallest scales.

Based on those understandings concerning vector orientations, Sirignano (2020), extended flamelet theory in a second significant aspect beyond the inclusion of both premixed and non-premixed flame structures; namely, a model was created of a three-dimensional field with both shear and normal strains. The three-dimensional problem is reduced to a two-dimensional form and then, for the counterflow or mixing-layer flow, to a one-dimensional similar form. The system of ordinary differential equations (ODEs) is presented for the thermo-chemical variables and the velocity components. Conserved scalars are determined and can become the independent variable if they behave in a monotonic fashion. Sirignano (2021c) also was able to use a velocity component as the independent variable for the flamelet model with shear strain and vorticity. The validity of the similar solution form for mixing layers with certain thin reaction zones was discussed using concepts from singular perturbation theory. The chemical-kinetic model appears as a source term for an ODE. These new findings are very helpful in improving the foundations for flamelet theory and its use in sub-grid modeling for turbulent combustion. Still, however, there has not been a flamelet model that connects well the scales on the resolved LES level to the sub-grid scales at the level of the flame structure.

Based on the observations of the needed improvements, the aim here is to develop a flamelet model that (i) determines rather than prescribes the existence of non-premixed flames, premixed flames, or multi-branched flame structures; (ii) determines directly the effect of shear strain and vorticity on the flames; (iii) applies directly the resolved-scale strain rates and vorticity to the sub-grid level without the use of a contrived progress variable; (iv) employs a three-dimensional flamelet model; and (v) considers the effect of variable density. Furthermore, some discussion and primitive analysis of the in situ function of the flamelet model in a turbulent shear flow is presented. The analysis uses one-step kinetics to avoid complications in this initial study; however, a clear template will exist for the employment of multi-step kinetics. The choice for the in situ study will be a mixing layer with the use of mixing-length theory. Here, the goal is not to advance the portion of the analysis

for the resolved scale; rather, the coupling with the sub-grid closure model will be made clear.

In Section 2, the scaling and connections between the resolved shear flow and the flamelet behavior on the sub-grid scale are discussed. Section 3 has the description of a new sub-grid flame model that better handles connection with strain and vorticity on the resolved scale, three-dimensional character, and multibranched flame structure. The application of the sub-grid flamelet with a resolved shear flow is addressed in Section 4. Concluding comments are made in Section 5.

2 Scaling Between Flamelet Scale and Resolved Scale

Current flamelet theory for use in LES or RANS makes no substantial attempt to scale properly between the small scale of the flamelet and the larger flow scales which pertain to the computational fluid dynamics analysis. A theoretical basis is needed to prescribe how to determine vorticity, strain rates, and scalar gradients on the flamelet scale given those properties on the resolved scale. Certainly, as mentioned in Subsection 1.2 of the Introduction, a body of helpful literature exists on this subject; it shall be considered here. Specifically, we shall avoid the creation of arbitrary variables such as the flame progress variable (FPV) used in many publications. The FPV is actually not a good measure of progress. In order to relate increasing temperature during combustion to the flamelet theory, scalar dissipation rate is obliged to increase as the FPV increases. Instead, scalar dissipation rate on the flamelet scale should be related to temporally-varying and spatially-varying scalar and velocity gradients and not to temperature magnitude. The existing theory will not allow a hot gas to experience reductions in dissipation rates related to reductions in the values of velocity and scalar gradients which surely is not consistent with general flow patterns in turbulent combustors. Here, a new method will be developed for determining burning rate from the flamelet theory and applying it to the resolved scale for LES or to the averaged flow field for RANS. During the burning process, temperature will be able to increase even if strain rate and the associated scalar dissipation rate might be decreasing.

2.1 Scaling of Velocity, Strain Rate, and Vorticity

Here, at first, we use approximate concepts which perhaps are reasonably well suited for a use of mixing-length theory to describe the time-averaged turbulent flow in a shear layer. The aim is to provide a simple framework for the first application and test of a new flamelet theory. More sophisticated and modern statistical approaches can be found, e.g., Pope (2000), and can be used in the future for examination of turbulent flows using RANS or LES.

The shear-driven flow on the larger scale can be characterized by a length δ and a time-averaged velocity difference ΔU across that particular length that ultimately relate to the magnitudes of the largest eddy size and the turbulence kinetic energy. Then, the velocity, length, and time scales for the resolved scales are ΔU , δ , and $\delta/\Delta U$, respectively. The rms velocity fluctuation u' , the turbulence kinetic energy k , and the rate of dissipation of turbulence kinetic energy ϵ will have magnitudes of the order of ΔU , ΔU^2 , and $\Delta U^3/\delta$, respectively. The Kolmogorov scale is the smallest scale in the turbulence energy cascade where the inertial and viscous effects balance each other (Pope (2000); White (2005)). On that smallest scale, the characteristic velocity, length, and time scales become $u_\kappa = (\nu\epsilon)^{1/4}$, $\kappa = (\nu^3/\epsilon)^{1/4}$, and $t_\kappa = (\nu/\epsilon)^{1/2}$, respectively, where ν is the kinematic viscosity of the fluid. One can use these Kolmogorov scales to be the scales for flamelet analysis; a more refined approach might be to use the rate of dissipation for scalar quantities ϵ_c discussed by Elghobashi and Launder (1983) instead of ϵ .

Estimate a Reynolds number for the resolved flow using $Re \equiv \Delta U\delta/\nu$. Vorticity, rate of normal strain, and rate of shear strain will be $O(\Delta U/\delta)$. If we estimate the magnitudes of rate of strain and vorticity on the flamelet scale to be given as

$$S^* \equiv \frac{\partial u_\kappa}{\partial \kappa} = O\left(\frac{u_\kappa}{\kappa}\right) ; \quad \frac{u_\kappa}{\kappa} = \left(\frac{\epsilon}{\nu}\right)^{1/2} = \frac{\Delta U}{\delta} Re^{1/2} \quad (1)$$

Clearly, for high Re values, we may expect vorticity and rate of strain on the flamelet scale to be orders higher than found on the resolved scale. This scaling and the connection of the strain rates and vorticity on different scales has not been addressed in prior flamelet modeling.

Note that different estimates of a relevant resolved-scale or averaged-flow Reynolds number will be used at later points in this discussion. The intention, however, is to maintain the same order of magnitude.

If we examine a time-averaged shear flow, the quantity $\Delta U/\delta$ can be replaced by the magnitude of a velocity gradient for the averaged flow treated through RANS simulations following a mixing-length concept. For LES, that quantity can be related to a velocity gradient on the smallest resolved scale, following an approach similar to the Smagorinsky model for Reynolds stress. Specifically,

$$\begin{aligned} \frac{\Delta U}{\delta} &\equiv \left| \frac{\partial u}{\partial x} \right| ; \quad Re \equiv \left| \frac{\partial u}{\partial x} \right| \frac{\delta^2}{\nu} ; \\ \left| \frac{\partial u_\kappa}{\partial \kappa} \right| &= \left| \frac{\partial u}{\partial x} \right| Re^{1/2} = \left| \frac{\partial u}{\partial x} \right|^{3/2} \frac{\delta}{\nu^{1/2}} = \frac{S_{rs}^{*3/2} \delta}{\nu^{1/2}} \end{aligned} \quad (2)$$

Here, one can make a choice about the interpretation of the resolved scale strain rate $S_{rs}^* \equiv |\partial u/\partial x|$. The largest component of shear strain rate on the resolved scale or for the time-averaged flow is recommended for use. S_{rs}^* can vary with location in the flow and, for unsteady RANS and LES, can vary with time as well. The quantity $\partial u_\kappa/\partial \kappa$ will be imposed as the compressive normal strain rate in the flamelet model; it will be a negative number $-(S_1^* + S_2^*)$. Thus, Equation (2) can relate the normal strain rate on the flamelet scale to the strain rate on the resolved scale or for the time-averaged flow. In the case with the two-equation RANS model using k, ϵ theory, Equation (1) will yield $S^* = (\epsilon/\delta^2)^{1/3}$.

A relation must be created between the dimensional vorticity ω^* on the resolved scale and the dimensional vorticity ω_κ^* on the flamelet sub-grid scale. (Note that, in the development of the flamelet model, the sub-grid ω_κ is dimensionless.) A reasonable relationship, mimicking the strain rate relation, is given as $\omega_\kappa^* = \omega^{*3/2} \delta/\nu^{1/2} = O(\omega^* Re^{1/2}) \gg \omega^*$.

2.2 Scaling of the Scalar Properties

The inflow boundary conditions for the scalar quantities in the flamelet calculation must be determined from the resolved scale behavior. The scalar gradients are much larger on the flamelet scale due to the dynamics of the turbulent flow. As a first approximation, consider that the scalar gradients scale in proportion to the strain rates. For example, using the mass fraction

of species m , we state the rough approximation:

$$\frac{\frac{\partial Y_{m,\kappa}}{\partial \kappa}}{\frac{\partial Y_m}{\partial x}} = \frac{\frac{\partial u_\kappa}{\partial \kappa}}{\frac{\partial u}{\partial x}} = Re^{1/2} \quad (3)$$

where the subscript κ designates the flamelet scale. The domain sizes between the Kolmogorov scale and the resolved scale as $\kappa = \delta Re^{-3/4}$. Setting the change in scalar value across the given domain as the product of domain size and its gradient, the result is $\Delta Y_{m,\kappa} = \Delta Y_m Re^{-1/4}$. So, the variation in scalar properties across the smallest eddy is smaller than the variation across the larger eddies. Although the gradient of the scalar property is much greater on the flamelet scale due to turbulent mixing, the variation across the flamelet domain is smaller due to the greatly reduced domain size. Changes in enthalpy h and density ρ can be determined following the same pattern. The important implication is that, in general, the partial premixing on the smaller scales should be greater than experienced on the largest scales.

If, on the resolved scale at a particular point $\vec{x}, t$, the scalar property is Y_m , the bounding values for the inflow of the flamelet counterflow will be taken as $Y_{m,\kappa,\infty} = Y_m(\vec{x}, t) + \Delta Y_{m,\kappa}$ and $Y_{m,\kappa,-\infty} = Y_m(\vec{x}, t) - \Delta Y_{m,\kappa}$. Again, the boundary values for other scalars can be handled identically. A consequence here will be that the incoming streams of the flamelet counterflow are more likely to be fuel rich or fuel lean than pure fuel or pure oxidizer. Multi-branched-flame structures of the type found by Hamins et al. (1985); Rajamanickam et al. (2019); Sirignano (2019, 2021c); López-Cámara et al. (2020) can be expected.

2.3 Scaling of Energy Release Rate and Species Consumption and Production Rates

The resolved scale will require input from the flamelet model for the quantities giving consumption (or production) rates per unit volume for the chemical species and energy release rate per unit volume due to chemical reaction and perhaps also viscous dissipation rate. The production and consumption rates within the flame are substantially higher than the average values over the counterflow volume. It is the average over the counterflow volume that should be used in the resolved-scale calculations. The same approach should be used for the viscous dissipation rate in high-speed flows where that is considered to be important. These quantities to be used on the resolved scale

are given as integrals over the flamelet scale by Equation (27).

The dimensional form of the rates indicates that the integrated chemical rates are proportional to the magnitude of the compressive strain rate $S^* \equiv S_1^* + S_2^*$ for the counterflow. The portion of the dimensional energy release rate due to viscous dissipation is proportional to S^{*2} . That sub-grid strain rate is much larger than the strain rate on the resolved scale as indicated by Equation (3). The scalar gradients have similar scaling relation between the sub-grid and the resolved scale. They impact diffusion and therefore, in diffusion-controlled combustion, they determine burning rates.

3 Sub-grid Flamelet Analysis

We formulate the problem in a quasi-steady three-dimensional form. The following alignments will be assumed. The direction of major compressive principal strain is orthogonal to the vorticity vector direction. Specifically, the intermediate principal strain direction is aligned with the vorticity while the scalar gradient aligns with the principal compressive strain direction. These assumptions are consistent with the statistical findings of Nomura and Elghobashi (1993).

3.1 Coordinate Transformation

A transformation displayed in Figure 1 is made from the Newtonian frame with rotating material (due to vorticity) to a rotating, non-Newtonian frame. Let the vorticity direction be the z' direction in an orthogonal framework. Any x', y' plane contains the directions of scalar gradients, major principal axis for compressive strain, and major principal axis for tensile strain. Note that the x', y', z' directions are not correlated with coordinates on the resolved scale. ω_κ is the vorticity magnitude on this sub-grid (Kolmogorov) scale. x', y', z' are transformed to ξ, χ, z' wherein the material rotation is removed from the ξ, χ plane by having it rotate at angular velocity $d\theta/dt = \omega_\kappa/2$ relative to x', y' . Here, θ is the angle between the x' and ξ axes and simultaneously the angle between the y' and χ axes. Clearly, we take the sub-grid domain to be sufficiently small to consider a uniform value of ω across it.

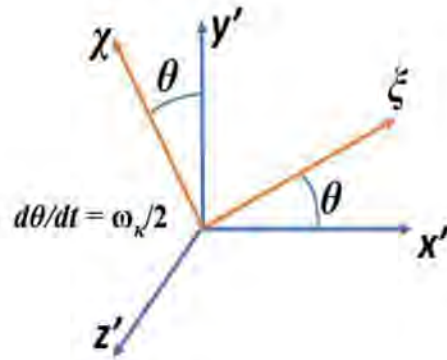


Figure 1: Transformation to ξ, χ, z' rotating coordinate system from x', y', z' Newtonian system. θ increases in the counterclockwise direction.

The following relations apply.

$$\begin{aligned}
 \xi &= x' \cos \theta + y' \sin \theta ; \quad \chi = y' \cos \theta - x' \sin \theta \\
 \frac{\partial \xi}{\partial x'} &= \cos \theta ; \quad \frac{\partial \xi}{\partial y'} = \sin \theta ; \quad \frac{\partial \chi}{\partial x'} = -\sin \theta ; \quad \frac{\partial \chi}{\partial y'} = \cos \theta \\
 u_{\xi} &= u \cos \theta + v \sin \theta + \chi \frac{\omega_{\kappa}}{2} ; \quad u_{\chi} = v \cos \theta - u \sin \theta - \xi \frac{\omega_{\kappa}}{2} \\
 \frac{\partial u}{\partial x'} &= \frac{\partial u}{\partial \xi} \cos \theta - \frac{\partial u}{\partial \chi} \sin \theta ; \quad \frac{\partial u}{\partial y'} = \frac{\partial u}{\partial \xi} \sin \theta + \frac{\partial u}{\partial \chi} \cos \theta \\
 \frac{\partial v}{\partial x'} &= \frac{\partial v}{\partial \xi} \cos \theta - \frac{\partial v}{\partial \chi} \sin \theta ; \quad \frac{\partial v}{\partial y'} = \frac{\partial v}{\partial \xi} \sin \theta + \frac{\partial v}{\partial \chi} \cos \theta
 \end{aligned} \tag{4}$$

Since

$$\frac{\partial v}{\partial x'} - \frac{\partial u}{\partial y'} = \omega_{\kappa} \tag{5}$$

it follows that

$$\frac{\partial u_{\chi}}{\partial \xi} - \frac{\partial u_{\xi}}{\partial \chi} = 0 \tag{6}$$

Namely, the flow in the rotating frame of reference does not have the vorticity imposed on it. However, two points must be understood. Firstly, the frame is not Newtonian and a reversed (centrifugal) force is imposed. Secondly, the expansions due to combustion and energy release can produce new vorticity but it will integrate to zero globally. The inflowing free-stream vorticity in the transformed coordinates is zero. Thus, in similar fashion to classical counterflow, the vorticity develops as an odd function so that the circulation on a contour surrounding the flow domain remains with zero value. This creation of vorticity is related to gas expansion with density variation; however, that expansion has a symmetry that yields an anti-symmetry in the vorticity.

3.2 Governing Equations

The governing equations for unsteady 3D flow in the non-Newtonian frame can be written with $u_i = u_\xi, u_\chi, w$; $x_i = \xi, \chi, z$. The centrifugal acceleration $a_i = \xi\omega_\kappa^2/4, \chi\omega_\kappa^2/4, 0$. The quantities $p, \rho, h, h_m, Y_m, \dot{\omega}, \mu, \lambda, D$, and c_p are pressure, density, specific enthalpy, heat of formation of species m , mass fraction of species m , chemical reaction rate of species m , dynamic viscosity, thermal conductivity, mass diffusivity, and specific heat, respectively. Furthermore, τ_{ij} is the viscous stress tensor and the Lewis number $Le \equiv \lambda/(\rho D c_p)$.

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (7)$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + \rho a_i \quad (8)$$

where, following the Stokes hypothesis for a Newtonian fluid,

$$\tau_{ij} = \mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] \quad (9)$$

$$\begin{aligned} \rho \frac{\partial h}{\partial t} + \rho u_j \frac{\partial h}{\partial x_j} - \frac{\partial p}{\partial t} - u_j \frac{\partial p}{\partial x_j} = & \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} \right) \\ & + \frac{\partial}{\partial x_j} \left(\rho D (1 - Le) \sum_{m=1}^N h_m \frac{\partial Y_m}{\partial x_j} \right) \\ & - \rho \sum_{m=1}^N h_{f,m} \dot{\omega}_m + \tau_{ij} \frac{\partial u_i}{\partial x_j} \end{aligned} \quad (10)$$

$$\rho \frac{\partial Y_m}{\partial t} + \rho u_j \frac{\partial Y_m}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_m}{\partial x_j} \right) + \rho \dot{\omega}_m ; \quad m = 1, 2, \dots, N \quad (11)$$

Equations (7) through (11) together with the equation of state and the relations describing fluid physico-chemical properties give a complete description of behavior in the non-Newtonian reference frame. These equations will be used in the remainder of this section.

Equation (10) is a thermodynamic statement wherein, following a material element, we are stating the differential relation $\rho dh - dp = \rho T ds$. The terms on the right side of (10) are entropy-producing terms. An alternative form of the energy equation can be developed to govern the total H of the specific enthalpy, specific chemical energy, and kinetic energy per unit mass. That is, $H \equiv h + \sum_{m=1}^N Y_m h_{f,m} + u_k u_k / 2$. Specifically, the vector dot product of u_i with Equation (8) is used to substitute for $u_j \partial p / \partial x_j$ in Equation (10) and Equation (11) is used to substitute for $\dot{\omega}_m$ there. The Lewis number $Le = 1$ is considered. It follows that

$$\rho \frac{\partial H}{\partial t} + \rho u_j \frac{\partial H}{\partial x_j} - \frac{\partial p}{\partial t} = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial (h + \sum_{m=1}^N Y_m h_{f,m})}{\partial x_j} \right) + \frac{\partial (u_i \tau_{ij})}{\partial x_j} + \rho u_j a_j \quad (12)$$

The energy source term $\rho u_j a_j = \rho (\omega_\kappa / 2)^2 (\xi u_\xi + \chi u_\chi)$. If we neglect terms of the order of the kinetic energy per mass, this effect disappears. We might still retain the viscous dissipation rate $\tau_{ij} \partial u_i / \partial x_j$ for special cases where large strain rates are expected on the sub-grid scale, as suggested by Drozda et al. (2020). The viscous dissipation rate will have exactly the same value whether it is calculated in the Newtonian frame or the rotating frame; this result is expected because it relates to the thermodynamics where the laws

are independent of the reference frame. The resulting equation becomes

$$\rho \frac{\partial h}{\partial t} + \rho u_j \frac{\partial h}{\partial x_j} - \frac{\partial p}{\partial t} \approx \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D (1 - Le) \sum_{m=1}^N h_m \frac{\partial Y_m}{\partial x_j} \right) - \rho \sum_{m=1}^N h_{f,m} \dot{\omega}_m + \tau_{ij} \frac{\partial u_i}{\partial x_j} \quad (13)$$

Here, we define the non-dimensional Prandtl, Schmidt, and Lewis numbers: $Pr \equiv c_p \mu / \lambda$; $Sc \equiv \mu / (\rho D)$; and $Le \equiv Sc / Pr$.

The non-dimensional forms of the above equations remain identical to the above forms if we choose certain reference values for normalization. In the remainder of this article, the non-dimensional forms of the above equations are considered. The superscript $*$ is used to designate a dimensional property. The variables u_i^* , t^* , x_i^* , ρ^* , h^* , p^* , and $\dot{\omega}_m^*$, and properties μ^* , λ^* / c_p^* , and D^* are normalized respectively by $[(S_1^* + S_2^*) \mu_\infty^* / \rho_\infty^*]^{1/2}$, $(S_1^* + S_2^*)^{-1}$, $[\mu_\infty^* / (\rho_\infty^* (S_1^* + S_2^*))]^{1/2}$, ρ_∞^* , $(S_1^* + S_2^*) \mu_\infty^* / \rho_\infty^*$, $(S_1^* + S_2^*) \mu_\infty^*$, μ_∞^* , μ_∞^* , and $\mu_\infty^* / \rho_\infty^*$. The dimensional strain rates S_1^* and S_2^* and vorticity ω_κ^* are normalized by $S_1^* + S_2^*$. It is understood that, for unsteady flow, the reference values for strain rates and far-stream variables and properties used for normalization are constants; for example, averages might be taken for fluctuating conditions. Note that the reference length $[\mu_\infty^* / (\rho_\infty^* (S_1^* + S_2^*))]^{1/2}$ is the estimate for the magnitude of the viscous-layer thickness. In the following flamelet analysis, the vorticity ω_κ and the velocity derivatives $\partial u_i / \partial x_j$ are non-dimensional quantities; their dimensional values can be obtained through multiplication by $S_1^* + S_2^*$. In Section 2, the algorithms are given that relate dimensional vorticity and velocity derivatives on the resolved scale to dimensional vorticity and velocity derivatives on the sub-grid scale.

3.3 Similar Form for the Velocity and Pressure

The stagnation point in the steady counterflow is taken as the origin $\xi = \chi = z = 0$. Along the line $\xi = z = 0$ normal to the interface, we can expect the first derivatives of u_χ , ρ , h , T , and Y_m with respect to either ξ or z to be zero-valued. For unsteady cases, only symmetric situations will be considered so that the stagnation point remains at the origin and the interface remains at $\chi = 0$. The velocity components u_ξ and w are odd functions of ξ and z , respectively, going through zero and changing sign at that line. Consequently, upon neglect of terms of $O(\xi^2)$ and $O(z^2)$, the variables u_χ , ρ , h , T , and Y_m can

be considered to be functions only of t and χ . For steady flow, the density-weighted Illingworth (1949) transformation of χ can be used to replace χ with $\eta \equiv \int_0^\eta \rho(\chi') d\chi'$. Neglect of the same order of terms implies that $u_\xi = S_1 \xi(df_1/d\eta)$ and $w = S_2 z(df_2/d\eta)$. Note u_ξ is independent of z and w is independent of ξ in this case where no shear strain is imposed on the incoming stream(s). At the edge of the viscous layer at large positive η , $df_1/d\eta \rightarrow 1$, $df_2/d\eta \rightarrow 1$, $f_1 \rightarrow \eta$, and $f_2 \rightarrow \eta$. Ordinary differential equations are created here through the variable η and the convenient definition is made that $()' \equiv d()/d\eta$. Note that other transformations of the χ coordinate can be made, e.g., weighting by transport properties Linan et al. (2017); Weiss et al. (2018) rather than density.

In the non-dimensional form given by Equations (7) through (13), the dimensional strain rates S_1^* and S_2^* are each normalized by the dimensional sum $S_1^* + S_2^*$. Thus, the non-dimensional relation is $S_2 = 1 - S_1$ and only one independent non-dimensional strain-rate parameter is needed. Nevertheless, two strain rates are presented above and in the following analysis with the understanding that one depends on the other such that $S_1 + S_2 = 1$. $S_1 + S_2$ are explicitly stated in our analysis without substitution of the unity value. This choice clarifies whether a particular term when converted to a dimensional form depends on S_1^* , S_2^* , or the sum of the two strain rates.

For steady state, the continuity equation (7) is readily integrated to give

$$\rho u_\chi = -S_1 f_1(\eta) - S_2 f_2(\eta) \quad (14)$$

For derivatives of variables that are functions of η only, the prime is used to indicate differentiation with respect to η . Then,

$$u'_\chi = \frac{S_1 f_1(\eta) + S_2 f_2(\eta)}{\rho^2} \rho' - \frac{S_1 f'_1(\eta) + S_2 f'_2(\eta)}{\rho} \quad (15)$$

Thus, the incoming inviscid flow outside the boundary layer is described by $u_\chi = -(S_1 + S_2)\eta$ for positive η and $u_\chi = -(S_1 + S_2)\eta/\rho_{-\infty}$ for negative η . Note that the same result is found for the unsteady or steady incompressible state where there is no need to use η in place of χ since $\rho = 1$ everywhere. Then, $u_\chi = -(S_1 + S_2)\chi$ for the external incoming flow.

Equations (14) and (15) may be substituted into Equation (8) to deter-

mine the pressure gradient.

$$\begin{aligned}
 \frac{\partial p}{\partial \xi} &= \rho[\rho\mu S_1 f_1''' + S_1 f_1''(\rho\mu)' + (S_1 f_1 + S_2 f_2) S_1 f_1'' + \left(\frac{\omega_\kappa}{2}\right)^2 - (S_1 f_1')^2]\xi \\
 \frac{\partial p}{\partial \eta} &= \frac{4}{3}(\rho\mu u_\chi')' - \frac{2}{3}(S_1 f_1' + S_2 f_2')\mu' + \frac{\mu}{3}(S_1 f_1'' + S_2 f_2'') + \left(\frac{\omega_\kappa}{2}\right)^2 \chi + (S_1 f_1 + S_2 f_2)u_\chi' \\
 \frac{\partial p}{\partial z} &= \rho[\rho\mu S_2 f_2''' + S_2 f_2''(\rho\mu)' + (S_1 f_1 + S_2 f_2) S_2 f_2'' - (S_2 f_2')^2]z
 \end{aligned} \tag{16}$$

It follows from the η pressure-gradient in Equation (16) that $\partial p/\partial \eta$ is a function only of η . Therefore, $\partial^2 p/\partial \xi \partial \eta = 0$ and $\partial^2 p/\partial z \partial \eta = 0$. Now, the coefficient of ξ on the right side of the ξ pressure-gradient in Equation (16) must be constant. The same conclusion is made for the coefficient of z on the right side of the z pressure-gradient in Equation (16). At $\eta = \infty$, $f_1' = f_2' = 1$ and $f_1'' = f_2'' = f_1''' = f_2''' = 0$ which allows the two constants to be determined. Specifically, we obtain

$$\begin{aligned}
 \rho\mu f_1''' + f_1''(\rho\mu)' + (S_1 f_1 + S_2 f_2) f_1'' + S_1 \left(\frac{1}{\rho} - (f_1')^2\right) + \frac{\omega_\kappa^2}{4S_1} \left(1 - \frac{1}{\rho}\right) &= 0 \\
 \rho\mu f_2''' + f_2''(\rho\mu)' + (S_1 f_1 + S_2 f_2) f_2'' + S_2 \left(\frac{1}{\rho} - (f_2')^2\right) &= 0
 \end{aligned} \tag{17}$$

The boundary conditions will use the assumption that two velocity components asymptote to the constant values $u_\xi(\infty)$, $u_\xi(-\infty)$, $w(\infty)$, and $w(-\infty)$ at large magnitudes of η . The stream function bounding the two incoming streams is arbitrarily given a zero value and placed at $\eta = 0$.

$$\begin{aligned}
 f_1'(\infty) &= 1 ; f_1'(-\infty) = \sqrt{\frac{1}{\rho(-\infty)} + \left(\frac{\omega_\kappa}{2S_1}\right)^2 \left(1 - \frac{1}{\rho(-\infty)}\right)} ; f_1(0) = 0 ; \\
 f_2'(\infty) &= 1 ; f_2'(-\infty) = \frac{1}{\sqrt{\rho(-\infty)}} ; f_2(0) = 0
 \end{aligned} \tag{18}$$

In the incompressible case where density is uniform throughout the flow, i.e. $\rho = 1$, the solutions become simply that $f_1'(\eta) = 1$ and $f_2'(\eta) = 1$ everywhere. When density varies through the flow because of heating or variation of composition, u_ξ and w vary with χ , thereby creating a shear stress and vor-

ticity albeit that the frame transformation removed vorticity and shear from the incoming flow. The vorticity will be created in an antisymmetric manner since the two velocity components are odd functions of ξ and z , respectively. Thereby, the circulation remains zero for the transformed counterflow.

For steady flows, $S_1 + S_2 = 1$. The dependence of u_χ on $f \equiv S_1 f_1 + S_2 f_2$ is shown by Equation (14). Thus, the function f will be important in determining both the field for u_χ and the scalar fields. From Equation (17), an equation for f can be formed.

$$\rho\mu f''' + f''(\rho\mu)' + ff'' + \frac{1}{\rho} - (f')^2 + \frac{\omega_\kappa^2}{4} \left(1 - \frac{1}{\rho}\right) = 2S_1 S_2 \left(\frac{1}{\rho} - f'_1 f'_2\right) \quad (19)$$

Consequently, f as well as f_1 and f_2 depend on both S_1 and S_2 , not merely on $S_1 + S_2$. That is, the particular distribution of the normal strain rate between the two transverse direction matters. f and f_1 also depend directly on ω_κ (unless $S_1 = 0$). f_2 depends on ω_κ through its coupling with f_1 . In our calculations, we consider a planar case ($S_1 = 1.0, S_2 = 0$) where the product $S_1 S_2$ is minimized and the vorticity vector is normal to the plane with strain. The case where $S_1 = S_2 = 0.5$ has the maximum value for the product $S_1 S_2$ would be axisymmetric if $\omega = 0$. However, symmetry is lost if the rotation exists.

In the outer flow where variability of viscosity and density may be neglected and $u_\chi \rightarrow \eta/\rho_\infty$ as $\eta \rightarrow \infty$, the χ -momentum equation from (16) becomes

$$\begin{aligned} \frac{\partial}{\partial \eta} \left[p - \frac{4\rho\mu}{3} u'_\chi \right] &\rightarrow (S_1 f_1 + S_2 f_2) u'_\chi + \left(\frac{\omega_\kappa}{2} \right)^2 \chi \rightarrow (S_1 + S_2) \eta u'_\chi + \left(\frac{\omega_\kappa}{2} \right)^2 \frac{\eta}{\rho_\infty} \\ \frac{\partial p}{\partial \eta} &\rightarrow \left[\left(\frac{\omega_\kappa}{2} \right)^2 - (S_1 + S_2)^2 \right] \frac{\eta}{\rho_\infty} \end{aligned} \quad (20)$$

The negative pressure gradient will be reduced by the centrifugal effect. Essentially, the pressure gradient serves to decelerate the incoming stream in a counterflow; here, it is helped by the imposed acceleration.

The variable-density-and-viscosity case requires some couplings with Equations (10) and (11) and with an equation of state and fluid-property laws which affect ρ and μ .

The pressure derivative can be determined by substituting from Equation

(14) and (15) into (16).

$$\begin{aligned}
 \frac{\partial p}{\partial \eta} &= \frac{4}{3} \left(\rho \mu \left[\frac{S_1 f_1(\eta) + S_2 f_2(\eta)}{\rho^2} \rho' - \frac{S_1 f_1'(\eta) + S_2 f_2'(\eta)}{\rho} \right] \right)' + \left(\frac{\omega_\kappa}{2} \right)^2 \chi \\
 &\quad + \frac{\mu}{3} (S_1 f_1'' + S_2 f_2'') - \frac{2}{3} (S_1 f_1' + S_2 f_2') \mu' \\
 &\quad + (S_1 f_1 + S_2 f_2) \left[\frac{S_1 f_1(\eta) + S_2 f_2(\eta)}{\rho^2} \rho' - \frac{S_1 f_1'(\eta) + S_2 f_2'(\eta)}{\rho} \right] \\
 p(x, \eta, z) &= p_{ref} + \frac{4\mu(\eta)}{3\rho(\eta)} \left[(S_1 f_1(\eta) + S_2 f_2(\eta)) \rho' - \rho(\eta) (S_1 f_1'(\eta) + S_2 f_2'(\eta)) \right] \\
 &\quad + \frac{4\mu(0)}{3} (S_1 f_1'(0) + S_2 f_2'(0)) \\
 &\quad + \int_0^\eta \left[\frac{\mu(\zeta)}{3} (S_1 f_1''(\zeta) + S_2 f_2''(\zeta)) - \frac{2}{3} (S_1 f_1'(\zeta) + S_2 f_2'(\zeta)) \mu' \right] d\zeta \\
 &\quad + \int_0^\eta (S_1 f_1(\zeta) + S_2 f_2(\zeta)) \left[\frac{S_1 f_1(\zeta) + S_2 f_2(\zeta)}{\rho(\zeta)^2} \rho' - \frac{S_1 f_1'(\zeta) + S_2 f_2'(\zeta)}{\rho(\zeta)} \right] d\zeta \\
 &\quad - \frac{S_1^2 x^2}{2} - \frac{S_2^2 z^2}{2} + \left(\frac{\omega_\kappa}{2} \right)^2 \int_0^\eta \chi(\zeta) d\zeta
 \end{aligned} \tag{21}$$

The viscous dissipation Φ can be determined as follows:

$$\begin{aligned}
 \Phi &\equiv \tau_{ij} \frac{\partial u_i}{\partial x_j} = \mu \left[\frac{4}{3} \left(\left(\frac{\partial u_\xi}{\partial \xi} \right)^2 + \left(\frac{\partial u_\chi}{\partial \chi} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 - \frac{\partial u_\xi}{\partial \xi} \frac{\partial u_\chi}{\partial \chi} - \frac{\partial w}{\partial z} \frac{\partial u_\chi}{\partial \chi} - \frac{\partial w}{\partial z} \frac{\partial u_\xi}{\partial \xi} \right) \right. \\
 &\quad \left. + \left(\frac{\partial u_\xi}{\partial \chi} \right)^2 + \left(\frac{\partial w}{\partial \chi} \right)^2 \right] \\
 &= \mu \left(4(S_1 f_1')^2 + 4(S_2 f_2')^2 + \frac{8}{3} S_1 S_2 f_1' f_2' - 4 \frac{(S_1 f_1 + S_2 f_2)(S_1 f_1' + S_2 f_2')}{\rho} \rho' \right. \\
 &\quad \left. + \frac{4}{3} \left(\frac{S_1 f_1 + S_2 f_2}{\rho} \rho' \right)^2 \right)
 \end{aligned} \tag{22}$$

Here, neglect is made of the quantities $\mu(\partial u_\xi / \partial \chi)^2$ and $\mu(\partial w / \partial \chi)^2$ because they are of $O(\xi^2)$ and $O(z^2)$, respectively.

An exact solution of the variable-density Navier-Stokes equation has been obtained subject to determination of ρ and μ through solutions of the energy and species equations as discussed below. There has been no need for use

of a boundary-layer approximation. Thus, the solution here is the natural solution, subject to neglect of terms of $O(\xi^2)$ and $O(z^2)$. Unlike the incompressible counterflow, a viscous layer exists with the three normal strains and normal viscous stresses varying through the layer due to varying density and viscosity. Shear strain does not appear explicitly in the incoming flow because it has been removed through the coordinate transformation to the rotating frame. Nevertheless, its effect appears through the rotational term.

3.4 Similar Form for the Scalar Fields

Consider the reacting, steady case keeping viscous dissipation. Assume Prandtl number Pr is constant. Substitution from Equations (10) and (11) yields the following ordinary differential equations:

$$\begin{aligned} (\rho\mu h')' + Prfh' + (\rho^2 D(Pr - Sc)\Sigma_{m=1}^N h_m Y_m')' &= Pr\Sigma_{m=1}^N h_{f,m}\dot{\omega}_m - Pr\frac{\Phi}{\rho} \\ (\rho^2 DY_m')' + fY_m' &= -\dot{\omega}_m \quad ; \quad m = 1, 2, \dots, N \end{aligned} \quad (23)$$

If $Le = 1$, i.e., $Pr = Sc$, the new scalar $\tilde{h} \equiv h + \Sigma_{m=1}^N h_{f,m} Y_m$ is governed by

$$(\rho\mu\tilde{h}')' + Prf\tilde{h}' = -Pr\frac{\Phi}{\rho} \quad (24)$$

When the viscous dissipation is negligible, $\tilde{h}$ is a conserved scalar indicating that the sum of thermal energy plus chemical energy is in an advective-diffusive balance. It remains to use thermodynamic relations to substitute for ρ and μ in terms of h and p .

Now, we will address the special case where $\rho\mu = 1$. The perfect gas law and the assumption of constant specific heat c_p will give the relation that

$1/\rho = h$. Then, Equations (17), (18), (23), and (24) yield

$$\begin{aligned}
 f_1''' + f f_1'' + S_1[h - (f_1')^2] + \frac{\omega_\kappa^2}{4S_1}(1 - h) &= 0 \\
 f_2''' + f f_2'' + S_2[h - (f_2')^2] &= 0 \\
 Y_m'' + Pr f Y_m' &= -Pr \dot{\omega}_m ; \quad m = 1, 2, \dots, N \\
 h'' + Pr f h' + (Pr - Sc) \sum_{m=1}^N h_m Y_m'' &= Pr \sum_{m=1}^N h_{f,m} \dot{\omega}_m - Pr \frac{\Phi}{\rho} \\
 \tilde{h}'' + Pr f \tilde{h}' &= -Pr \frac{\Phi}{\rho}
 \end{aligned} \tag{25}$$

The boundary conditions are

$$\begin{aligned}
 f_1'(\infty) &= 1 ; \quad f_1'(-\infty) = \sqrt{h_{-\infty} + \left(\frac{\omega_\kappa}{2S_1}\right)^2 (1 - h_{-\infty})} ; \quad f_1(0) = 0 ; \\
 f_2'(\infty) &= 1 ; \quad f_2'(-\infty) = \sqrt{h_{-\infty}} ; \quad f_2(0) = 0 ; \\
 h(\infty) &= 1 ; \quad h(-\infty) = \frac{1}{\rho_{-\infty}} ; \\
 Y_m(\infty) &= Y_{m,\infty} ; \quad Y_m(-\infty) = Y_{m,-\infty} ; \\
 \tilde{h}(\infty) &= 1 + \sum_{m=1}^N h_{f,m} Y_{m,\infty} ; \quad \tilde{h}(-\infty) = h_{-\infty} + \sum_{m=1}^N h_{f,m} Y_{m,-\infty}
 \end{aligned} \tag{26}$$

Equations (17) indicates a dependence of the heat and mass transport on $f \equiv S_1 f_1 + S_2 f_2$. Manipulation of the first two equations of (25) leads to an ODE for f with $S_1 S_2$ and $S_1 S_2 f_1' f_2'$ as parameters, clearly indicating that generally f will have a dependence on $S_1 S_2$. Thus, the behavior for the counterflow can vary from the planar value of $S_1 = 1, S_2 = 0$ (or vice versa) or from the case $S_1 = S_2 = 1/2$. This clearly shows that distinctions must be made amongst the various possibilities for three-dimensional strain fields as $S_1 S_2$ varies between large negative numbers and $1/4$. An exception will be the incompressible case with constant properties where the $S_1 S_2$ terms cancel in the equation for f .

The vorticity ω_κ impacts directly f_1 and f ; thereby, it is affecting the velocity field. Then, through the advection of the scalar properties, there is impact on mass fractions and enthalpy. If the vorticity $\omega_\kappa = 0$, a simple inspection of the governing ODEs leads to the conclusion that the values for $f_1, f_1', f_2, f_2', u/x$, and w/z can be interchanged with the values for

$f_2, f'_2, f_1, f'_1, w/z$, and u/x , respectively, when S_1 and S_2 are replaced by $1 - S_1$ and $1 - S_2$, respectively.

Note that, for $S_1 > 1$ or $S_2 > 1$ (which imply $S_2 < 0$ or $S_1 < 0$, respectively), there would be incoming streams from two directions. One incoming stream would have a prescribed velocity profile in the viscous layer determined as a local exact solution to the Navier-Stokes conditional on its matching the profile determined by upstream conditions for the flow in that direction; this situation is too highly contrived and is not considered here. Thus, S_1 and S_2 are always each non-negative and bounded above by unity value in our considerations here. The figures show results for three strain rates; $S_1 = 0$ (planar case); $S_1 = 0.25$ (3D strain); and $S_1 = 0.5$ (axisymmetric case).

If the viscous dissipation is negligible, $\tilde{h}$ becomes a conserved scalar. Other conserved scalars can be created. Mixture fraction is a popular choice. For case of one-step kinetics with $Le = 1$ and negligible viscous dissipation, the Shvab-Zel'dovich variables, $\alpha \equiv Y_F - \nu_S Y_O$ and $\beta \equiv h - \nu_S Y_O Q$ become conserved scalars. Y_F, Y_O, ν_S , and Q are fuel mass fraction, oxygen mass fraction, stoichiometric mass ratio, and chemical energy per unit mass of fuel, respectively. For steady-state and time-averaged flows, these conserved scalars vary monotonically across a flow field and can be used to replace one of the spatial coordinates. This coordinate transformation in the counterflow configuration results in a new form of the scalar equations where the advective term is not present; a reactive-diffusive balance results. This result has classically been used (Peters, 2000; Pierce and Moin, 2004) together with an incompressible-flow assumption which gives an overly simplistic solution for the velocity field. Sirignano (2019, 2021a,c) has shown the transformation gains little when the variable density is considered; furthermore, the variable density significantly affects the reacting counterflow.

Consider the production or consumption rate of a particular species over the counterflow volume. We can either integrate over a volume using the original form in Equation (11) or, more conveniently, using Equation (25) to get exactly the same result. Consider the volume $-a < \xi < a, -b < y < b, -c < z < c$. The choices of lengths a and c will not matter on a per-unit-volume basis since mass fraction Y_m and reaction rate $\dot{\omega}_m$ do not vary with x or z . c is chosen to be of the order of the Kolmogorov scale. Volume $V = 8abc$, $\tilde{\Phi}$ is the volume averaged viscous dissipation rate; and $\rho \tilde{\omega}_m$ is the average mass production rate over the volume. It follows from integration of

Equation (23) after multiplication by density ρ and division by PrV that

$$\begin{aligned}
 \int_{-a}^a \int_{-b}^b \int_{-c}^c \frac{\rho}{PrV} [Y_m'' + Pr f Y_m' + Pr \dot{\omega}_m] dx dy dz &= 0 \quad ; \quad m = 1, 2, \dots, N \\
 \widetilde{\rho \dot{\omega}_m} &\equiv \frac{1}{V} \int_V \rho \dot{\omega}_m dV = -\frac{1}{2b} \int_{\eta(-b)}^{\eta(b)} f Y_m' d\eta \quad ; \quad m = 1, 2, \dots, N \\
 \int_{-a}^a \int_{-b}^b \int_{-c}^c \frac{\rho}{PrV} [h'' + Pr f h' - Pr \sum_{m=1}^N h_{f,m} \dot{\omega}_m + Pr \frac{\Phi}{\rho}] dx dy dz &= 0 \\
 \sum_{m=1}^N h_{f,m} \widetilde{\rho \dot{\omega}_m} - \tilde{\Phi} &= \frac{1}{2b} \int_{\eta(-b)}^{\eta(b)} f h' d\eta
 \end{aligned} \tag{27}$$

The quantity $\widetilde{\rho \dot{\omega}_m}$ is the only value that need be transferred from the sub-grid flamelet analysis to the resolved-scale simulation. Note the reaction rate is invariant under the change of reference frame. Here, b has been considered large enough so that $Y_m' = 0$ and $h' = 0$ at those boundaries are good approximations. However, the value for $\widetilde{\rho \dot{\omega}_m}$ depends on the chosen domain size $2b$, which has a value of $O(10)$ typically in our analysis. Future studies should examine the optimization of the domain-size b . $Le = 1$ has also been considered. The volume-averaged viscous dissipation rate $\tilde{\Phi}$ may be obtained by integration of Equation (22).

Consider a species m that is flowing inward away from $\eta = \infty$ towards $\eta = 0$. If it is being produced (consumed), the derivative Y_m' in Equation (27) will be negative (positive) for $\eta > 0$ where velocity $v < 0$ and $f > 0$. The signs are opposite for a species flowing inward away from $\eta = -\infty$ and towards $\eta = 0$. The equation provides two ways to evaluate the average production (consumption) rate for species m . The volume integral of the reaction rate has highly nonuniform integrand values over the space while the outflow integral over η has a smoother variation of the integrand.

The flamelet model requires inputs that are scaled from the resolved flow. Specifically, rate of strain and vorticity, pressure, and the inflowing scalar values for the counterflow are needed. The magnitude of the resolved scale velocity is not relevant because the sub-grid velocities are measured relative to a frame moving with a Galilean transformation. The flamelet can give back to the resolved flow the instantaneous value for energy release rate.

3.5 Chemical Kinetics Model

The above equations can be readily applied for diffusion-flame counterflows and partially-premixed-flame counterflows as will be explained in the following sections. They can also describe situations where multi-branched flames exist. For case of zero vorticity, i.e., $\omega = 0$, the generality has been shown by Sirignano (2021a, 2019). Although the analysis allows for the use of detailed chemical kinetics in the future, we will focus here on propane-oxygen flows with one-step kinetics. However, results are expected to be qualitatively more general, applying to situations with more detailed kinetics and to other hydrocarbon /oxygen-or-air combination. Westbrook and Dryer (1984) kinetics are used; they were developed for premixed flames but any error for nonpremixed flames is viewed as tolerable often here because diffusion would generally be rate-controlling. Using asterisks to denote dimensional quantities, one may deduce that

$$\omega_F^* = -A^* \rho^{*0.75} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}} \quad (28)$$

where the ambient temperature is set at 300 K and density ρ^* is given in units of kilograms per cubic meter. Here, $A^* = 4.79 \times 10^8 (kg/m^3)^{-0.75}/s$. The dimensional strain rate $S_1^* + S_2^*$ (at the sub-grid scale) is used to normalize time and reaction rate. In non-dimensional terms,

$$\begin{aligned} \dot{\omega}_F &= -\frac{A^* \rho_\infty^{*0.75}}{S_1^* + S_2^*} \tilde{h}^{-0.75} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}} \\ \dot{\omega}_F &= -\frac{Da}{\tilde{h}^{0.75}} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}} \end{aligned} \quad (29)$$

The above equation defines the Damköhler number Da . Furthermore, we set $Da \equiv K Da_{ref}$ where

$$Da_{ref} \equiv \frac{\tilde{A} (10 kg/m^3)^{0.75}}{(10^4/s)} = 2.693 \times 10^5 ; \quad K \equiv \left[\frac{\rho_\infty^*}{10 kg/m^3} \right]^{0.75} \frac{10^4/s}{S_1^* + S_2^*} \quad (30)$$

$10 kg/m^3$ and $10,000/s$ are conveniently chosen as reference values for density and strain rate, respectively. The reference value for density implies an elevated pressure. The strain-rate reference value is in the middle of an interesting range for this chemical reaction. Suppose the resolved scale has a velocity, a mixing length, and kinematic viscosity with the following re-

spective orders of magnitude: $10m/s$, $0.1m$, and $10^{-4}m^2/s$. Then, we may estimate $Re = 10^4$ and resolved scale strain rate $\partial u/\partial x = 100/s$. Thereby, Equation (3) yields that $\partial u_\kappa/\partial \kappa = Re^{1/2}\partial u/\partial x = S_1^* + S_2^* = 10^4/s$.

Clearly, there is no need to set pressure (or its proxy, density) and the strain rate separately for a one-step reaction. For propane and oxygen, the mass stoichiometric ratio $\nu = 0.275$.

The non-dimensional parameter K increases (decreases) as the strain rate decreases (increases) and/ or the pressure increases (decreases). $K = 1$ is our reference case and the range covered includes $O(10^{-1}) \leq K \leq O(10^2)$, allowing for the needed variation in strain rate and pressure to sustain premixed flamelets, diffusion flamelets, and multi-branched flamelets.

The system of ordinary differential equations is solved numerically using a relaxation method and central differences. Solution over the range $-5 \leq \eta \leq 5$ provides adequate fittings to the asymptotic behaviors. The parameters that are varied are K , Pr , and S_1 (and thereby $S_2 = 1 - S_1$). Most calculations have $Pr = 1$ with emphasis on the effect of variation in K , i.e., pressure and strain rate.

3.6 Uncoupled Diffusion Flamelet Calculations

Now, we treat a situation with a three-dimensional diffusion-flame structure at the sub-grid level. Figures 2 and 3 show the influence of vorticity on the flamelet stability near the extinction limit. The rotation of the flamelet due to vorticity causes a centrifugal effect on the counterflow velocity and thereby on the residence time in the vicinity of the reaction zone. The dash red and solid red curves represent K values of 0.195 and 0.196, respectively, both without vorticity. Despite the very modest difference in K , one survives as a strong flame and the other is basically extinguished. By applying $K = 0.195$ and $\omega_\kappa = 1.0$ and therefore rotational speed of value $d\theta/dt = 0.5$, the solid blue curve is obtained, indicating a strong flame with regard to both reaction rate and peak temperature or enthalpy is induced by the rotation. Actually, the $K = 0.196$, $\omega_\kappa = 1.0$ curve falls right on the solid blue curve as well, except in Figure 2d where it appears as a dash purple curve. The rotation causes a lower mass flux f than was obtained without rotation. The inflow rate is diminished because the centrifugal effect creates a more adverse pressure gradient. However, the slower flow rate allows a longer residence time and modifies the extinction limit. As K is lowered to values of 0.180 or 0.185, the flame is essentially extinguished in spite of the increased residence time

due to the rotational effects.

The rotation also causes a decrease in f'_1 and therefore in the ξ -component of velocity as shown in Figure 3. There is an associated increase in f'_2 and therefore an increase in the z -component of velocity. Basically, the low-density products of combustion more easily flow in the z -direction wherein no centrifugal effect is applied. This gives some physical explanation to the findings of Nomura and Elghobashi (1993) where, for reacting flows but not for non-reacting flows, the major extensional axis tends to align parallel with the vorticity vector. Specifically, when reaction and energy release occur, the outflow for the counterflow configuration will have the greater extensional strain rate in the principal direction aligned with the vorticity. The outflow velocity in the principal direction orthogonal to the vorticity might still experience a higher magnitude than the inflow velocity in the compressive-strain direction due to the density decrease in the flow. However, its increase will be less profound than for the velocity component aligned with the vorticity.

The asymptotic value as $\eta \rightarrow \infty$ in subfigure 2d gives the integrated burning rate in the sub-grid volume. Realize that the factor $2b$ from Equation (27) has not yet been factored into the integral result in the figures; it will reduce the values by an order of magnitude in order to give the average over the volume. It is seen that rotation affects burning and burning rate is negligible in several cases. The decrease in mass flux rate with increasing rotation rate (i.e., vorticity) results in a decreased burning rate through the sub-grid volume.

The values of S_1 and S_2 do have some consequence on the behavior. In Figures 4 and 5, S_1 varies between 0.750 and 0.333. $S_2 = 1 - S_1$ and varies accordingly. As S_1 decreases and S_2 increases, the flame zone moves slightly, the integrated burning rate decreases, and the normalized mass flux f through the counterflow decreases. Very interestingly, as S_1 decreases, both the u_ξ velocity component and f'_1 decrease while the w velocity component and f'_2 increase. u_χ also decreases. As the S_1 value moves from 0.500 to 0.333, some reversal of the u_ξ velocity occurs in the region of highest temperature and lowest density. In that region, there is inflow (compressive strain) in two directions with outflow (tensile strain) only in the z -direction. This implies that, for $S_1 = 0.333$, an inflowing particle of material enters at first with decreasing magnitude of χ and increasing values of ξ and z in Lagrangian time. Then, it changes to decreasing values of both χ and ξ in that time but remaining with an increasing value for z . Note that a case with $K = 0.195$, $\omega_\kappa = 1.0$, and $S_1 = 0.250$ is not plotted here. It resulted in extinction

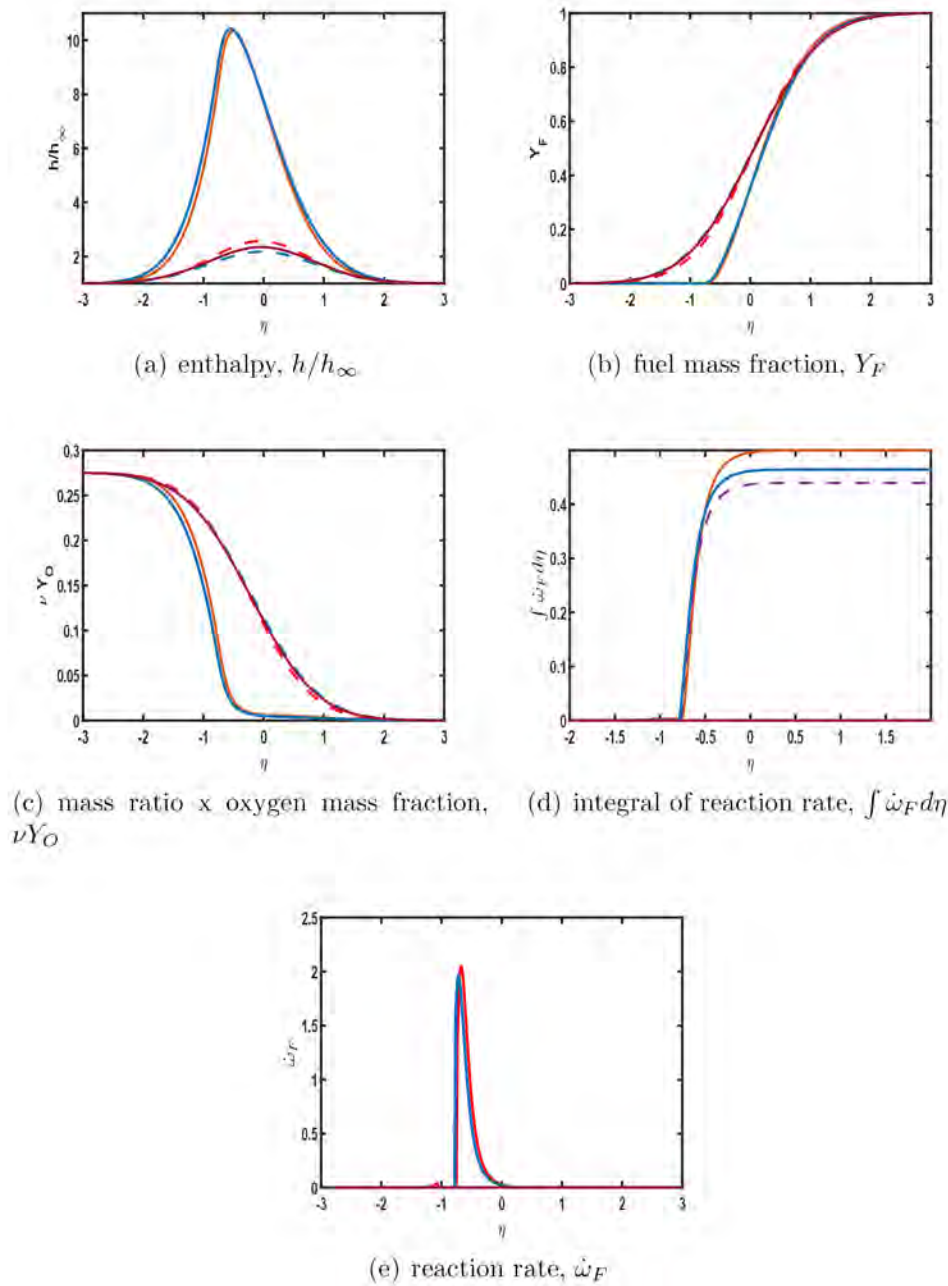


Figure 2: Diffusion flame with varying vorticity and Damköhler number. $S_1 = 0.75$; $S_2 = 0.25$. dash red, $K = 0.195$, $\omega_\kappa = 0$; solid red, $K = 0.196$, $\omega_\kappa = 0$; solid blue, $K = 0.196$, $\omega_\kappa = 1.0$; solid purple, $K = 0.185$, $\omega_\kappa = 1.0$; dash blue, $K = 0.180$, $\omega_\kappa = 1.0$. The $K = 0.195$, $\omega_\kappa = 1.0$ case is covered by the solid blue curve, except in subfigure d where it is given by the dash purple curve.

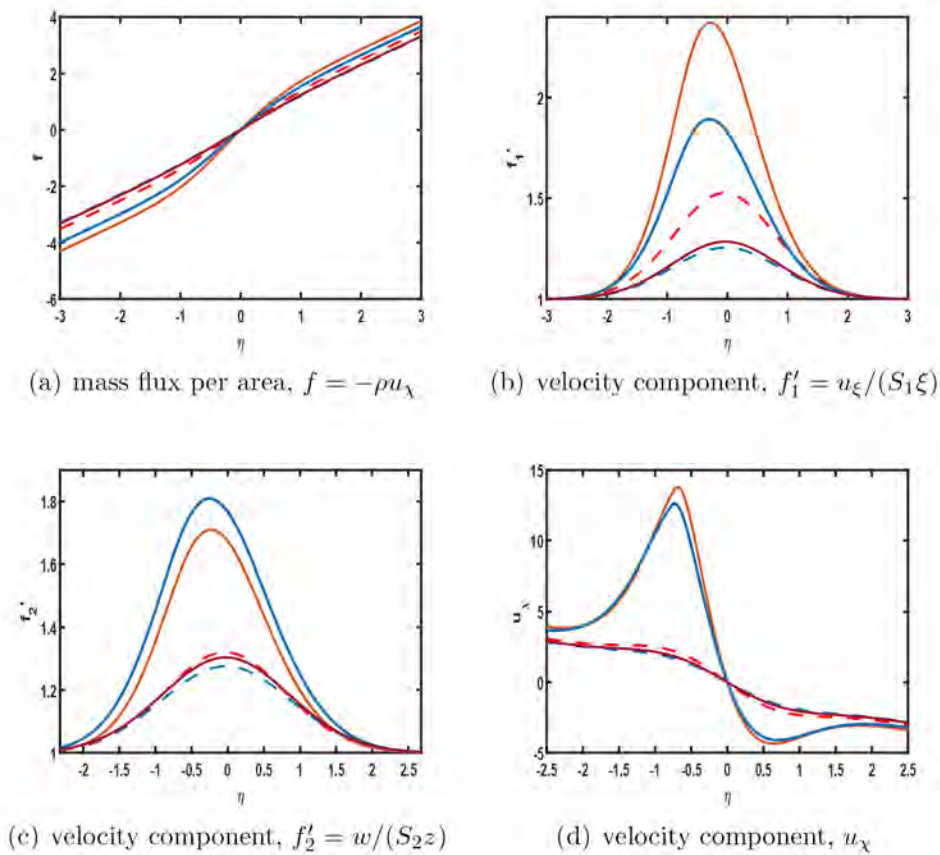


Figure 3: Diffusion flame with varying vorticity and Damköhler number. $S_1 = 0.75$; $S_2 = 0.25$. dash red, $K = 0.195$, $\omega_\kappa = 0$; solid red, $K = 0.196$, $\omega_\kappa = 0$; solid blue, $K = 0.196$, $\omega_\kappa = 1.0$; solid purple, $K = 0.185$, $\omega_\kappa = 1.0$; dash blue, $K = 0.180$, $\omega_\kappa = 1.0$. The $K = 0.195$, $\omega_\kappa = 1.0$ case is covered by the solid blue curve.

of the flame.

As seen from Figures 3 and 5, because of density gradients, velocity gradients exist in the new rotating coordinate system such that vorticity components result in the z and ξ direction from f_1'' and f_2'' , respectively. However, those velocity components and thereby the associated vorticity components have an antisymmetry. Thus, the induced circulation around the flamelet due to density gradients is zero. Only the circulation due to the imposed vorticity ω_κ will exist. These findings are consistent with the results of Sirignano (2021a, 2019).

Clearly, the combination of fluid rotation, variable-density, and three-dimensional structure have major consequences for flamelet behavior.

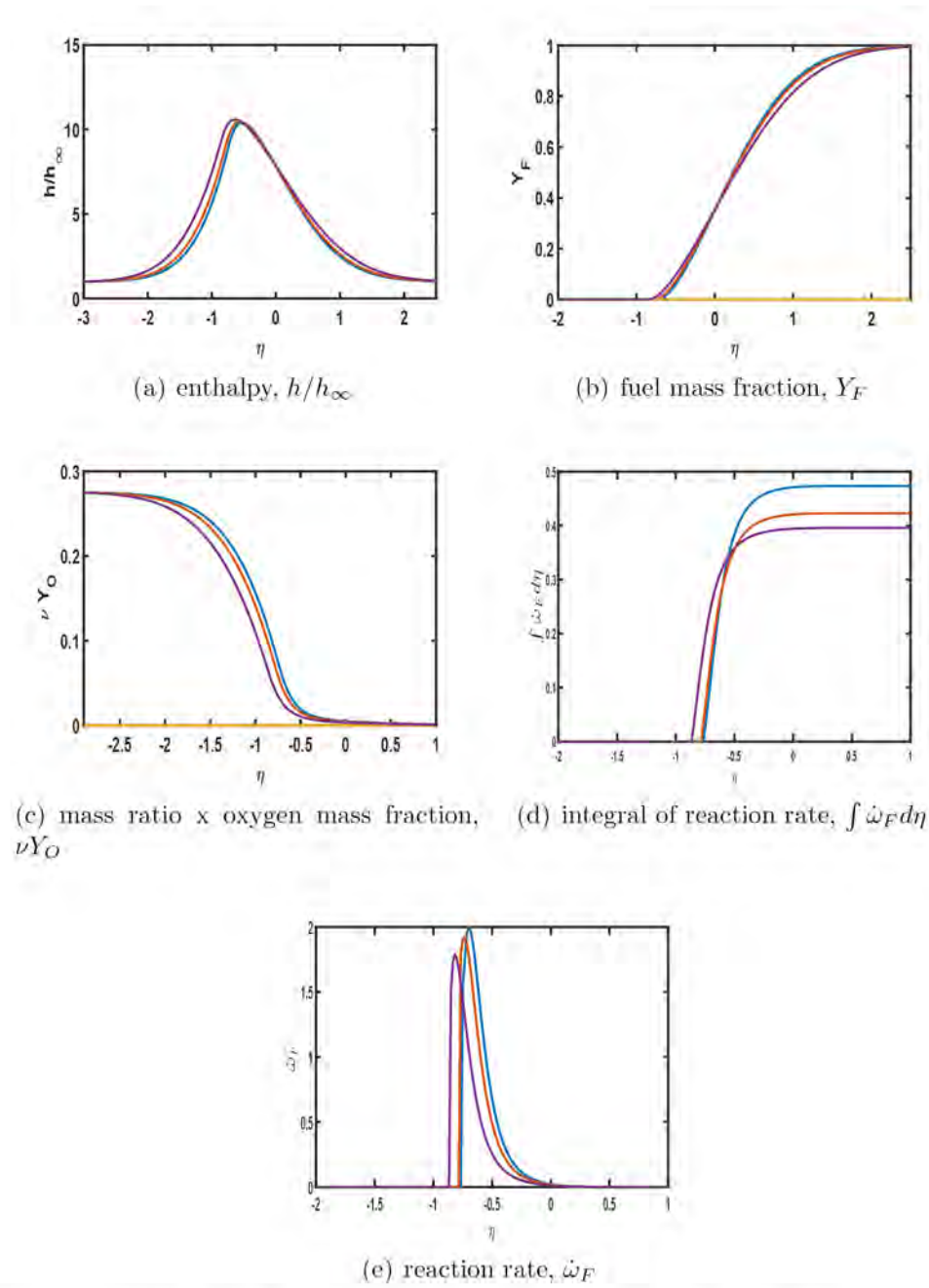


Figure 4: Diffusion flame with varying strain rate. $K = 0.195$, $\omega_\kappa = 1.0$. blue $S_1 = 0.750$, $S_2 = 0.250$; red $S_1 = 0.500$, $S_2 = 0.500$; purple $S_1 = 0.333$, $S_2 = 0.667$.

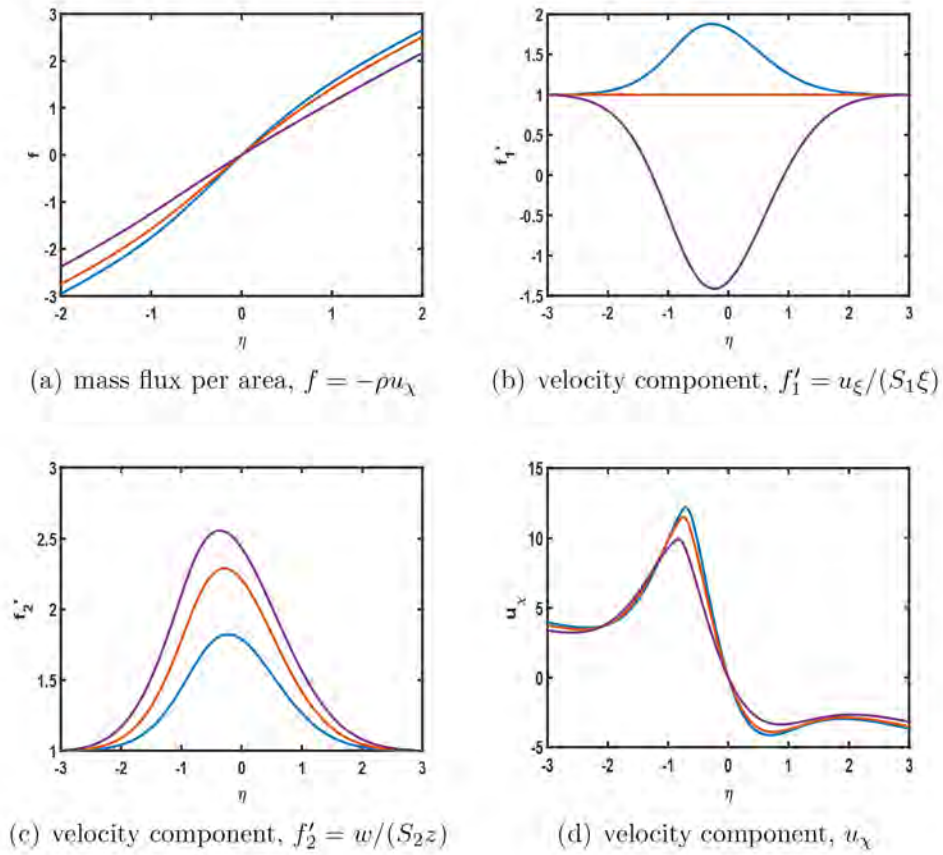


Figure 5: Diffusion flame with varying strain rate. $K = 0.195$, $\omega_\kappa = 1.0$. blue $S_1 = 0.750$, $S_2 = 0.250$; red $S_1 = 0.500$, $S_2 = 0.500$; purple $S_1 = 0.333$, $S_2 = 0.667$.

3.7 Uncoupled Premixed Flame Calculations

The premixed flame is treated with consideration of a mixture that is 12 per cent propane by mass and 43.5 per cent oxygen by mass (stoichiometric proportion), with the remainder an inert gas. This flame structure requires a much larger Damköhler number to exist when compared to the diffusion flame. It extinguishes under high strain rate (i.e., low residence time in the counterflow). In Figures 6 and 7, the rate of strain values are held constant at $S_1 = 0.750$ and $S_2 = 0.250$ while Da and/ or ω_κ are varied. K varies between 15 and 40 while ω_κ varies between 0 and 1. At lower values of the imposed vorticity, the flame extinguishes. Increased vorticity strengthens the centrifugal effect, increasing the efflux of the counterflow in the z -direction aligned with the vorticity vector.

Figure 6 shows that modest changes for the Damköhler number Da can result in differences in burning rate while Figure 7 shows modification in the flame velocity. As Da increases, the flame shifts to a position in the counterflow with higher incoming velocity and mass flux. All three components of the velocity generally increase as Da increases. There is an increase in the chemical reaction rate leading to an increase in the premixed flame speed and a flame position farther from the counterflow interface where the incoming velocity is larger in magnitude. At the lowest value of Da shown in the plots, the flame extinguishes as the reaction rate decreases because, in the spatially varying velocity field, it cannot obtain the needed residence time. The higher velocities result from the combination of an increase in mass burning rate and a decrease in density.

Vorticity produces the centrifugal effect that decreases outflow rate in the x direction while increasing the outflow rate in the z direction. It also causes the flame to stabilize at a larger distance from the interface at $\eta = 0$. The inflow mass flux, reflected through f , decreases as ω_κ increases, implying an increase in the residence time.

It is noteworthy that the premixed flames require Da values that are orders of magnitude larger than required for diffusion flames. We can expect that they therefore are less likely to appear in highly strained turbulent flows.

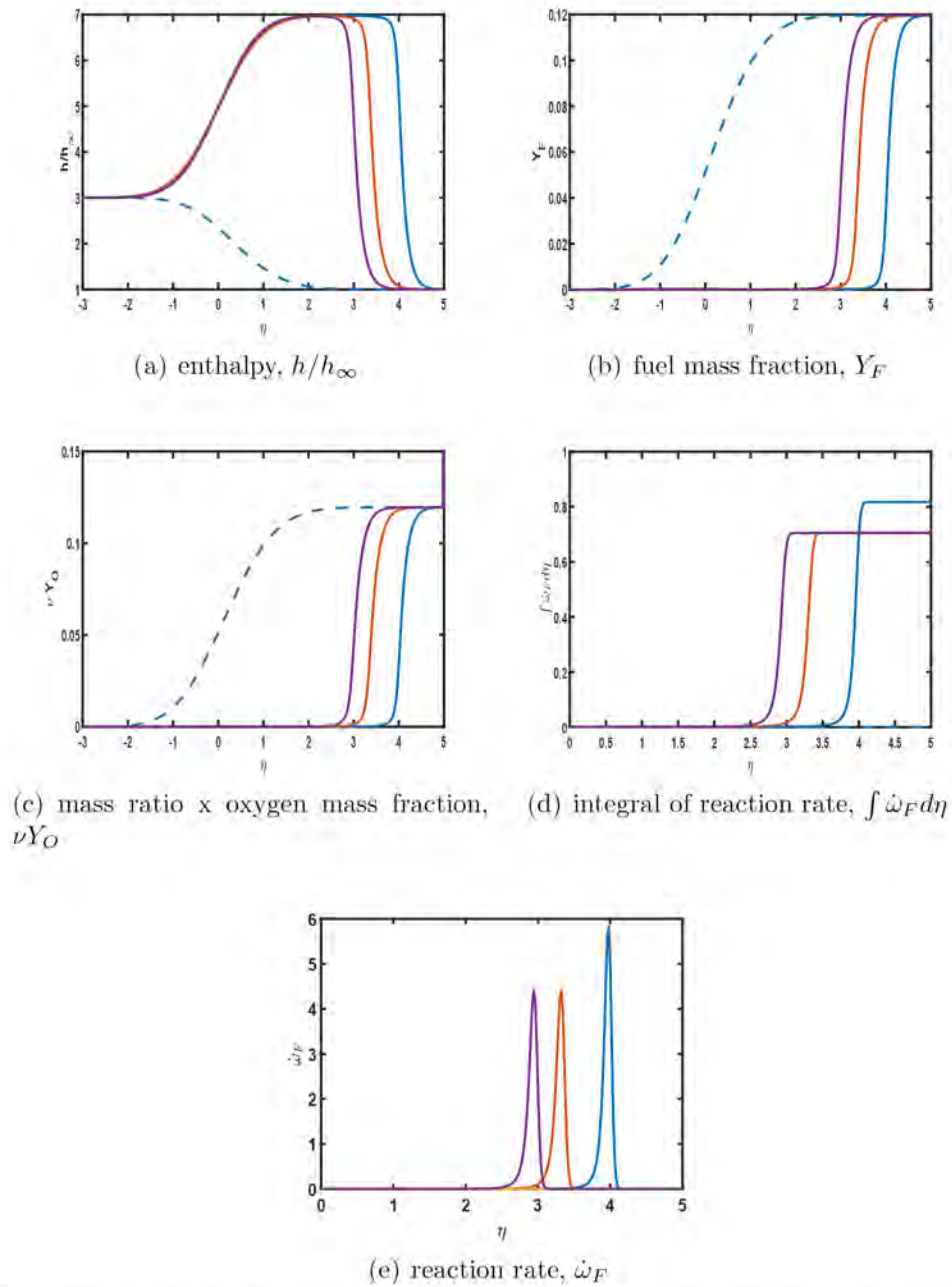


Figure 6: Premixed flame: influence of Damköhler number and vorticity. $S_1 = 0.750$, $S_2 = 0.250$. Blue, $\omega_\kappa = 1.0$, $K = 40$; red, $\omega_\kappa = 1.0$, $K = 30$; dash blue, $\omega_\kappa = 1.0$, $K = 15$; purple, $\omega_\kappa = 0$, $K = 30$.

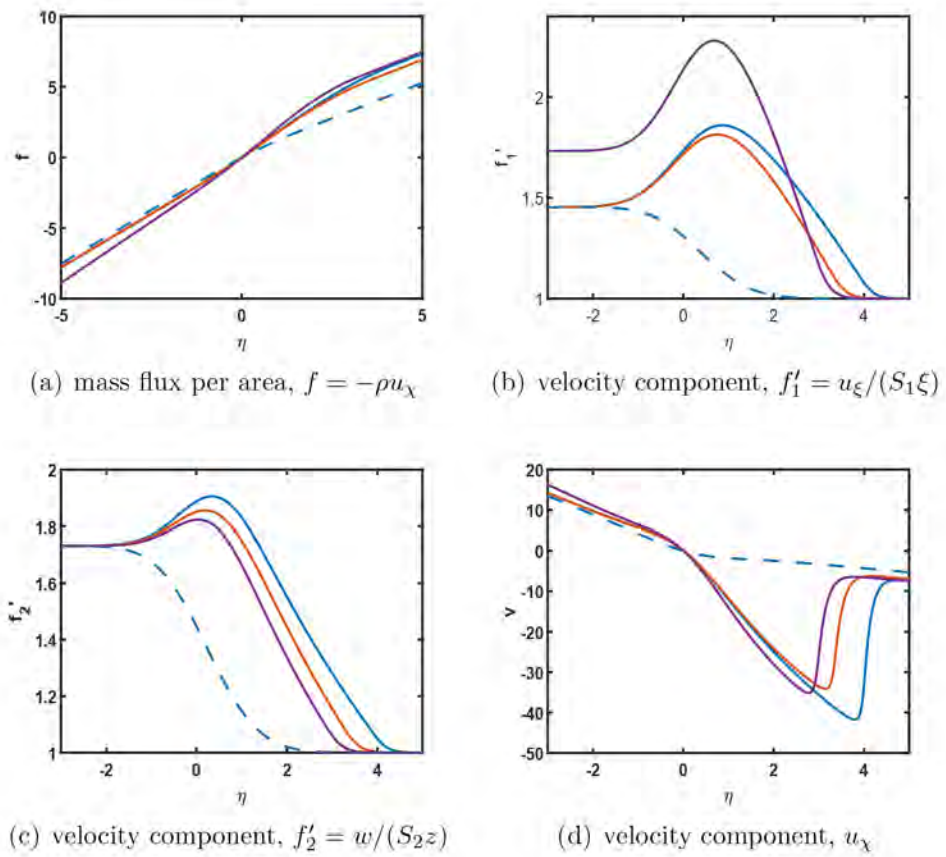


Figure 7: Premixed flame: influence of Damköhler number and vorticity. $S_1 = 0.750$, $S_2 = 0.250$. Blue, $\omega_\kappa = 1.0$, $K = 40$; red, $\omega_\kappa = 1.0$, $K = 30$; dash blue, $\omega_\kappa = 1.0$, $K = 15$; purple, $\omega_\kappa = 0$, $K = 30$.

3.8 Uncoupled Multibranched Flamelet Calculations

In Figures 8 and 9, results are shown for a multi-flame configuration with $K = 0.200$ where a fuel-rich mixture with $Y_F = 2/3$ and $Y_O = 1/3$ exists on one side of the counterflow flame and a fuel-lean mixture with $Y_F = 1/12$ and $Y_O = 11/12$ exists on the other side. This allows for the possibility of multi-flame structures as found by Sirignano (2021a), in contrast to the FPV approach which disallows multi-branched or premixed flame behavior by using a mixture fraction Z domain that extends for $0 \leq Z \leq 1$. The figures show that three flame structures appear based on this new theory: a fuel-lean premixed flame on the left, a diffusion flame in the center, and a fuel-rich premixed flame on the right. As noted by Sirignano (2021b), the two premixed flames are not independent structures but rather depend substantially on heat flux from the diffusion flame. The figures also show that, as vorticity and rotation rate increase, the burning rate for each of the three flame branches and mass-flux through the counterflow decrease. The location of each of the flames shifts towards the fuel-lean side as rotation rate increases. Also, the fraction of the outflow in the direction aligned with the vorticity increases substantially with increasing rate of rotation.

For the multi-branched flame as well as the simple diffusion flame, fluid rotation, variable-density, and three-dimensional structure combine to have major consequences for the behavior.

For both the multi-branched flame and the single diffusion flame, values of S_1 and S_2 have consequence on the behavior. In Figures 10 and 11, S_1 varies between 0.750 and 0.333. $S_2 = 1 - S_1$ and varies accordingly. Again, as S_1 decreases and S_2 increases, the flame zone moves slightly, the integrated burning rate decreases, and the normalized mass flux f through the counterflow decreases. As S_1 decreases, the u_χ velocity component increases while the u_ξ velocity component decreases and, below $S_1 = 0.500$, the u_ξ velocity reverses direction in the region of highest temperature and lowest density. So, again in that low-density region, there is inflow (compressive strain) in two directions with outflow (tensile strain) only in the z -direction. The results show in Figure 12 that for $S_1 = 0.333$, an inflowing particle of material enters at first with decreasing magnitude of χ with Lagrangian time and increasing values of ξ and z in time. However, a reversal for the ξ direction is seen with all the outflow going in the z direction. As noted earlier, the behavior is consistent with DNS findings concerning alignment of vorticity and principal strain axes for reacting flows by Nomura and Elghobashi (1993).

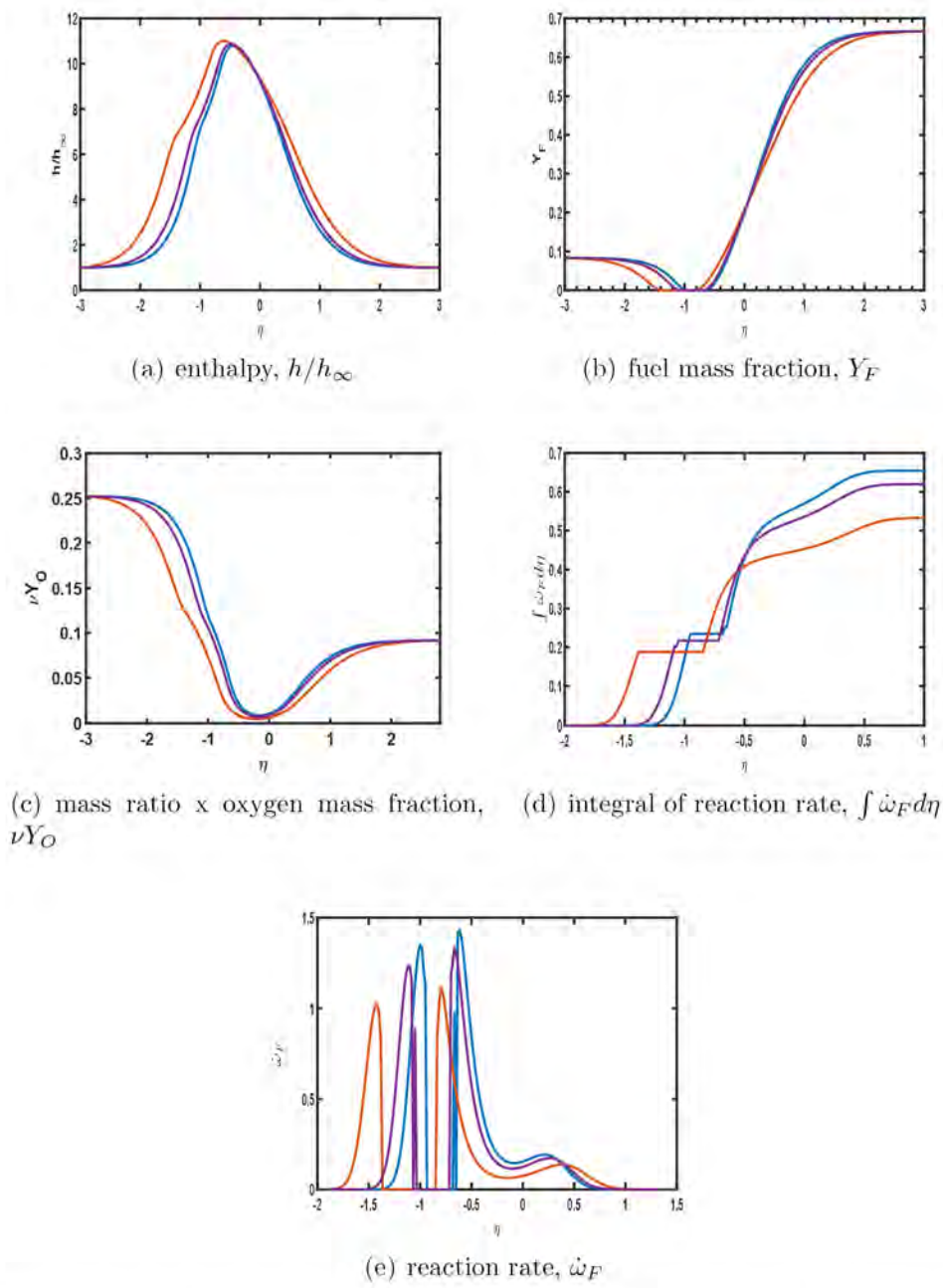


Figure 8: Multi-branched flame with $K = 0.200$ and varying vorticity. $S_1 = 0.75$; $S_2 = 0.25$. blue, $\omega_K = 0$; red, $\omega_K = 1.50$; purple, $\omega_K = 1.0$.

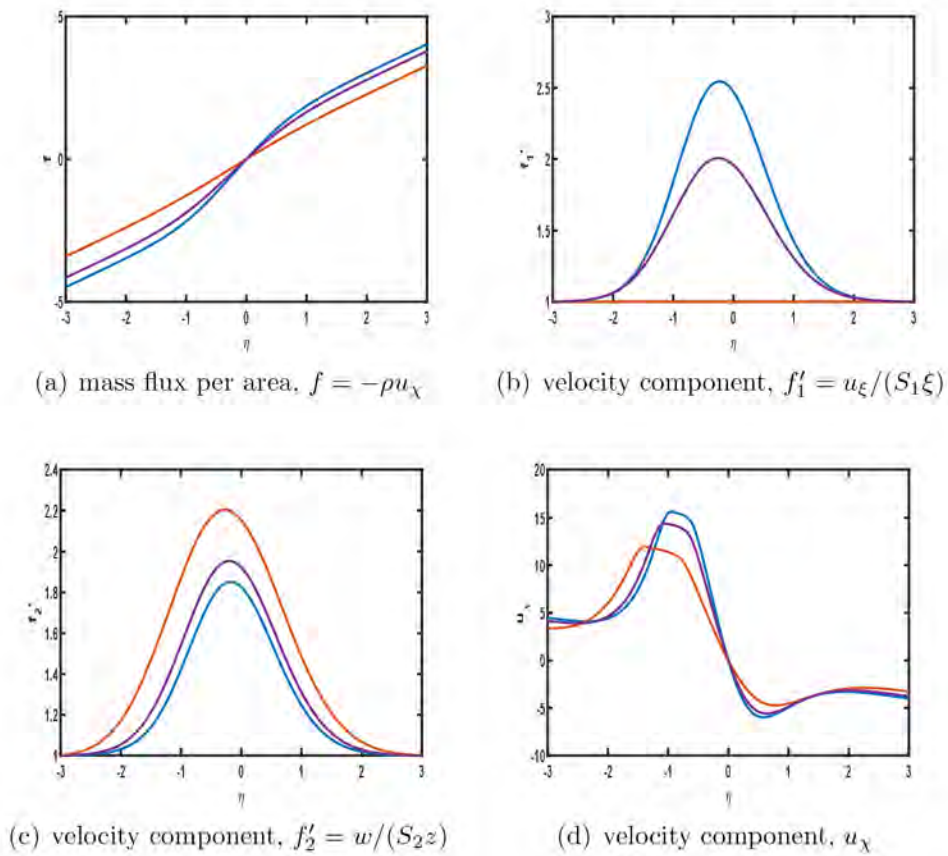


Figure 9: Multi-branched flame with $K = 0.200$ and varying vorticity. $S_1 = 0.75$; $S_2 = 0.25$. blue, $\omega_\kappa = 0$; red, $\omega_\kappa = 1.50$; purple, $\omega_\kappa = 1.0$.

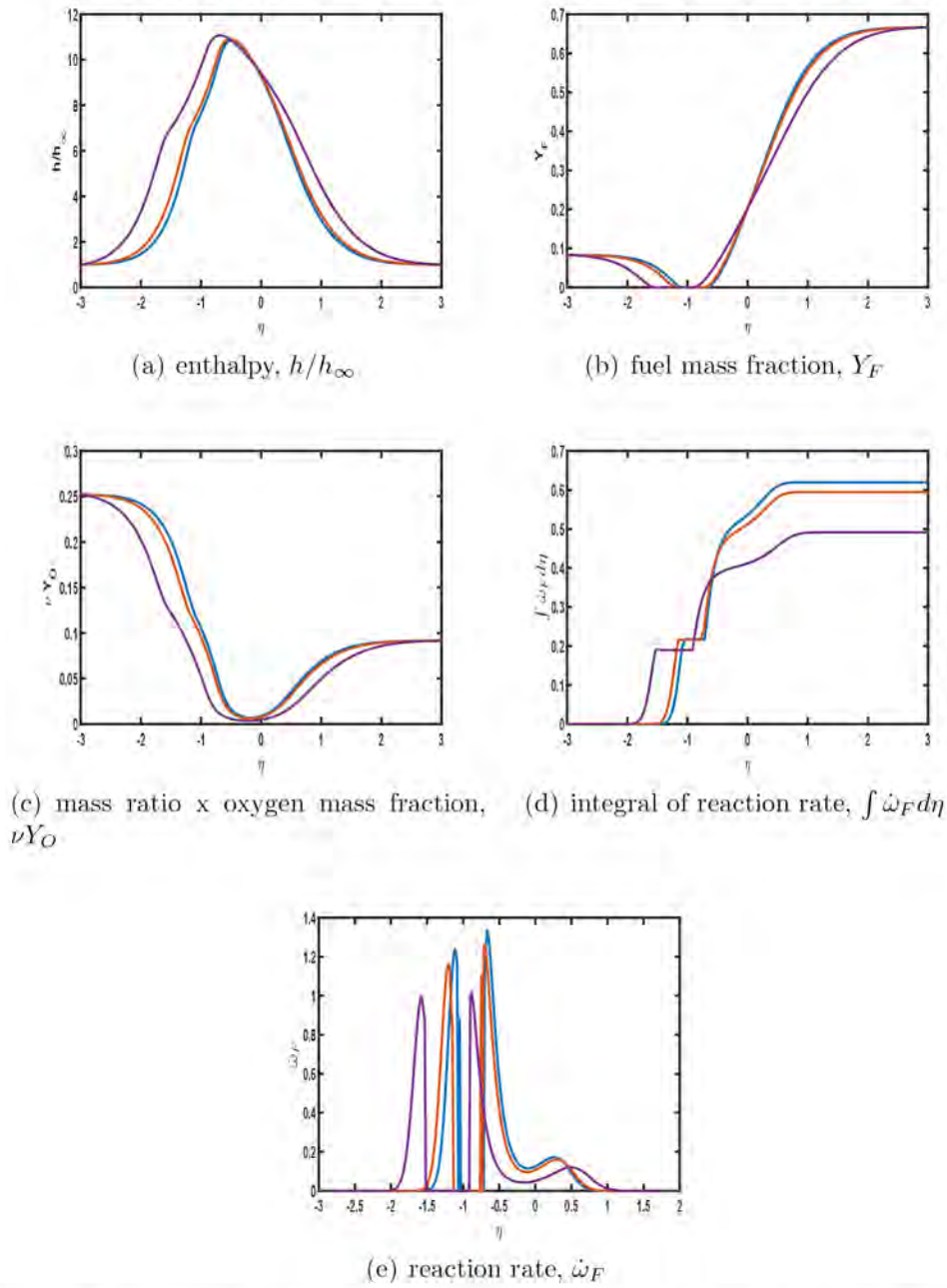


Figure 10: Multi-branched flame with varying strain rate. $K = 0.200, \omega_\kappa = 1.0$. blue $S_1 = 0.750, S_2 = 0.250$; red $S_1 = 0.500, S_2 = 0.500$; purple $S_1 = 0.333, S_2 = 0.667$.

Interestingly, the partially premixed flames in the multi-branched structure are driven by heat flux from the diffusion flame as shown by Sirignano (2021b). Thus, they survive extinction at much lower Da values than independent premixed flames can.

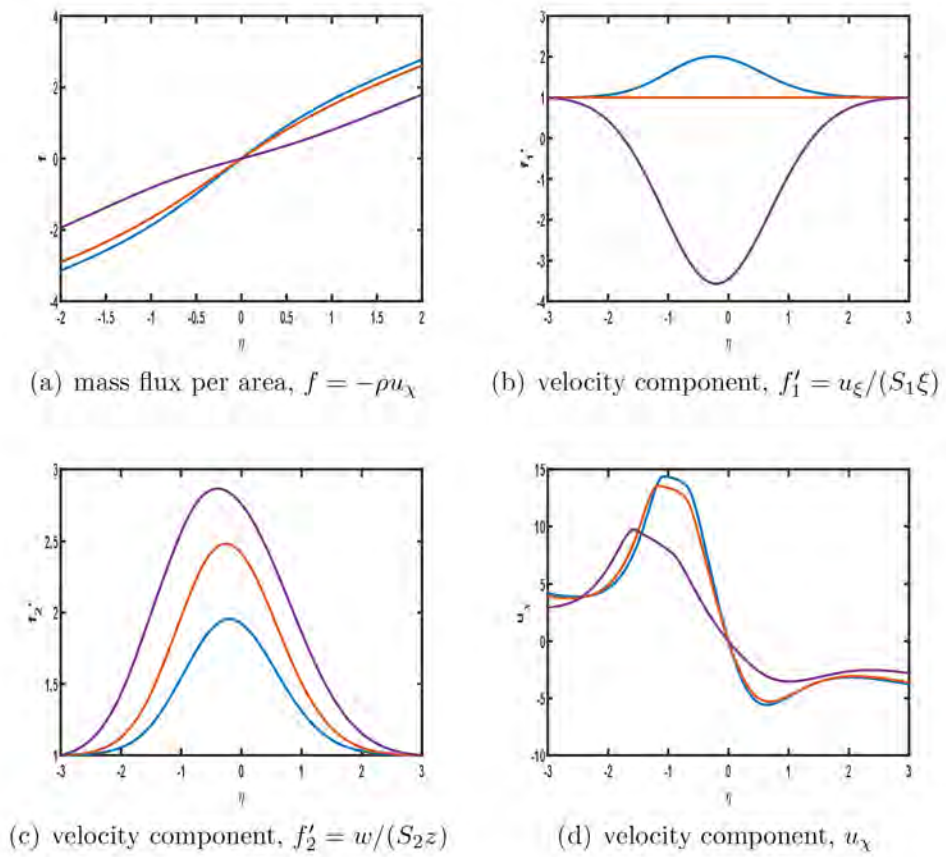


Figure 11: Multi-branched flame with varying strain rate. $K = 0.200, \omega_\kappa = 1.0$. blue $S_1 = 0.750, S_2 = 0.250$; red $S_1 = 0.500, S_2 = 0.500$; purple $S_1 = 0.333, S_2 = 0.667$.

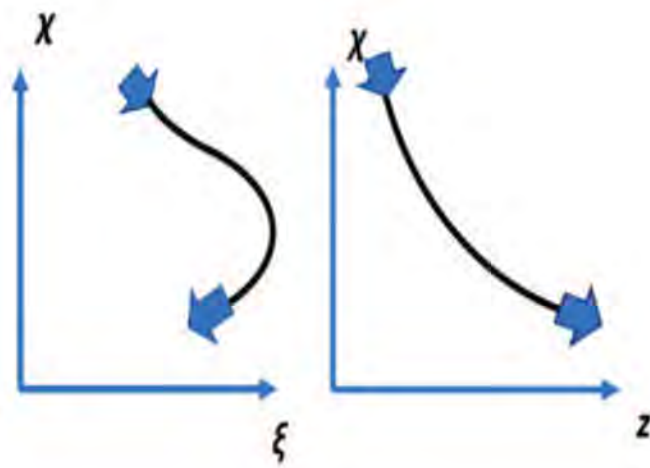


Figure 12: Multi-branched flamelet with reversed flow. $K = 0.200$, $\omega_K = 1.0$. $S_1 = 0.333$, $S_2 = 0.667$.

4 Shear Flow on the Resolved Scale - Planar Jet

The ultimate objective is to connect this new flamelet model with RANS, unsteady RANS, and LES computations. Thereby, a limit on dimensionality or time dependence of the large-scale resolved flow would not be sought. The longer-term goal is to couple the sub-grid flamelet model to a multiscale, fully unsteady LES. However, in this first application which is aimed towards gathering understanding of the method and not yet towards solving a new problem, a much simpler resolved scale is sought. So, we seek a resolved scale that is time-averaged with minimal dimensionality. This drives the consideration towards a simple mixing-length examination of two-dimensional mixing and reacting flows. This simple example is only a demonstration of the use of the new flamelet model; in the longer term, many of the simplifying assumptions in this section should be abandoned for the model to achieve its full potential. In the following discussion, the turbulent planar mixing layer is considered.

We desire a solution for the two-dimensional, time-averaged, turbulent shear layer with variable density. The density can vary due to variations in temperature and/or composition. Pressure gradients in the mixing layer are considered negligible and the boundary-layer approximation is employed. Pope (2000) and White (2005) present useful overviews on the topic. Görtler (1942) treated a non-reacting incompressible case, finding a one-dimensional similar solution with y/x as the independent similarity variable. We have a long-standing Illingworth (1949) template with laminar flow to modify the relations for the similar compressible flow. However, the reacting flow does not allow for a similar solution in either a laminar or a turbulent case (except for infinite reaction rate with diffusion flames). Here, we take a pathway using a time-averaged two-dimensional turbulent planar mixing layer. We use a mixing-length concept for the eddy viscosity and diffusivities.

4.1 Reacting Shear-layer Analysis

We consider the averaged turbulent flow, e.g., steady-state 2D. The density is variable. The pressure gradient is zero and the boundary-layer approximation is used. The governing equations for the time-averaged velocity components

u, v in x, y space are

$$\begin{aligned}
 \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} &= 0 \\
 u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= \frac{1}{\rho} \frac{\partial}{\partial y} \left(\rho \nu_t \frac{\partial u}{\partial y} \right) \\
 u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} &= \frac{1}{\rho Pr_t} \frac{\partial}{\partial y} \left(\rho \nu_t \frac{\partial h}{\partial y} \right) - \sum_{m=1}^N h_{f,m} \dot{\omega}_{m,rs} + \frac{1}{\rho} \Phi \\
 u \frac{\partial Y_m}{\partial x} + v \frac{\partial Y_m}{\partial y} &= \frac{1}{\rho Sc_t} \frac{\partial}{\partial y} \left(\rho \nu_t \frac{\partial Y_m}{\partial y} \right) + \dot{\omega}_{m,rs} ; \quad m = 1, 2, \dots, N \quad (31)
 \end{aligned}$$

Here, $\nu_t = \mu_t / \rho$ and μ_t are the kinematic turbulent viscosity and dynamic turbulent viscosity, respectively. It is assumed that the turbulent Prandtl number Pr_t and turbulent Schmidt number Sc_t are uniform through the flow. The above equations are in a non-dimensional form that uses the resolved scales as reference length and velocity. Thus, quantities such as $\dot{\omega}_{m,rs}$ and Φ must be properly scaled before calculations. See Section 2. Note that we can replace ν_t in the equations by $\nu + \nu_t$ where ν is the molecular kinematic viscosity. In most portions of the flow, $\nu_t \gg \nu$. For low mean velocities, the dissipation Φ can be neglected.

Transform in standard fashion from x, y to $\bar{x} \equiv x, \bar{y} \equiv \int_0^y (\rho / \rho_\infty) dy'$. v , the transverse component of velocity, is transformed to the variable w to mimic incompressible flow.

$$\begin{aligned}
 w &\equiv \frac{\rho}{\rho_\infty} v + \frac{u}{\rho_\infty} \int_{y_{ref}}^y \frac{\partial \rho}{\partial x} dy' \\
 \frac{\partial u}{\partial \bar{x}} + \frac{\partial w}{\partial \bar{y}} &= 0 \\
 u \frac{\partial u}{\partial \bar{x}} + w \frac{\partial u}{\partial \bar{y}} &= \frac{\partial}{\partial \bar{y}} \left(\frac{\rho^2}{\rho_\infty^2} \nu_t \frac{\partial u}{\partial \bar{y}} \right) \\
 u \frac{\partial h}{\partial \bar{x}} + w \frac{\partial h}{\partial \bar{y}} &= \frac{1}{Pr_t} \frac{\partial}{\partial \bar{y}} \left(\frac{\rho^2}{\rho_\infty^2} \nu_t \frac{\partial h}{\partial \bar{y}} \right) - \sum_{m=1}^N h_{f,m} \dot{\omega}_{m,rs} + \frac{1}{\rho} \Phi \\
 u \frac{\partial Y_m}{\partial \bar{x}} + w \frac{\partial Y_m}{\partial \bar{y}} &= \frac{1}{Sc_t} \frac{\partial}{\partial \bar{y}} \left(\frac{\rho^2}{\rho_\infty^2} \nu_t \frac{\partial Y_m}{\partial \bar{y}} \right) + \dot{\omega}_{m,rs} ; \quad m = 1, 2, \dots, N \quad (32)
 \end{aligned}$$

With the knowledge from Equations (1), (3), and (27) about the impact of the Kolmogorov strain rate on the reaction rate and the relation between

strain rates at different levels, we may write

$$\begin{aligned}\rho\dot{\omega}_{m,rs} &= \rho_{\text{dimensional}}\dot{\omega}_{m,\text{dimensional}} = \rho_{\infty,\text{dimensional}}S^*\widetilde{\rho\dot{\omega}_m} \\ &= \rho_{\infty,\text{dimensional}}\frac{S_{rs}^{*3/2}\delta}{\nu^{1/2}}\widetilde{\rho\dot{\omega}_m}\end{aligned}\quad (33)$$

Note that the resolved scale reaction rate $\dot{\omega}_{m,rs}$ is dimensional while the sub-grid averaged term $\widetilde{\rho\dot{\omega}_m}$ is non-dimensional in Equation (33).

Here, the layer thickness is described by a constant value of the slope $d\delta/dx$ since a linear growth rate is expected. The constant value can be estimated and adjusted based on the results but is expected to be close to the value for the incompressible, non-reacting mixing layer. Experiments have indicated the range of 0.06 to 0.11 according to Pope (2000). Here, a constant σ is considered as the reciprocal of the slope so that $\delta(x) = x/\sigma$.

$$\begin{aligned}S_{rs}^* &\equiv \left| \frac{du}{dy} \right| = \frac{\rho}{\rho_\infty} \left| \frac{du}{d\bar{y}} \right| \\ \nu_t &= (\delta(x))^2 \left| \frac{du}{dy} \right|\end{aligned}\quad (34)$$

Accordingly, the value of ν_t will vary with both x and y .

From Equations (33) and (34), the dimensional resolved-scale reaction rate $\dot{\omega}_{m,rs}$ can be related to the non-dimensional sub-grid-scale reaction rate $\widetilde{\rho\dot{\omega}_m}$. Equation (27) indicates that the non-dimensional reaction rate is proportional to an integral with f in the integrand. Thus, the dimensional reaction rate is proportional to the sub-grid-scale strain rate $S_1^* + S_2^*$. That sub-grid strain rate is larger than the resolved-scale strain rate by a factor $Re^{1/2}$ as shown by Equation (1).

The boundary conditions on each of the second-order partial differential equations are given by prescribing the u -component of velocity and the scalar properties in the two free streams. In addition, there are the upstream inflow conditions.

The system of equations given as (32) can be made nondimensional by using u_∞ to normalize velocity components, a downstream length x_0 to normalize the $\bar{x}$ and $\bar{y}$ coordinates, and ρ_∞ and h_∞ to normalize the corresponding scalar quantities. The turbulent viscosity ν_t is non-dimensionalized using the kinematic viscosity ν . The perfect-gas assumption and constant specific heat are assumed so the nondimensional relation $\rho = 1/h$ holds through this

shear layer where the pressure is approximately uniform. We also define here a Reynolds number $Re \equiv u_\infty \delta_0 / \nu = u_\infty x_0 / (\sigma \nu)$. We consider cases where the fractional difference between $\Delta U = u_\infty - u_{-\infty}$ and u_∞ is not major. The viscous dissipation is considered negligible because the Mach number is low.

$$\begin{aligned}
 \frac{\partial u}{\partial \bar{x}} + \frac{\partial w}{\partial \bar{y}} &= 0 \\
 u \frac{\partial u}{\partial \bar{x}} + w \frac{\partial u}{\partial \bar{y}} &= \frac{\partial}{\partial \bar{y}} \left(\frac{1}{h^2} \left(\frac{x}{x_0} \right)^2 \frac{1}{\sigma^2} \left| \frac{\partial u}{\partial \bar{y}} \right| \frac{\partial u}{\partial \bar{y}} \right) \\
 u \frac{\partial h}{\partial \bar{x}} + w \frac{\partial h}{\partial \bar{y}} &= \frac{1}{Pr_t} \frac{\partial}{\partial \bar{y}} \left(\frac{1}{h^2} \left(\frac{x}{x_0} \right)^2 \frac{1}{\sigma^2} \left| \frac{\partial u}{\partial \bar{y}} \right| \frac{\partial h}{\partial \bar{y}} \right) \\
 &\quad - \sum_{m=1}^N h_{f,m} \frac{Re^{1/2}}{(\sigma h)^{1/2}} \frac{x}{x_0} \left| \frac{\partial u}{\partial \bar{y}} \right|^{3/2} \widetilde{\rho \dot{\omega}_m} \\
 u \frac{\partial Y_m}{\partial \bar{x}} + w \frac{\partial Y_m}{\partial \bar{y}} &= \frac{1}{Sc_t} \frac{\partial}{\partial \bar{y}} \left(\frac{1}{h^2} \left(\frac{x}{x_0} \right)^2 \frac{1}{\sigma^2} \left| \frac{\partial u}{\partial \bar{y}} \right| \frac{\partial Y_m}{\partial \bar{y}} \right) \\
 &\quad + \frac{Re^{1/2}}{(\sigma h)^{1/2}} \frac{x}{x_0} \left| \frac{\partial u}{\partial \bar{y}} \right|^{3/2} \widetilde{\rho \dot{\omega}_m} ; \quad m = 1, 2, \dots, N \quad (35)
 \end{aligned}$$

Here, in the non-dimensional processing, we have taken

$$\begin{aligned}
 (x_0/u_\infty) \dot{\omega}_{m,rs} &= (x_0/u_\infty) (1/\rho) \frac{S_{rs}^{*3/2} \delta}{\nu^{1/2}} \widetilde{\rho \dot{\omega}_m} \\
 &= [(x_0/u_\infty) \frac{u_\infty^{3/2}}{x_0^{3/2}} \frac{\delta}{\nu^{1/2}}]_{dimensional} (\rho^{3/2}/\rho) \left| \frac{du}{d\bar{y}} \right|^{3/2} \widetilde{\rho \dot{\omega}_m} \\
 &= \left(\frac{u_\infty x_0}{\nu} \right)^{1/2} \frac{x}{x_0} \frac{1}{\sigma h^{1/2}} \left| \frac{du}{d\bar{y}} \right|^{3/2} \widetilde{\rho \dot{\omega}_m} \\
 &= Re^{1/2} \frac{x}{x_0} \frac{1}{(\sigma h)^{1/2}} \left| \frac{du}{d\bar{y}} \right|^{3/2} \widetilde{\rho \dot{\omega}_m} \quad (36)
 \end{aligned}$$

The resolved-scale calculation will provide certain information as inputs to the sub-grid flamelet computation. Specifically, some information is needed to determine through reasonable scaling principles (i) constraints on the scalar properties (mass fractions of the reactants and the temperature) and (ii) strain rates and vorticity. Then, the sub-grid calculation can give the burning rate and associated energy release rate to the resolved scale. Since the sub-grid calculations are quasi-steady, they may be performed in ad-

vanced with the input-output relation organized in the form of a look-up table or a neural network (NN). Then, the table or NN may be coupled with the resolved-scale computation.

4.2 Shear-layer Results and Discussion

Computations are performed for a turbulent diffusion flame in the shear layer. One free stream is pure propane gas while the other is pure oxygen. We assume that the flamelet scale also displays a diffusion-flame character. (Clearly, a need exists for further DNS studies to inform us about the degree of partial mixing in the turbulence cascade.) At the flamelet scale, we take $\int \tilde{\omega}_F d\eta = 0.4$ which is consistent with results shown in Figures 2 and 4. Furthermore, considering $2b = O(10)$ in Equation (27), we assign $\tilde{\rho}\tilde{\omega}_F = 0.04$. The burning rate is determined by scaling the flamelet-scale burning rate based upon the large-scale strain rate S_{rs}^* ; thus, the averaged, large-scale burning rate will vary with x and y . Implicitly, the dimensional sub-grid-scale burning rate is thereby varying with x and y . The burning rate is forced to zero value where $Y_F = 0$ and / or $Y_O = 0$. In the regions where both mass fractions have positive values, the burning rate is prescribed by Equation (36). Thereby, discontinuities of the resolved-scale reaction rate can result. This can be rectified in the future by relating boundary conditions for the sub-grid flamelet calculation to resolved-scale mass fractions.

The eddy diffusivity is estimated based on the assumption that the shear-layer density-weighted width grows linearly as $0.11x$. Solutions start at $x_0 = 10$ and are marched to $x = 20$. Hyperbolic tangents are used for the $\bar{y}$ profiles at x_0 , except for the enthalpy where a Gaussian profile is superimposed to serve as an igniter. $Re = 1000$ based on layer width at x_0 . One free stream, at positive Y values, is five times faster than the other free stream at negative y values.

Figures 13 and 14 give results for a case where the fuel stream is the faster free stream while the oxygen stream is the slower stream. The profiles widen with increasing downstream distance for both velocity and scalar properties. The peak enthalpy and temperature values remain approximately unchanged but the locations of the peak value and of the center of the reaction zone shift towards the oxygen-stream side. The sharp cutoffs in burning rate at certain tranverse positions occur because the rate is nonzero only where both reactants exist on the large scale but that rate does not depend on the precise mass-fraction values on that scale.

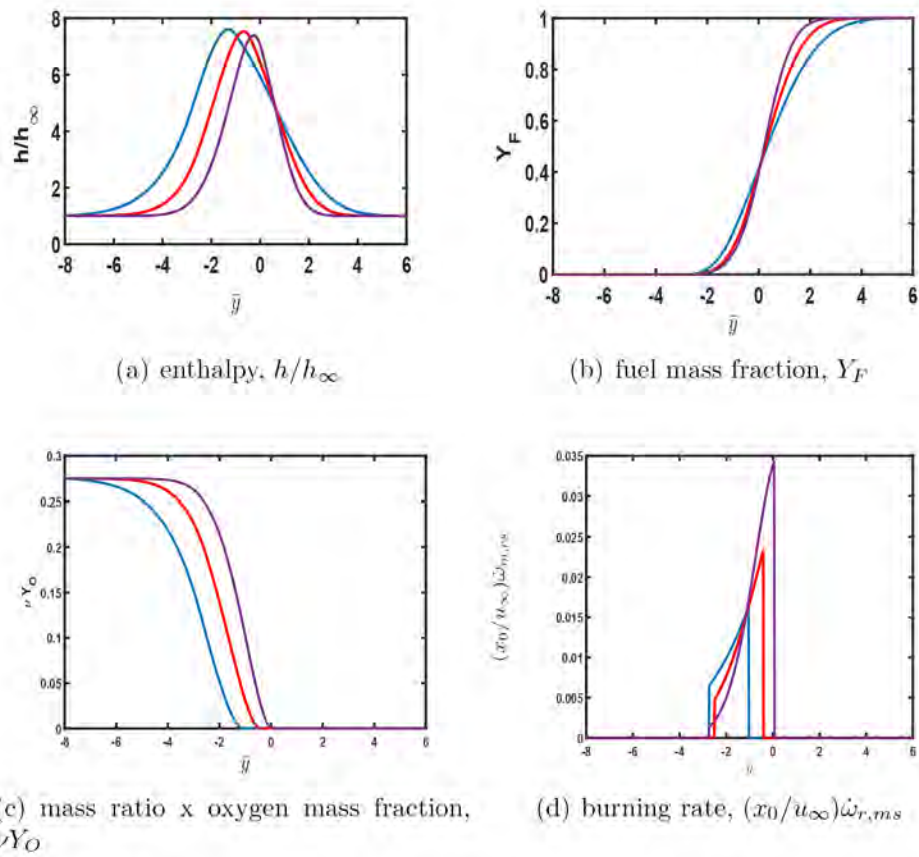


Figure 13: Flow-scale diffusion flame: blue $x = 20$, red $x = 15$, purple $x = 12.5$; fuel in higher-speed stream, oxygen in lower-speed stream.

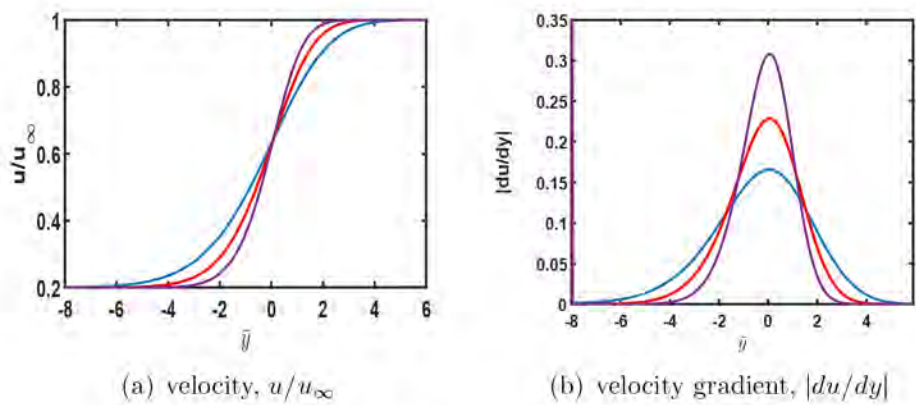


Figure 14: Flow-scale diffusion flame: blue $x = 20$, red $x = 15$, purple $x = 12.5$; fuel in higher-speed stream, oxygen in lower-speed stream.

Figures 15 and 16 give results for a case where the oxygen stream is the faster free stream while the fuel stream is the slower stream. Again, the profiles widen with increasing downstream distance for both velocity and scalar properties. The peak enthalpy and temperature values increase slightly as the locations of the peak value and of the center of the reaction zone shift towards the oxygen-stream side. Note that the burning zone moves towards the oxygen-rich side with increase of the downstream distance whether that stream is the faster or slower stream. This presumably occurs because nearly four times the mass of oxygen (compared to propane mass) is consumed in the reaction.

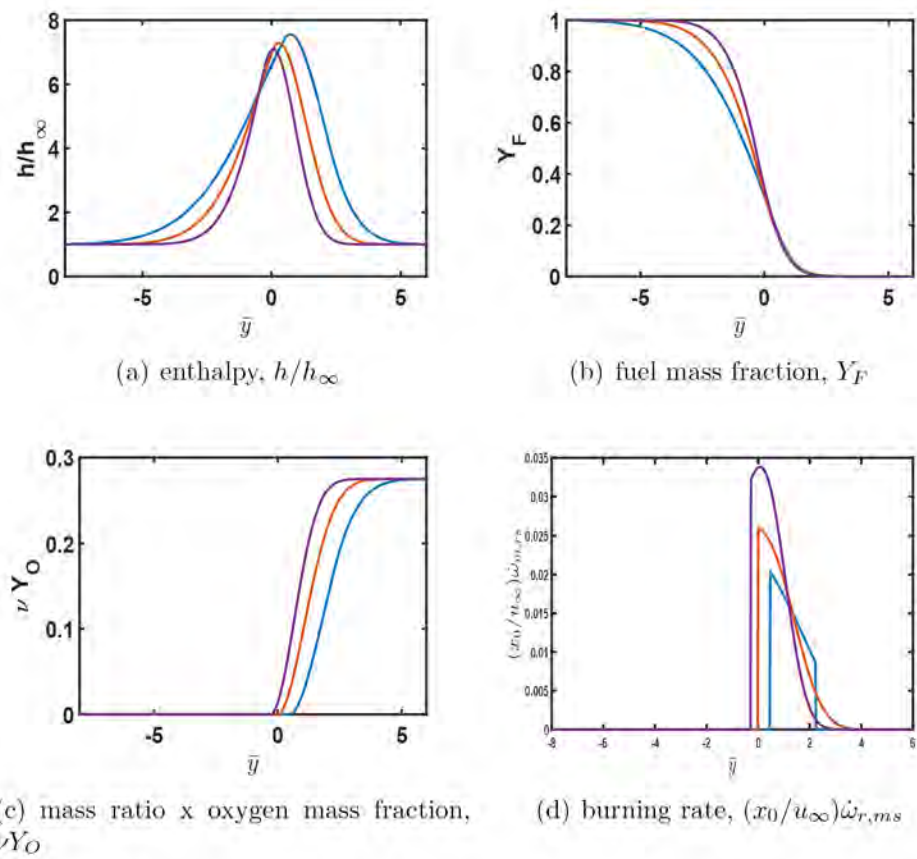


Figure 15: Flow-scale diffusion flame: blue $x = 20$, red $x = 15$, purple $x = 12.5$; oxygen in higher-speed stream, fuel in lower-speed stream.

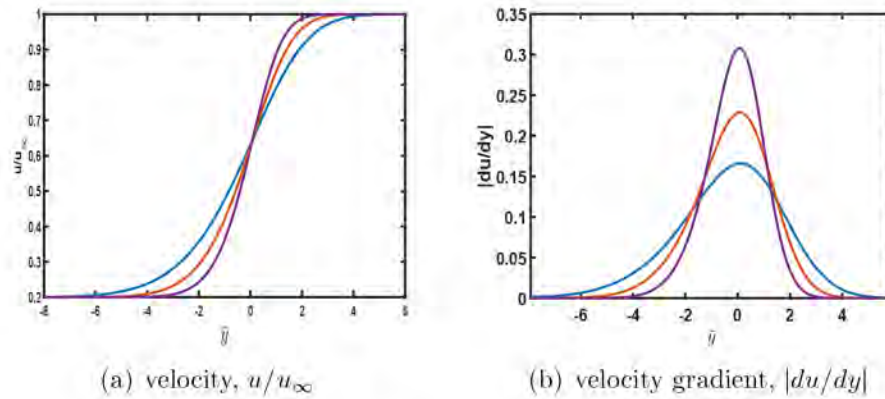


Figure 16: Flow-scale diffusion flame: blue $x = 20$, red $x = 15$, purple $x = 12.5$; oxygen in higher-speed stream, fuel in lower-speed stream.

5 Concluding Remarks

A new flamelet model is developed for use in sub-grid modelling for analysis of turbulent combustion by RANS and LES. This flamelet model presents certain key advances: (i) non-premixed flames, premixed flames, or multi-branched flame structures are allowed to appear naturally without prescription; (ii) the impacts of shear strain and vorticity (and associated centrifugal effects) on the flames are determined; (iii) the applied sub-grid strain rates and vorticity are directly related to the resolved-scale strain rates and vorticity without the use of a contrived progress variable; (iv) the flamelet model is three-dimensional without need for assuming axisymmetry or planar geometry, allowing the physically correct counterflow under the vorticity constraint; and (v) variable density is addressed in the flamelet model. The results indicate that each of these five features introduces consequential, vital physics that is missed by current two-dimensional, irrotational, constant-density flamelet models that assume a priori a nonpremixed- or premixed-flame structure and make no direct connection to shear strain or vorticity on the larger turbulence scales.

Information from direct numerical simulations concerning the relative alignments of the vorticity vector, scalar gradients, and principal strain axes provides a basis for a set of assumptions. The analytical framework allows for multi-step, detailed kinetics although the calculations here are limited

to one-step propane-oxygen kinetics. The quasi-steady assumption used in previous flamelet models is maintained here.

A similar solution is found for the flamelet model. Sample computations of the flamelet model without coupling to the resolved flow are presented first to demonstrate the importance of the new features of the model. The rotation due to vorticity creates a centrifugal force that generally decreases the mass-flux through the flamelet counterflow. Thereby, an increase in residence time and a decrease in burning rate occur. Rotation can thereby allow flames, which would otherwise extinguish, to survive. Premixed flames can only exist with orders-of-magnitude larger values of Da compared to diffusion flamelets or multibranched flames. Thereby, we can expect that premixed flames will be less likely to survive extinction in a turbulent situation with high strain rates. The partially premixed flames in a multibranched flame structure are driven by heat flux from the diffusion flame; thereby, they survive at lower values of Da .

Scaling laws relate sub-grid strain rates and vorticity to resolved-scale quantities for coupling with large-eddy simulations or Reynolds-averaged flows. Given these relations, the burning rate is determined by the rotational-flamelet physics and the energy release rate and rate of change of species mass fraction are given to the resolved scale by the rotational-flamelet algorithms. The theory does not introduce any new contrived variable such as a flamelet progress variable. Connection between the two scales is made using long established variables.

For this initial study, a highly challenging turbulent flow is deliberately avoided. Rather, a simple turbulent flow is resolved with coupling to the rotational-flamelet model in order to explore the interaction across the different scales. A two-dimensional, multicomponent, time-averaged planar shear layer with variable density and energy release uses a mixing-length description for the eddy viscosity and is coupled to the new rotational-flamelet model. The eddy diffusivity is proportional to the local magnitude of the velocity gradient and grows with downstream distance. These simplifying assumptions are only used in this first demonstration of the application of the sub-grid flamelet model. They should not be generalized to be an inherent component of the approach.

The profiles for velocity and scalar properties are seen to broaden with downstream distance in the shear layer, indicating the growing width of that layer. With increasing downstream distance, the zone where burning occurs moves towards the oxygen-rich side (for the chosen propane-oxygen kinetics)

whether or not it is the faster stream. That burning zone becomes more narrow with increasing downstream position.

In the future, multi-step kinetics should be utilized with the rotational-flamelet model. The model can be used to produce look-up tables or neural networks that can be employed with LES or RANS calculations.

There are several important issues that should be addressed in future studies to allow better matching between the closure model for the sub-grid mixing and combustion with the resolved-scale (or time-averaged) flow: (1) the lags, due to the turbulence cascade, in spatial position and time for the coupling between the large-scale strain and the energy release that it affects; (2) the degree of partial mixing of reactants during the cascade; (3) the proper choice of the b parameter to represent the optimal sub-grid volume-size for averaging; and (4) relative magnitudes of the vorticity and normal principal strain rates on the sub-grid scale. These matters can be examined through carefully designed DNS and perhaps clever experiments. Attention is needed to improve our knowledge of the statistical relations between resolved-scale quantities for vorticity, strain rates, and scalar gradients and those quantities on the flamelet scale. Of course, flamelets can in principle exist across a range of the smaller scales, not just the smallest scales. Perhaps more attention is needed for the details of the turbulence cascade; for example, strain-rate self-amplification as well as vortex stretching could be relevant (Johnson, 2021). Also, better determination is needed of the range of scales where mixing and reaction are prominent.

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RESEARCH ARTICLE

Inward Swirling Flamelet Model

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A new rotational flamelet model with inward swirling flow through a stretched vortex tube is developed for sub-grid modeling to be coupled with the resolved flow for turbulent combustion. The model has critical new features compared to existing models. (i) Non-premixed flames, premixed flames, or multi-branched flame structures are determined rather than prescribed. (ii) The effects of vorticity and the related centrifugal acceleration are determined. (iii) The strain rates and vorticity applied at the sub-grid level can be directly determined from the resolved-scale strain rates and vorticity without a contrived progress variable. (iv) The flamelet model is three-dimensional. (v) The effect of variable density is addressed. (vi) The inward swirl is created by vorticity combined with two compressive normal strain components; this feature distinguishes the model from counterflow flamelet models. Solutions to the multicomponent Navier-Stokes equations governing the flamelet model are obtained. By coordinate transformation, a similar solution is found for the model, through a system of ordinary differential equations. Vorticity creates a centrifugal force on the sub-grid counterflow that modifies the molecular transport rates, burning rates, and flammability limits. Sample computations of the inward swirling rotational flamelet model without coupling to the resolved flow are presented to demonstrate the importance of the new features. Premixed, nonpremixed, and multi-branched flame structures are examined. Parameter surveys are made with rate of normal strain, vorticity, Damköhler number, and Prandtl number. The centrifugal effect has interesting consequences when combined with the variable-density field. Flow direction can reverse; burning rates can be modified; flammability limits can be extended.

1. Introduction

Combustion in high mass-flux chambers is the practical and major method for energy conversion for mechanical power and heating. Inherently, the high mass-flow rate leads to turbulent flow. Thereby, many length and time scales appear in the physics making serious challenges for both computational and experimental analyses. For computations where the smallest scales typically cannot be resolved, the method of large-eddy simulations (LES) is employed wherein the smaller scales are filtered via integration over a window size commensurate with the computational mesh size that allows affordable computations. Consequently, the essential, rate-controlling, physical and chemical processes that occur on shorter scales than the filter size must be modelled. Those sub-grid models must be properly coupled to the resolved LES flow field.

Current flamelet models that are used for LES or Reynolds-averaged Navier-Stokes (RANS) methods have some advantages. Typically, the flamelet equations are a system of ordinary differential equations (ODEs) that can be solved offline with solutions available in tabular form or through neural networks (NN). The flamelet models can handle multi-species, multi-step oxidation kinetics without requiring small time steps during the solution of the resolved-scale fluid dynamics. Thus, for several reasons, savings of computational resources can be huge compared to direct numerical simulation. We aim here to retain these very attractive features while removing some less desirable features. Already, some progress has been made

in extending the fundamental flamelet theory beyond its long-term limitation of a single-flame structure, two-dimensional (or axisymmetric) configuration, and use of the uniform-density assumption. However, those advances still must be applied to LES or RANS. In addition, the flamelet theory must be advanced to consider shear strain and vorticity at the small scale of the flamelet; these are the vital forgotten physics in current flamelet modelling. Furthermore, the strain rates in the flamelet model are far from properly connected to the strain rates at the resolved scale. Attempts at corrections of some of these weaknesses are made here.

The goals in this paper are to improve the flamelet model by including several important physical effects that are commonly neglected in present models and to identify other issues, related to the coupling between the sub-grid-scale physics and the resolved-scale (or time-averaged) physics, that require further study.

1.1 Existing Flamelet Theory

The laminar mixing and combustion that commonly occur within the smallest turbulent eddies is important in determining the performance for many power and propulsion applications. These laminar flamelet sub-domains experience significant strain of all types, shear, tensile, and compressive. Some important works exist here but typically for either counterflows with only normal strain or simple vortex structures in planar or axisymmetric geometry and often with a constant-density approximation. See Linan [1], Williams [2], Marble [3], Karagozian and Marble [4]), Cetegen and Sirignano [5, 6], Peters [7], and Pierce and Moin [8]. An interesting review of the early flamelet theory is given by Williams [9]. Williams [2] first established the concept of laminar flamelets in the turbulent diffusion flame structure. Flamelet studies have focused on either premixed or nonpremixed flames; a unifying approach to premixed, nonpremixed, and multi-branched flames has not been developed until the recent counterflow-based rotational flamelet study by Sirignano [10]. Here, we attempt a unification for the vortex-tube-based flamelet.

Most flamelet studies have not directly considered vorticity interaction with the flamelet [1, 7–9]. Williams [2] first recognized the advantage of separating rotation (due to vorticity) and stretching by transformation to a rotating, non-Newtonian reference frame. However, the momentum consequences in the new reference frame were not examined. Some other works that have examined vortex-flame interaction have not separated the effects of stretching and rotation [3, 5, 6, 11]. Karagozian and Marble [4] examined a three-dimensional flow with radial inward velocity, axial jetting, and a vortex centered on the axis. The flame sheet wrapped around the axis due to the vorticity; an incompressible-flow velocity field was used with an ad hoc adjustment for the variable density effect.

Our interest on practical, high-mass-flux turbulent combustors leads to a focus on situations with a wide range of length and time scales where shearing, reactant mixing, and exothermic reaction occur together. So, we avoid detailed mention here of many interesting areas of turbulent-combustion literature, e.g, corrugated (i.e., wrinkled) premixed, laminar flames.

The two-dimensional planar or axisymmetric counterflow configuration is generally a foundation for a flamelet model. Local conversion to a coordinate system based on the principal strain-rate directions can provide the counterflow configuration in a general flow. Furthermore, the quasi-steady counterflow can be analyzed by ordinary differential equations because the dependence on the transverse coordinate is either constant or linear, depending on the variable. Pierce and Moin [8] modified the nonpremixed-flamelet counterflow configuration by fixing domain size and forcing flux to zero at the boundaries. Flamelet theory as a closure model

for turbulent combustion is typically based on the tracking of two variables: a normalized conserved scalar and the strain rate; the latter is generally given indirectly through a progress variable. Mixture fraction is traditionally used for the conserved scalar. The flamelet model for LES developed by Pierce and Moin [8] was a substantial advancement through the introduction of the flamelet progress variable (FPV). Their approach has also been used widely, e.g., [12], [13–15]. Some [12, 16, 17] introduced the use of neural networks in place of the look-up table. Mueller [18] presented the flamelet model in a somewhat different mathematical framework but without the addition of new physical description.

There are concerns about incompleteness and contradiction in the above models. (i) The models are designed specifically for non-premixed flames or premixed flames. The flame structure should be determined rather than prescribed. Multi-branched flames should be allowed. (ii) The effects of vorticity are commonly neglected with a very few exceptions identified above. Yet, the models are applied to turbulent flows where the strain rates and vorticity magnitudes are known to be larger at the small scales than at the large scales. (iii) The above flamelet models are two-dimensional or axisymmetric although key three-dimensional behavior can be shown to exist. (iv) The effect of variable density is not thoroughly addressed. (v) Clear connections are not given between the strain rates and vorticity at the flamelet level and those variables at the resolved scale of the combustor. Sirignano [10] has addressed the incompleteness and contradiction for counterflow flamelets with the presentation of a rotational flamelet closure model. Here, we attempt to follow with consideration of flamelets in vortex tubes.

1.2 Stretched Vortex with Inward Swirl

In one part of their paper, Karagozian and Marble [4] treated a flame within a stretched vortex tube with an inward swirling flow. Their incompressible velocity field was defined by Burgers [19] and Rott [20] and is commonly known as Burgers vortex. In particular, with u_r , u_z , and u_θ as the velocity components in cylindrical coordinates and parameter a and kinematic viscosity ν taken as constants, we have

$$\begin{aligned} u_r &= ar \quad ; \quad u_z = 2az \\ u_\theta &= \frac{\Gamma}{4\pi r} \left[1 - \exp\left(-\frac{ar^2}{2\nu}\right) \right] \end{aligned} \quad (1)$$

where Γ is the circulation taken through the far field surrounding the vortex tube. Note that $u_\theta \rightarrow \Gamma/(2\pi r)$ as $r \rightarrow \infty$, yielding potential flow for the far field. This description gives an exact steady-state solution to the incompressible Navier-stokes equations. Although the tube is being stretched in the z direction, diffusion of momentum and vorticity in the r direction allows a balance with radial advection that results in a steady solution.

Karagozian and Marble [4] made an ad hoc adjustment to correct for expansion by variable density; however, by not accounting for spatial variation of density, the effect of centrifugal acceleration was not considered. They also focused on diffusion flames. Here, a stretched vortex will be considered but with full account of variable density and allowance for a premixed flame, multibranched flame, or diffusion flame as determined by the boundary conditions. We will not use the incompressible Burgers vortex velocity field; however, it does provide useful guidance. In particular, note that for small r values, the Burgers vortex gives wheel motion for the fluid, i.e., $u_\theta \approx (\Gamma ar)/(4\pi\nu)$.

1.3 *Relative Orientations of Principal Strain Axes, Vorticity, and Scalar Gradients*

Both normal strain rate and shear strain rate are imposed on the flamelet and are important. Shear strain can, in general, be decomposed into a normal strain and a rotation (whose rate is half of the vorticity magnitude). The magnitudes of strain rate and vorticity increase as the eddy size decreases in the turbulence energy cascade. The strain and rotation become especially important on the smallest scales of turbulence where mixing and chemical reaction occur. The smallest (i.e., Kolmogorov) scale size is determined by the dissipation rate of turbulence kinetic energy. The final molecular mixing and chemical reaction occur on this smaller scale, where there will be an axis (or direction) of principal compressive normal strain and an orthogonal axis for principal tensile strain, the third orthogonal axis could be either tensile or compressive. These axes rotate due to vorticity. Thereby, the direction of the scalar gradient rotates. A useful flamelet model must have a statistically accurate representation of the relative orientations on this smallest scale of the vorticity vector, scalar gradients, and the directions of the three principal axes for strain rate. Several studies exist that are helpful in understanding this important alignment issue.

Generally (and always for incompressible flow), one principal strain rate γ locally will be compressive (corresponding to inflow in a counterflow configuration), another principal strain rate α will be tensile (also named extensional and corresponding to outflow), and the third can be either extensional or compressive and will have an intermediate strain rate β of lower magnitude than the other like strain rate. Specifically, $\alpha > \beta > \gamma$, $\alpha > 0$, $\gamma < 0$, and, for incompressible flow, $\alpha + \beta + \gamma = 0$. If the intermediate strain rate $\beta < 0$, there is inflow from two directions with outflow in one direction; a contracting jet flow occurs locally. Conversely, with $\beta > 0$, there is outflow in two directions and inflow in one direction; a counterflow or, in other words, the head-on collision of two opposed jets occurs.

Several interesting findings result from direct numerical simulations (DNS) for incompressible flows. Both Ashurst et al. [21] and Nomura and Elghobashi [22] compared a case of homogeneous sheared turbulence with a case of isotropic turbulence. They report that the vorticity alignment with the intermediate strain direction is most probable in both cases but especially in the case with shear. Furthermore, the intermediate strain rate is most likely to be extensive (positive) implying a counterflow configuration.

Nomura and Elghobashi [23] studied reacting flow and show that in regions of exothermic reaction and variable density, alignment of the vorticity with the most tensile strain direction can occur. Still though as the strain rates increase, the intermediate direction becomes more favored for alignment with vorticity; that direction is also preferred in regions where mixing occurs without substantial divergence of the velocity due to chemical reaction.

A material interface most probably aligns to be normal to the direction of the compressive normal strain. That is, the scalar gradient and the direction of compressive strain are aligned [21–25]. Authors agree that the most common intermittent vortex structures in regions of high strain rate are sheets or ribbons rather than tubes. Nevertheless, the agreement is that vortex tubes can exist in a combustor and can be relevant.

Based on those understandings concerning vector orientations, Sirignano [26] extended flamelet theory in a second significant aspect beyond the inclusion of both premixed and non-premixed flame structures; namely, a model was created of a three-dimensional field with both shear and normal strains. The three-dimensional problem is reduced to a two-dimensional form and then, for the counterflow or

mixing-layer flow, to a one-dimensional similar form. The system of ordinary differential equations (ODEs) is presented for the thermo-chemical variables and the velocity components. Conserved scalars are determined and can become the independent variable if they behave in a monotonic fashion. These new findings are very helpful in improving the foundations for flamelet theory and its use in sub-grid modeling for turbulent combustion.

Based on the observations of the needed improvements, Sirignano [10] has developed a rotational flamelet model based on a counterflow with rotation. The model (i) determines rather than prescribes the existence of non-premixed flames, premixed flames, or multi-branched flame structures; (ii) determines directly the effect of shear strain and vorticity on the flames; (iii) applies directly the resolved-scale strain rates and vorticity to the sub-grid level without the use of a contrived progress variable; (iv) employs a three-dimensional flamelet model; (v) considers the effect of variable density. The analysis uses one-step kinetics to avoid complications in this initial study; however, a clear template will exist for the employment of multi-step kinetics. The goal with the new inward-swirl flamelet model presented here is to extend the rotational flamelet concept to a vortex-tube configuration with inward spiralling flow rather than the traditional counterflow. Elements of the counterflow character will remain because fluid of differing compositions will be strained to move towards each other enhancing transport and reaction.

Section 2 presents the analysis supporting a new sub-grid flame model that better addresses effects of rotation, variable density, three-dimensional character, and multibranched flame structure for the stretched vortex tube. Computational results are discussed in Section 2. Results and the related discussion are presented in Section 3. Concluding comments are made in Section 4.

2. Sub-grid Flamelet Analysis

The problem is stated here in a quasi-steady, three-dimensional form where variable density is allowed. These assumed orientations are consistent with the statistical findings of [23]. The direction of major compressive principal strain aligns with the scalar gradient and is orthogonal to the vorticity vector direction; an extensional principal strain direction is aligned with the vorticity. The stretched vortex character is created by imposing compressive normal strain in both coordinate direction that are orthogonal to the vorticity vector. Thus, we have a stretched vortex tube that qualitatively relates to the incompressible-flow configurations of [19], [20], and [4].

2.1 Coordinate Transformation

In Figure 1, the Newtonian frame is transformed to a rotating, non-Newtonian frame where the curl of the velocity is zero. The vorticity aligns with the z' direction. ω_κ is the vorticity magnitude on this sub-grid (Kolmogorov) scale. x, y, z are transformed to ξ, χ, z wherein the material rotation is removed from the ξ, χ plane by having it rotate at angular velocity $d\theta/dt = \omega_\kappa/2$ relative to x, y . Here, θ is the angle between the x and ξ axes and simultaneously the angle between the y and χ axes. The sub-grid domain is sufficiently small to consider a uniform value of ω across it, consistent with the truncated Taylor series expansion used elsewhere in the flamelet analysis. The scalar gradients align with the major principal axis for compressive strain. In many of our calculations, the two compressive normal strains will have equal magnitude; so, the choice of the normal strain direction

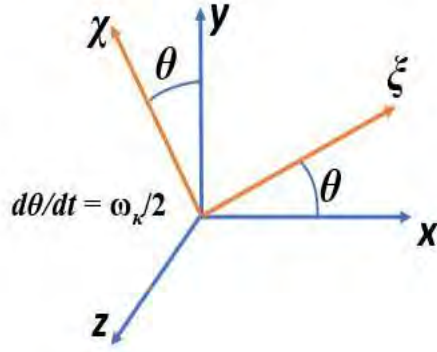


Figure 1.: Transformation to ξ, χ, z' rotating coordinate system from x', y', z' Newtonian system. θ increases in the counterclockwise direction.

which aligns with the scalar gradient is arbitrary. The scalar gradient is always aligned with the χ direction in the analysis here.

Thereby,

$$\begin{aligned}
 \xi &= x \cos\theta + y \sin\theta ; \quad \chi = y \cos\theta - x \sin\theta \\
 \frac{\partial \xi}{\partial x} &= \cos\theta ; \quad \frac{\partial \xi}{\partial y} = \sin\theta ; \quad \frac{\partial \chi}{\partial x} = -\sin\theta ; \quad \frac{\partial \chi}{\partial y} = \cos\theta \\
 u_\xi &= u \cos\theta + v \sin\theta + \chi \frac{\omega_\kappa}{2} ; \quad u_\chi = v \cos\theta - u \sin\theta - \xi \frac{\omega_\kappa}{2} \\
 \frac{\partial u}{\partial x} &= \frac{\partial u}{\partial \xi} \cos\theta - \frac{\partial u}{\partial \chi} \sin\theta ; \quad \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi} \sin\theta + \frac{\partial u}{\partial \chi} \cos\theta \\
 \frac{\partial v}{\partial x} &= \frac{\partial v}{\partial \xi} \cos\theta - \frac{\partial v}{\partial \chi} \sin\theta ; \quad \frac{\partial v}{\partial y} = \frac{\partial v}{\partial \xi} \sin\theta + \frac{\partial v}{\partial \chi} \cos\theta
 \end{aligned} \tag{2}$$

Since

$$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = \omega_\kappa \tag{3}$$

it follows that

$$\frac{\partial u_\chi}{\partial \xi} - \frac{\partial u_\xi}{\partial \chi} = 0 \tag{4}$$

Thus, the rotating frame of reference does not have vorticity appearing explicitly. However, the frame is not Newtonian and a reversed (centrifugal) force is imposed. The expansions due to energy release produce new vorticity but it will integrate to zero globally; the flow will be antisymmetric and have zero circulation in the new reference frame.

In the new reference frame, the normal rates of strain, imposed in the far field, in the ξ, χ , and z directions are $S_1, -(S_1 + S_2)$, and S_2 , respectively. Sirignano [10], for the rotational flamelet with counterflow, considered both S_1 and S_2 to be positive. Here, with the inward swirl flamelet, $S_1 < 0$, $S_2 > 0$, and $S_1 + S_2 > 0$. In

the next sub-section, these strain rates will be non-dimensionalized.

2.2 Governing Equations

Quasi-steady behavior is considered. The governing equations for steady 3D flow in the non-Newtonian frame can be written with $u_i = u_\xi, u_\chi, w$; $x_i = \xi, \chi, z$. The centrifugal acceleration $a_i = \xi\omega_\kappa^2/4, \chi\omega_\kappa^2/4, 0$. The quantities $p, \rho, h, h_m, Y_m, \dot{\omega}, \mu, \lambda, D$, and c_p are pressure, density, specific enthalpy, heat of formation of species m , mass fraction of species m , chemical reaction rate of species m , dynamic viscosity, thermal conductivity, mass diffusivity, and specific heat, respectively. Furthermore, the Newtonian viscous stress tensor with the Stokes hypothesis is considered. The boundary-layer approximation is not needed and the Navier-Stokes equations for a multicomponent field will be solved. The system is described as

$$\frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (5)$$

$$\rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] \right) + \rho a_i \quad (6)$$

$$\begin{aligned} \rho u_j \frac{\partial h}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D (1 - Le) \sum_{m=1}^N h_m \frac{\partial Y_m}{\partial x_j} \right) \\ - \rho \sum_{m=1}^N h_{f,m} \dot{\omega}_m \end{aligned} \quad (7)$$

$$\rho u_j \frac{\partial Y_m}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_m}{\partial x_j} \right) + \rho \dot{\omega}_m ; \quad m = 1, 2, \dots, N \quad (8)$$

The viscous dissipation, the energy source term $\rho u_j a_j = \rho(\omega_\kappa/2)^2(\xi u_\xi + \chi u_\chi)$ in the new reference frame, and other terms of the order of the kinetic energy per mass have been neglected.

Here, we define the non-dimensional Prandtl, Schmidt, and Lewis numbers: $Pr \equiv c_p \mu / \lambda$; $Sc \equiv \mu / (\rho D)$; and $Le \equiv Sc / Pr$. These numbers will be assumed to be constants. Furthermore, $Pr = Sc$ (i.e., $Le = 1$).

The non-dimensional forms of the above equations remain identical to the above forms if we choose certain reference values for normalization. In the remainder of this article, the non-dimensional forms of the above equations will be considered. The superscript $*$ is used here to designate a dimensional property. The variables $u_i^*, t^*, x_i^*, \rho^*, h^*, p^*$, and $\dot{\omega}_m^*$, and properties $\mu^*, \lambda^*/c_p^*$, and D^* are normalized respectively by $[(S_1^* + S_2^*)\mu_\infty^*/\rho_\infty^*]^{1/2}, (S_1^* + S_2^*)^{-1}, [\mu_\infty^*/(\rho_\infty^*(S_1^* + S_2^*))]^{1/2}, \rho_\infty^*, (S_1^* + S_2^*)\mu_\infty^*/\rho_\infty^*, (S_1^* + S_2^*)\mu_\infty^*, (S_1^* + S_2^*), \mu_\infty^*, \mu_\infty^*$, and $\mu_\infty^*/\rho_\infty^*$. The dimensional strain rates S_1^* and S_2^* and vorticity ω_κ^* are normalized by $S_1^* + S_2^*$. The reference values for strain rates and far-stream variables and properties used for normalization will be constants. The reference length $[\mu_\infty^*/(\rho_\infty^*(S_1^* + S_2^*))]^{1/2}$ is the estimate for the magnitude of the viscous-layer thickness. In the following flamelet analysis, the vorticity ω_κ and the velocity derivatives $\partial u_i / \partial x_j$ are non-dimensional quantities; their dimensional values can be obtained through multiplication by $S_1^* + S_2^*$. Now, $S_1 + S_2 = 1$.

In the rotating reference frame, two different gaseous mixtures exist the far field, one for large positive values of χ and another for large negative values of χ . They both advect and diffuse towards each other. For the study of a diffusion (non-premixed) flame, one mixture is fuel and the other is an oxidizer. With a premixed flame, one far field has a combustible mixture of fuel and oxidizer while the other has a hot inert gas (e.g., combustion products). In another case where multiple flame branches may occur, both streams can be combustible; one can be fuel rich while the other is fuel lean.

2.3 Similar Form for the Equations

The stagnation point is taken as the origin $\xi = \chi = z = 0$. Along the line $\xi = z = 0$ normal to the interface, we can expect the first derivatives of u_χ, ρ, h, T , and Y_m with respect to either ξ or z to be zero-valued. The velocity components u_ξ and w will be odd functions of ξ and z , respectively, going through zero and changing sign at that line. v also changes sign, going through zero at the origin; however, generally the reaction zone will be offset and an odd function does not result for v . Upon neglect of terms of $O(\xi^2)$ and $O(z^2)$, the variables u_χ, ρ, h, T , and Y_m can be considered to be functions only of t and χ . The density-weighted Illingworth transformation [27] of χ replaces χ with $\eta \equiv \int_0^\chi \rho(\chi') d\chi'$. Neglect of the same order of terms implies that $u_\xi = S_1 \xi (df_1/d\eta)$ and $w = S_2 z (df_2/d\eta)$. Note u_ξ is independent of z and w is independent of ξ . At the edge of the viscous layer at large positive η , $df_1/d\eta \rightarrow 1$, $df_2/d\eta \rightarrow 1$, $f_1 \rightarrow \eta$, and $f_2 \rightarrow \eta$. Ordinary differential equations are created here through the variable η and the convenient notation is used so that $(\cdot)' \equiv d(\cdot)/d\eta$.

In the non-dimensional form given by Equations (5) through (8), the dimensional strain rates S_1^* and S_2^* are each normalized by the dimensional sum $S^* = S_1^* + S_2^*$. If the far field has uniform density, S^* is the magnitude of the major compressive normal strain. Thus, the non-dimensional relation is $S_2 = 1 - S_1$ and only one independent non-dimensional strain-rate parameter is needed. Two strain rates are presented above and in the following analysis with the understanding that one depends on the other such that $S_1 + S_2 = 1$. $S_1 + S_2$ will be explicitly stated in our analysis without substitution of the unity value in order to emphasize the summation which is consequential in the dimensional formulation. This choice clarifies whether a particular term when converted to a dimensional form depends on S_1^*, S_2^* , or the sum of the two strain rates.

The analysis follows closely the method of [10]. Here, that method is presented in a summary fashion since details are readily available. For the steady state, the continuity equation (5) is integrated to give

$$\rho u_\chi = -S_1 f_1(\eta) - S_2 f_2(\eta) \quad (9)$$

and then

$$u'_\chi = \frac{S_1 f_1(\eta) + S_2 f_2(\eta)}{\rho^2} \rho' - \frac{S_1 f'_1(\eta) + S_2 f'_2(\eta)}{\rho} \quad (10)$$

Thus, the incoming inviscid flow outside the boundary layer is described by $u_\chi = -(S_1 + S_2)\eta$ for positive η and $u_\chi = -(S_1 + S_2)\eta/\rho_{-\infty}$ for negative η .

At $\eta = \infty$, $f'_1 = f'_2 = 1$ and $f''_1 = f''_2 = f'''_1 = f'''_2 = 0$ which allows the two constants to be determined. A perfect gas with $\rho\mu = 1$ is assumed. The perfect gas law and the assumption of constant specific heat c_p will give the relation that

$1/\rho = h$. Specifically, we obtain

$$\begin{aligned} f_1''' + f f_1'' + S_1[h - (f_1')^2] + \frac{\omega_\kappa^2}{4S_1}(1 - h) &= 0 \\ f_2''' + f f_2'' + S_2[h - (f_2')^2] &= 0 \end{aligned} \quad (11)$$

The boundary conditions use the assumption that two velocity components asymptote to the constant values $u_\xi(\infty)$, $u_\xi(-\infty)$, $w(\infty)$, and $w(-\infty)$ at large magnitudes of η . The stream function bounding the two incoming streams is arbitrarily given a zero value and placed at $\eta = 0$.

$$\begin{aligned} f_1'(\infty) = 1 \ ; \ f_1'(-\infty) &= \sqrt{h_{-\infty} + \left(\frac{\omega_\kappa}{2S_1}\right)^2(1 - h_{-\infty})} \ ; \ f_1(0) = 0 \ ; \\ f_2'(\infty) = 1 \ ; \ f_2'(-\infty) &= \sqrt{h_{-\infty}} \ ; \ f_2(0) = 0 \end{aligned} \quad (12)$$

When density varies through the flow because of heating or variation of composition, u_ξ and w vary with χ , thereby creating a shear stress and vorticity albeit that the frame transformation removed vorticity and shear from the incoming flow.

The dependence of u_χ on $f \equiv S_1 f_1 + S_2 f_2$ is shown by Equation (9). Thus, the function f will be important in determining both the field for u_χ and the scalar fields.

Consequently, f as well as f_1 and f_2 depend on both S_1 and S_2 , not merely on $S_1 + S_2$. That is, the particular distribution of the normal strain rate between the two transverse direction matters. f and f_1 also depend directly on ω_κ (unless $S_1 = 0$). f_2 depends on ω_κ indirectly through its coupling with f_1 .

Here, an exact solution of the variable-density Navier-Stokes equation is obtained subject to determination of h through solutions of the energy and species equations as discussed below. Thus, the solution here is the natural solution, subject to neglect of terms of $O(\xi^2)$ and $O(z^2)$.

The similar form of the scalar equations becomes

$$\begin{aligned} Y_m'' + Pr f Y_m' &= -Pr \dot{\omega}_m \ ; \ m = 1, 2, \dots, N \\ h'' + Pr f h' + (Pr - Sc) \sum_{m=1}^N h_m Y_m'' &= Pr \sum_{m=1}^N h_{f,m} \dot{\omega}_m \end{aligned} \quad (13)$$

The boundary conditions are

$$\begin{aligned} h(\infty) = 1 \ ; \ h(-\infty) &= \frac{1}{\rho_{-\infty}} \ ; \\ Y_m(\infty) = Y_{m,\infty} \ ; \ Y_m(-\infty) &= Y_{m,-\infty} \ ; \end{aligned} \quad (14)$$

Equations (13) indicate a dependence of the heat and mass transport on $f \equiv S_1 f_1 + S_2 f_2$. Manipulation of the first two equations of (13) leads to an ODE for f with $S_1 S_2$ and $S_1 S_2 f_1' f_2'$ as parameters, clearly indicating that generally f will have a dependence on $S_1 S_2$. Thus, the behavior for the counterflow can vary from the planar value of $S_1 = 1, S_2 = 0$ (or vice versa) or from the case $S_1 = S_2 = 1/2$. This clearly shows that distinctions must be made amongst the various possibilities for three-dimensional strain fields as $S_1 S_2$ varies between large negative numbers and $1/4$. An exception is the incompressible case with constant properties where

the $S_1 S_2$ terms cancel in the equation for f .

The vorticity ω_κ impacts directly f_1 and f ; thereby, it is affecting the velocity field. Then, through the advection of the scalar properties, there is impact on mass fractions and enthalpy. If the vorticity $\omega_\kappa = 0$, a simple inspection of the governing ODEs leads to the conclusion that the values for $f_1, f'_1, f_2, f'_2, u/x$, and w/z can be interchanged with the values for $f_2, f'_2, f_1, f'_1, w/z$, and u/x , respectively, when S_1 and S_2 are replaced by $1 - S_1$ and $1 - S_2$, respectively.

The analysis is formulated in identical fashion to the approach of [10]. However, there, with two directions for extensional strain rate in the rotating frame of reference, both S_1 and S_2 are positive numbers. However, in the computations here, we consider the vortex tube with inward swirl so that, in the far field, there are two directions of compressive strain and only one direction of extensional strain. That extensional strain is aligned with the vorticity vector. Thus, here, $S_1 \leq 0$ and $S_2 \geq 1$. The basic case takes the two compressive strain rates to be equal; thereby, $S_1 = -1.0$ and $S_2 = 2.0$.

Consider the production or consumption rate of a particular species over the counterflow volume. We can either integrate over a volume using the original form in Equation (8) or, more conveniently, using Equation (13) to get exactly the same result. Consider the volume $-a < \xi < a, -b < y < b, -c < z < c$. The choices of lengths a and c do not matter on a per-unit-volume basis since mass fraction Y_m and reaction rate $\dot{\omega}_m$ do not vary with x or z . c is chosen to be of the order of the Kolmogorov scale. Volume $V = 8abc$ and $\widetilde{\rho\dot{\omega}_m}$ is the average mass production rate over the volume. From integration of the Equations (13) after multiplication by density ρ and division by PrV ,

$$\begin{aligned} \int_{-a}^a \int_{-b}^b \int_{-c}^c \frac{\rho}{PrV} [Y_m'' + Pr f Y_m' + Pr \dot{\omega}_m] dx dy dz &= 0 \quad ; \quad m = 1, 2, \dots, N \\ \widetilde{\rho\dot{\omega}_m} &\equiv \frac{1}{V} \int_V \rho \dot{\omega}_m dV = -\frac{1}{2b} \int_{\eta(-b)}^{\eta(b)} f Y_m' d\eta \quad ; \quad m = 1, 2, \dots, N \\ \int_{-a}^a \int_{-b}^b \int_{-c}^c \frac{\rho}{PrV} [h'' + Pr f h' - Pr \sum_{m=1}^N h_{f,m} \dot{\omega}_m] dx dy dz &= 0 \\ \sum_{m=1}^N h_{f,m} \widetilde{\rho\dot{\omega}_m} &= \frac{1}{2b} \int_{\eta(-b)}^{\eta(b)} f h' d\eta \end{aligned} \quad (15)$$

Here, b is considered large enough so that $Y_m' = 0$ and $h' = 0$ at those boundaries are good approximations. However, the value for $\widetilde{\rho\dot{\omega}_m}$ depends strongly on the chosen domain size $2b$, which has a value of $O(10)$ typically in our analysis.

Consider a species m that is flowing inward away from $\eta = \infty$ towards $\eta = 0$. If it is being produced (consumed), the derivative Y_m' in Equation (15) will be negative (positive) for $\eta > 0$ where velocity $v < 0$ and $f > 0$. The signs are opposite for a species flowing inward away from $\eta = -\infty$ and towards $\eta = 0$. The equation provides two ways to evaluate the average production (consumption) rate for species m . The volume integral of the reaction rate has highly nonuniform integrand values over the space while the outflow integral over η has a smoother variation of the integrand.

2.4 Chemical Kinetics Model

The above analysis applies for both diffusion-flame and partially-premixed-flame configurations. Multi-branched flames can also be described. While the analysis

allows for the use of detailed chemical kinetics, we focus here on propane-oxygen flows with one-step kinetics. Westbrook-Dryer [28] kinetics are used; they were developed for premixed flames but any error for nonpremixed flames is often viewed as tolerable here because diffusion generally is rate-controlling. Using asterisks to denote dimensional quantities,

$$\dot{\omega}_F^* = -A^* \rho^{*0.75} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}} \quad (16)$$

where the ambient temperature is set at 300 K and density ρ^* is to be given in units of kilograms per cubic meter. $A^* = 4.79 \times 10^8 (kg/m^3)^{-0.75}/s$. The dimensional strain rate $S_1^* + S_2^*$ (at the sub-grid scale) is used to normalize time and reaction rate. In non-dimensional terms,

$$\begin{aligned} \dot{\omega}_F &= -\frac{A^* \rho_\infty^{*0.75}}{S_1^* + S_2^*} \tilde{h}^{-0.75} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}} \\ \dot{\omega}_F &= -\frac{Da}{\tilde{h}^{0.75}} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}} \end{aligned} \quad (17)$$

The equation defines the Damköhler number Da . We define K so that $Da \equiv K Da_{ref}$ where

$$Da_{ref} \equiv \frac{\tilde{A}(10kg/m^3)^{0.75}}{(10^4/s)} = 2.693 \times 10^5 ; \quad K \equiv \left[\frac{\rho_\infty^*}{10kg/m^3} \right]^{0.75} \frac{10^4/s}{S_1^* + S_2^*} \quad (18)$$

$10 kg/m^3$ and $10,000/s$ are conveniently chosen as reference values for density and strain rate, respectively.

It is not necessary to set pressure (or its proxy, density) and the strain rate separately for a one-step reaction. For propane and oxygen, the mass stoichiometric ratio $\nu = 0.275$. The non-dimensional parameter K will increase (decrease) as the strain rate decreases (increases) and/ or the pressure increases (decreases). $K = 1$ is our reference case. The value of K will be varied as needed to address the variations in strain rate and pressure that affect premixed flamelets, diffusion flamelets, and multi-branched flamelets.

3. Computational Results and Discussion

The ordinary differential equations are solved numerically using a relaxation method with a pseudo-time variable and central differences. The parameters that are varied are K, Pr, ω_κ and S_1 (and thereby $S_2 = 1 - S_1$). Here, calculations have $Sc = Pr = 1$ with emphasis on the effect of variation in K , i.e., pressure and strain rate.

Here, the effects of vorticity on three types of oxygen-propane flame structure will be examined. In Subsection 3.1, a diffusion flame near its flammability is considered. The premixed flame is discussed in Subsection 3.2 while the multi-branched flame calculations are shown in Subsection 3.3. The basic calculations pertain to the inward swirling flow with $Pr = Sc = 1$ and equal compressive strain rate in the far field from two directions in the rotating frame of reference, i.e., $S_1 = -1.0$ and $S_2 = 2.0$. Note that the same code for these calculations was used by [10] where both S_1 and S_2 were positive. Values for $K = Da/Da_{ref}$ and thereby for the Damköhler number Da are deliberately chosen in the vicinity of the flammability limit where vorticity and its centrifugal effect can have a significant role. In addition

to boundary values at $\eta = \infty$ and $\eta = -\infty$, the system of equations has four independent, non-dimensional parameters as inputs: ω_κ , $S_1 = 1 - S_2$, $Pr = Sc$, and $Da = KDa_{ref}$.

3.1 Diffusion Flamelet Calculations

First, we treat a situation with a three-dimensional diffusion-flame structure. Figures 2 and 3 show the influence of vorticity on the flamelet stability near the extinction limit. The rotation of the flamelet due to vorticity causes a centrifugal effect on the counterflow velocity and thereby on the residence time in the vicinity of the reaction zone. $K = 0.275$ with values of $\omega_\kappa = 0, 0.5$, and 1.0 are examined and reported here.

Figure 2 shows that, without rotation and also with $\omega_\kappa = 0.5$, there is negligible reaction rate and heat release, essentially yielding extinction. Fuel and oxidizer just diffuse and mix without significant exothermic reaction. Further increase of the rotational rate with $\omega_\kappa = 1.0$, however, yields a strong flame with a narrow reaction zone.

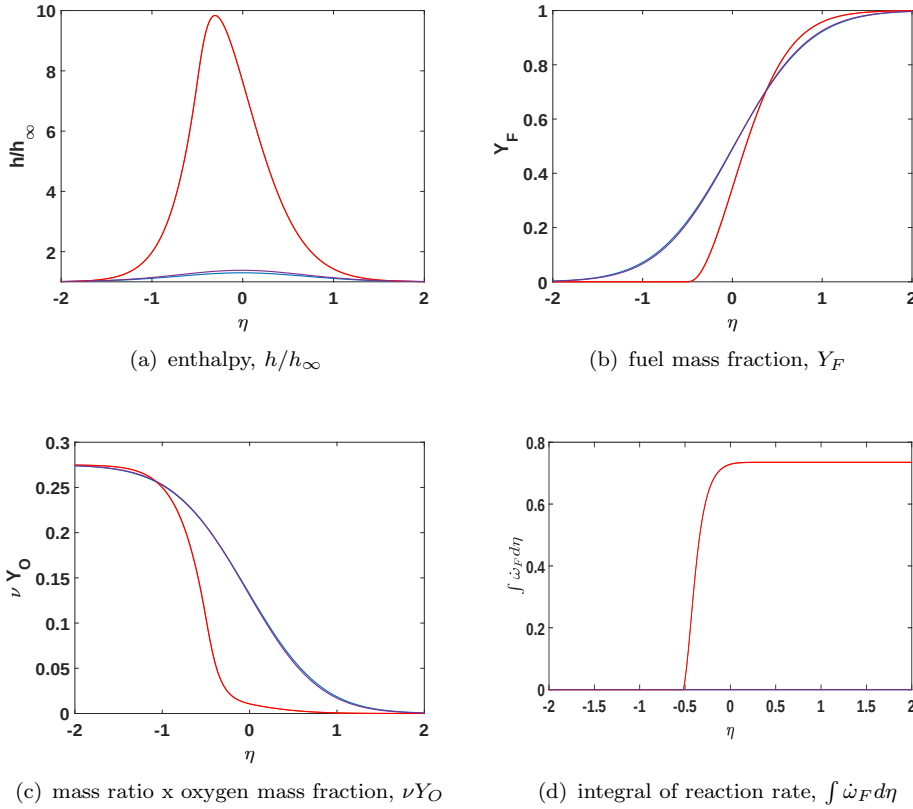


Figure 2.: Scalar properties for diffusion flame with varying vorticity.

$S_1 = -1.00$; $S_2 = 2.00$; $K = 0.275$. $\omega_\kappa = 0$, blue, no flame; $\omega_\kappa = 0.5$, purple, no flame; $\omega_\kappa = 1.0$, red, flame.

The heat release causes a decrease of the density in the vicinity of the flame. A plane still exists in the rotating reference frame where two different mixtures come together in a direction aligned with the scalar gradient while turning into the z direction aligned with the vorticity. The expanding gas can cause a flow reversal of the inward flow from the ξ -direction, orthogonal to the scalar gradient, as shown in Figure 3. The increased rotational rate produces the centrifugal acceleration that inhibits radially inward flow of the heavier gas and allows the expansion and velocity reversal for the lighter, hotter gas. Note that the development of negative

values for f_1' means that with the value $S_1 \leq 0$, the direction of the velocity component u_ξ becomes radially outward, i.e., $u_\xi > 0$ for $\xi > 0$ and $u_\xi < 0$ for $\xi < 0$.

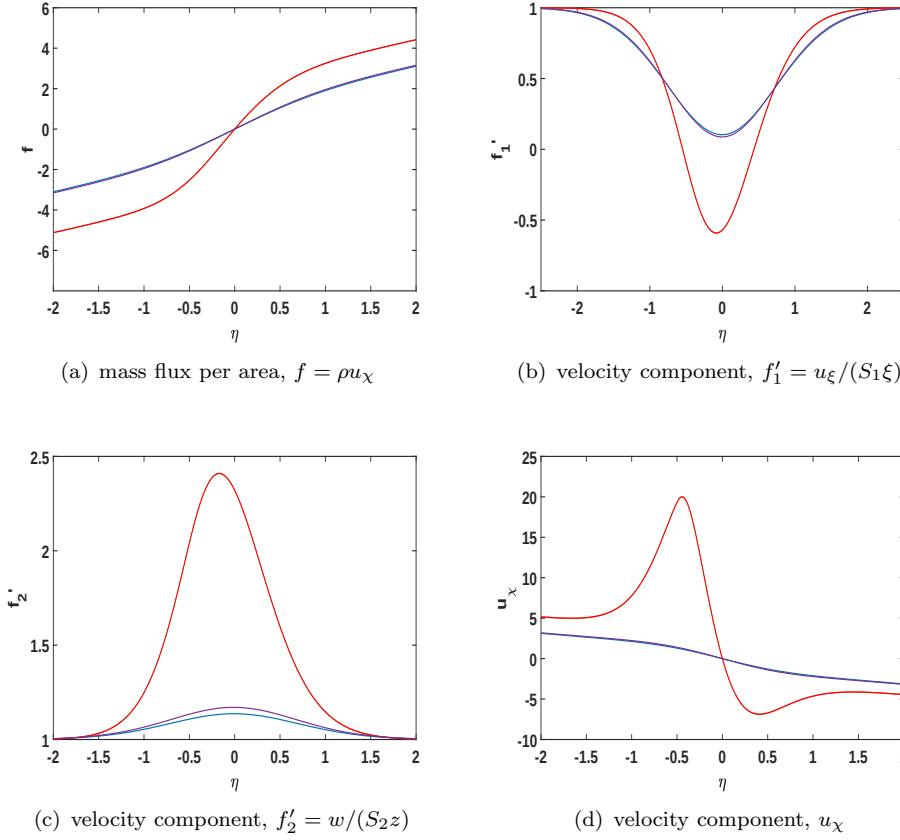


Figure 3.: Velocity behavior for diffusion flame with varying vorticity. $S_1 = -1.00$; $S_2 = 2.00$; $K = 0.275$. $\omega_\kappa = 0$, blue, no flame; $\omega_\kappa = 0.5$, purple, no flame; $\omega_\kappa = 1.0$, red, flame, flow reversal.

Clearly, the combination of fluid rotation, variable density, and three-dimensional structure have major consequences for flamelet behavior. The specific mechanism is not immediately obvious but can be inferred from the results. Figure 3b and 3c indicate that the strong swirl causes the reversal of the u_ξ velocity and an increase in the w velocity, both now being outward flows from the combustion zone. However, the fractional decrease in density implied by Figure 2a is significantly larger than the fractional increase in outward velocity. So, the outward mass flow rate is reduced which is consistent with the reduction of the inward mass flow rate when the inward flow ceases to come from both the ξ and χ directions and is limited to only the χ direction. Thereby, an increase in residence time of the flow in the reaction domain is allowed. This increase in vorticity and thereby in swirl rate changes the flammability limit.

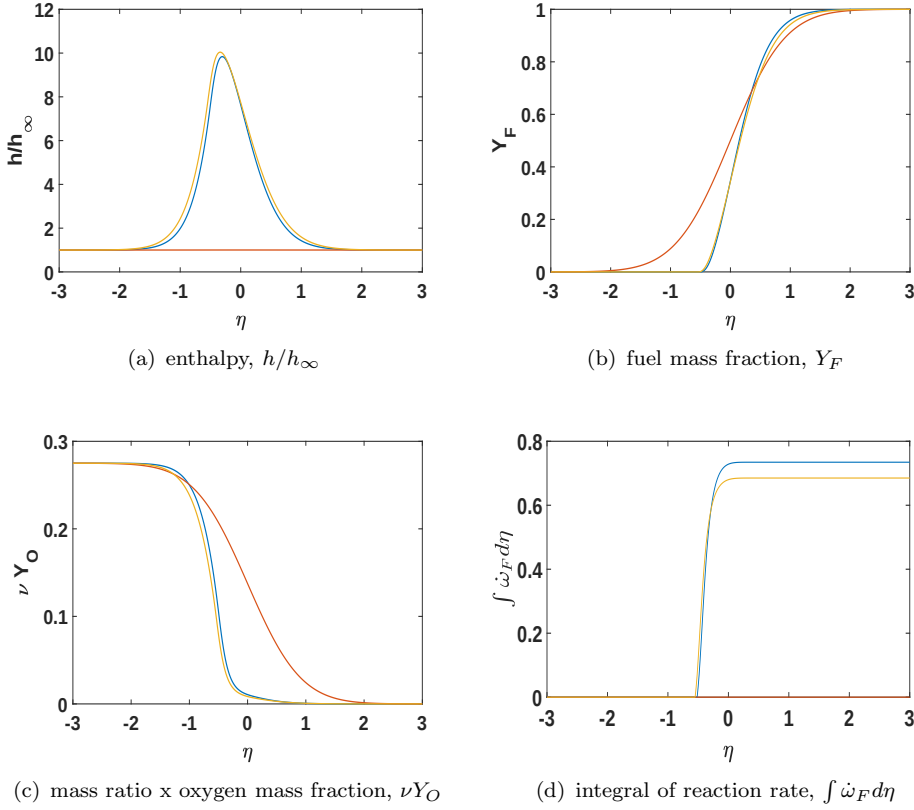


Figure 4.: Effects of normal strain on scalar properties for diffusion flame. $K = 0.275$; $\omega_\kappa = 1.0$. $S_1 = -1.25$, $S_2 = 2.25$: red, no flame. $S_1 = -1.00$, $S_2 = 2.00$: blue, flame. $S_1 = -0.75$, $S_2 = 1.75$: orange, flame.

In Figures 4 and 5, the effect of the imposed ambient normal strain rates is examined for a situation with $\omega_\kappa = 1$. Flame extinction results in this example with an increase of the magnitude of the ξ normal strain rate S_1 beyond the value of the χ normal strain rate. So, $S_1 + S_2 = 1 < |S_1| = 1.25$ yields no flame while a strong flame is established for the two cases where $S_1 + S_2 = 1 \geq |S_1|$. Modest decreases in the integrated reaction rate, the mass flux f , and the amount of flow reversal occur with a reduction of imposed strain in the ξ direction from the base case where $S_1 = -1.0$; simultaneously, a modest increase in peak temperature and enthalpy occurs. Apparently, the reduced mass flux and associated increase in residence time allows for a slightly greater temperature rise although the reaction rate is slightly reduced. On the other hand, the increase in the magnitude of S_1 from the base case would, if density were reduced because of an established flame, yield too low a residence time to hold a flame; so, no flame occurs.

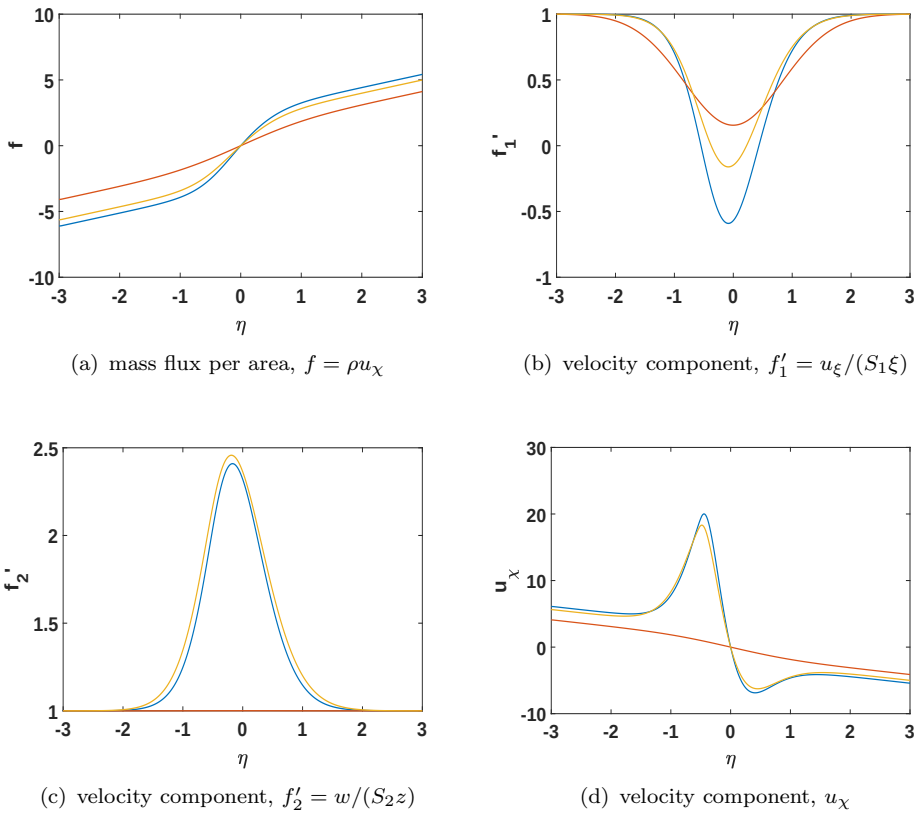


Figure 5.: Effects of normal strain on flow properties for diffusion flame. $K = 0.275$; $\omega_\kappa = 1.0$. $S_1 = -1.25$, $S_2 = 2.25$: red, no flame. $S_1 = -1.00$, $S_2 = 2.00$: blue, flame, flow reversal. $S_1 = -0.75$, $S_2 = 1.75$: orange, flame, flow reversal.

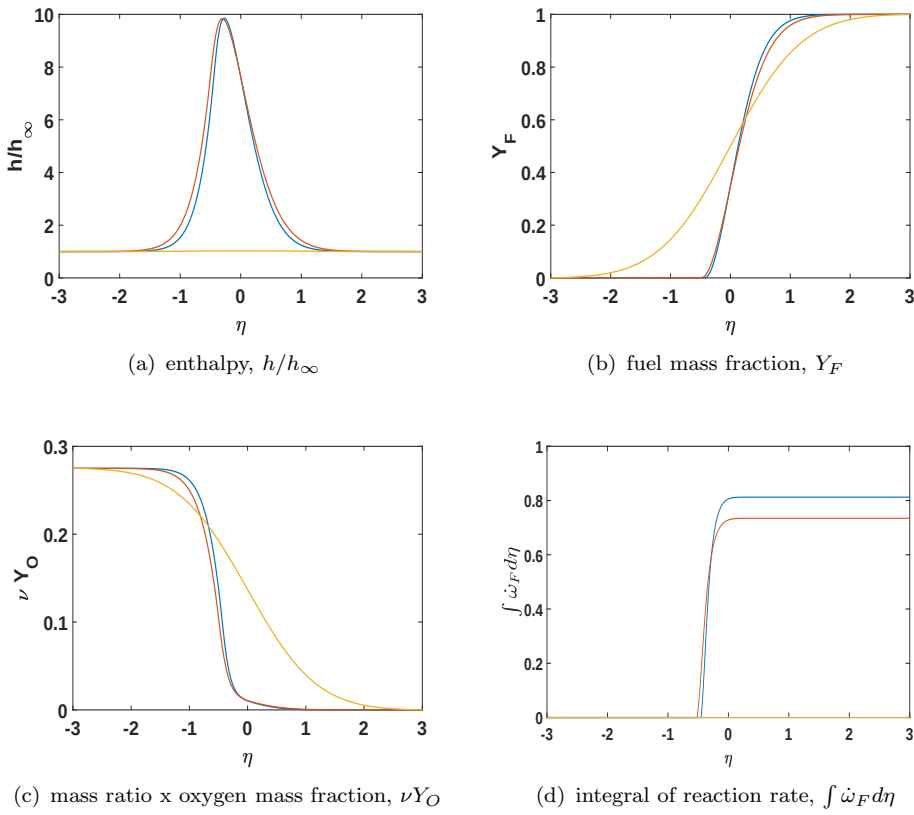


Figure 6.: Effects of Prandtl number on scalar properties for diffusion flame.
 $K = 0.275$; $\omega_\kappa = 1.0$; $S_1 = -1.00$; $S_2 = 2.00$. $Pr = 1.3$: blue, flame.
 $Pr = 1.0$: red, flame. $Pr = 0.7$: orange, no flame.

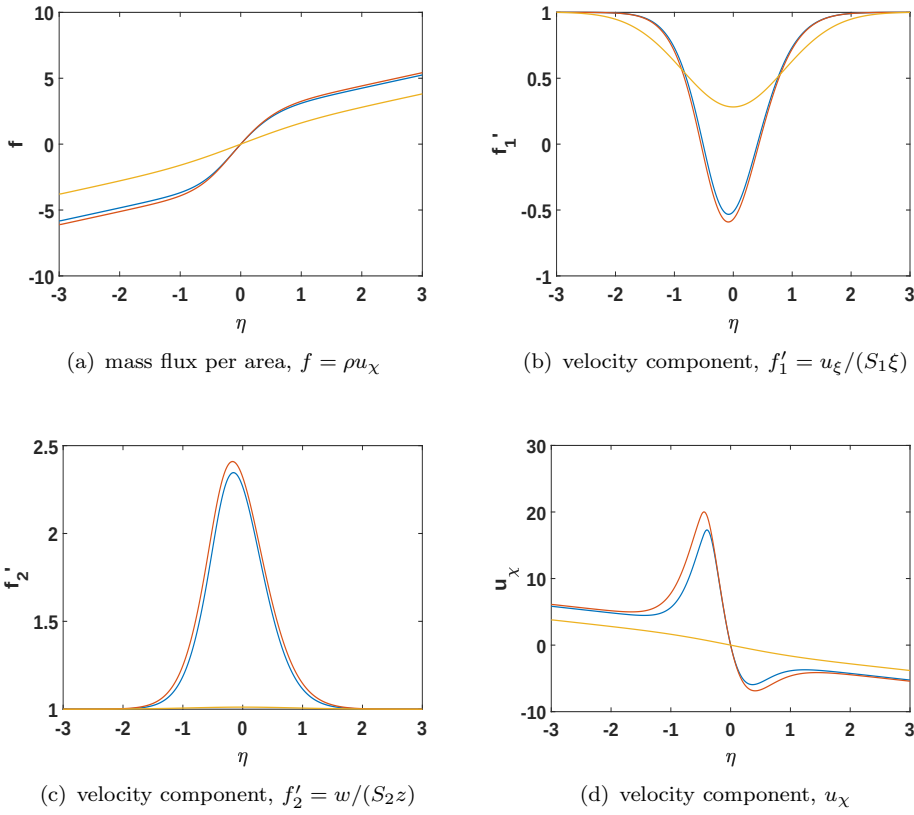


Figure 7.: Effects of Prandtl number on flow properties for diffusion flame. $K = 0.275$; $\omega_\kappa = 1.0$; $S_1 = -1.00$; $S_2 = 2.00$. $Pr = 1.3$: blue, flame, flow reversal. $Pr = 1.0$: red, flame, flow reversal. $Pr = 0.7$: orange, no flame, no flow reversal.

The sensitivity to thermal and mass diffusivities is shown in Figures 6 and 7. These diffusivities increase as Prandtl number Pr decreases. Thus, higher Pr results in thinner diffusion layers as shown in the figures. However, when the diffusivity is too large, heat is carried away over too large a domain to maintain a flame.

3.2 Premixed Flamelet Calculations

The analysis can apply to a situation where the inward swirling fluid has opposing streams of a combustible mixture and a hot inert gas (likely combustion products). A premixed flame can be established. As noted in an early study for counterflow flamelet [10], the premixed flame requires a Da value that is orders of magnitude larger than the required value for a diffusion flame. The vorticity and centrifugal motion can have consequence, especially near a flammability limit. Figures 8 and 9 have some interesting results. At a Da value of one-hundred to two-hundred-fifty times the reference value, i.e., $K = 100, 200, 250$, a strong premixed flame is shown to exist with or without a vorticity field. Application of swirl through the vorticity results in the same peak enthalpy or temperature and nearly the same flame speed (in the χ direction). The ξ component of velocity is seen to reverse direction with or without imposed vorticity. However, the increase in rotational rate and centrifugal acceleration decreases the magnitude of the reversal. The premixed flame moves slightly farther upstream as measured by the η value as swirl is applied. It likely occurs because, with less reversal in the ξ direction, the expansion in the η direction is enhanced.

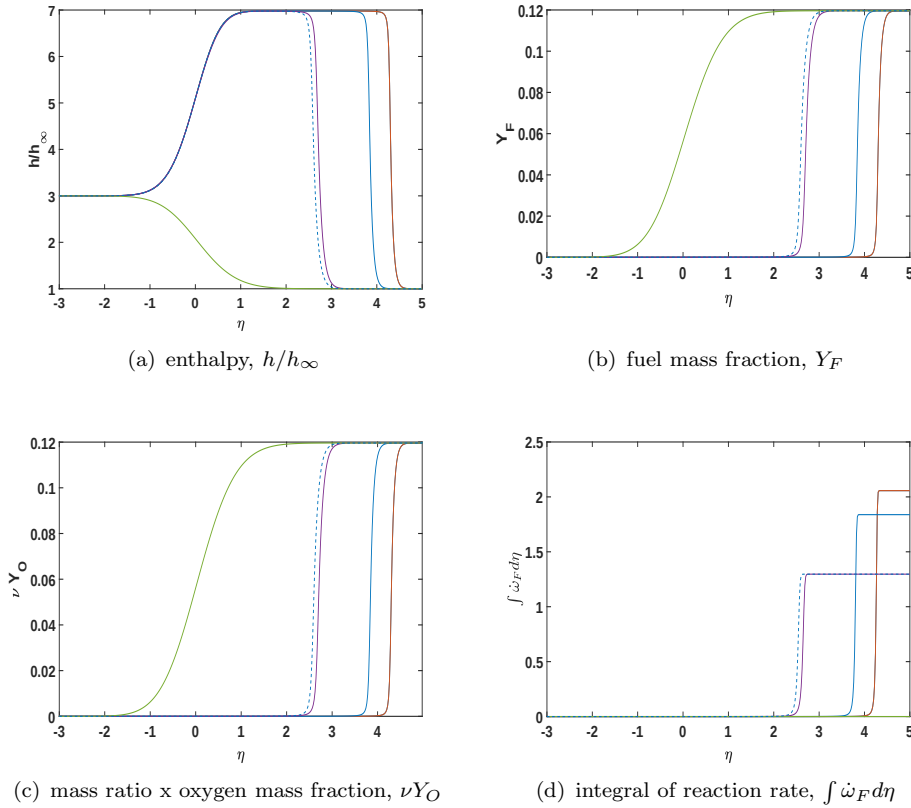


Figure 8.: Scalar properties for premixed flame with varying Damköhler number and vorticity. $S_1 = -1.00$, $S_2 = 2.00$. $K = 250$, $\omega_\kappa = 1.0$, red, flame; $K = 200$, $\omega_\kappa = 1.0$, blue, flame; $K = 100$, $\omega_\kappa = 1.0$, purple, flame; $K = 100$, $\omega_\kappa = 0$, dash blue, flame; $K = 20$, $\omega_\kappa = 1.0$, green, no flame.

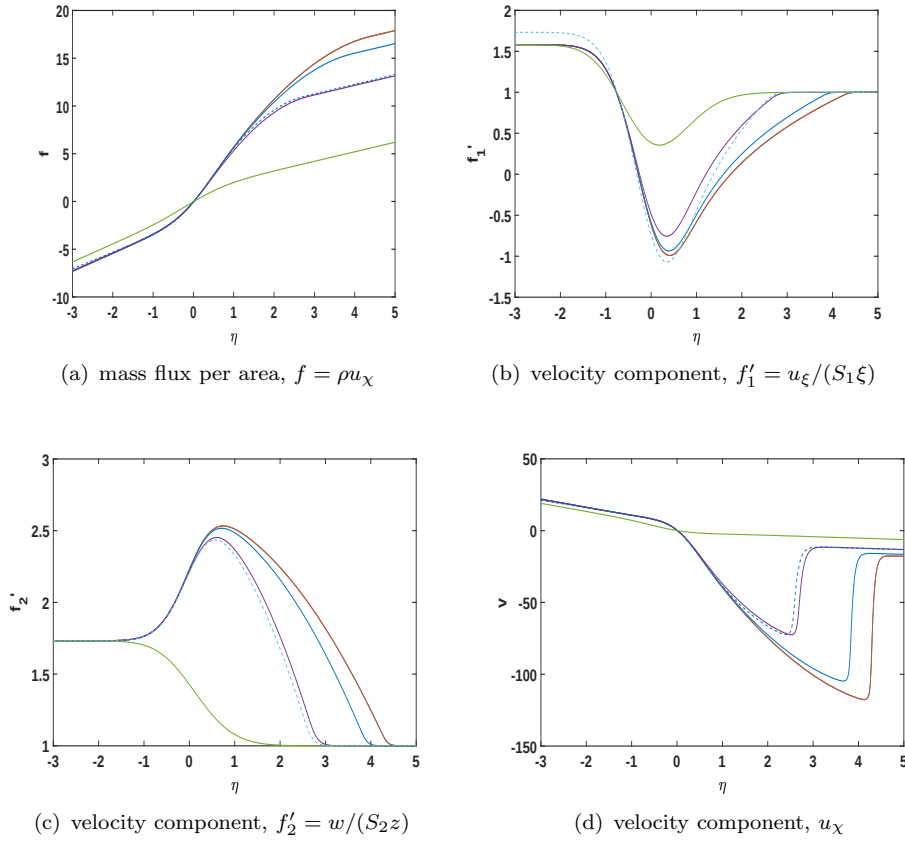


Figure 9.: Velocity behavior for premixed flame with varying Damköhler number and vorticity. $S_1 = -1.00$, $S_2 = 2.00$. $K = 250$, $\omega_\kappa = 1.0$, red, flame; $K = 200$, $\omega_\kappa = 1.0$, blue, flame; $K = 100$, $\omega_\kappa = 1.0$, purple, flame; $K = 100$, $\omega_\kappa = 0$, dash blue, flame; $K = 20$, $\omega_\kappa = 1.0$, green, no flame.

A decrease in Da to a situation where $K = 20$ results in extinction with vorticity in the range up to $\omega_\kappa = 1.0$. That situation is studied further with examination of the effect of vorticity on the extinction of the flame. In Figures 10 and 11, results are shown for four cases with $K = 37.5$ and ω_κ varying between 0 and 1.5. For $0.5 \geq \omega_\kappa \geq 0$, a flame does not survive while For $\omega_\kappa \geq 1.0$, a strong premixed flame can survive. In the range where a flame exists, the burning rate flame speed increases slight as the vorticity magnitude increases. Due to the centrifugal effect, u_ξ decreases in the flame region as ω_κ increases. In fact, it reverses direction near the flame. However, u_χ increases with ω_κ so the mass flux and burning rate increase as well.

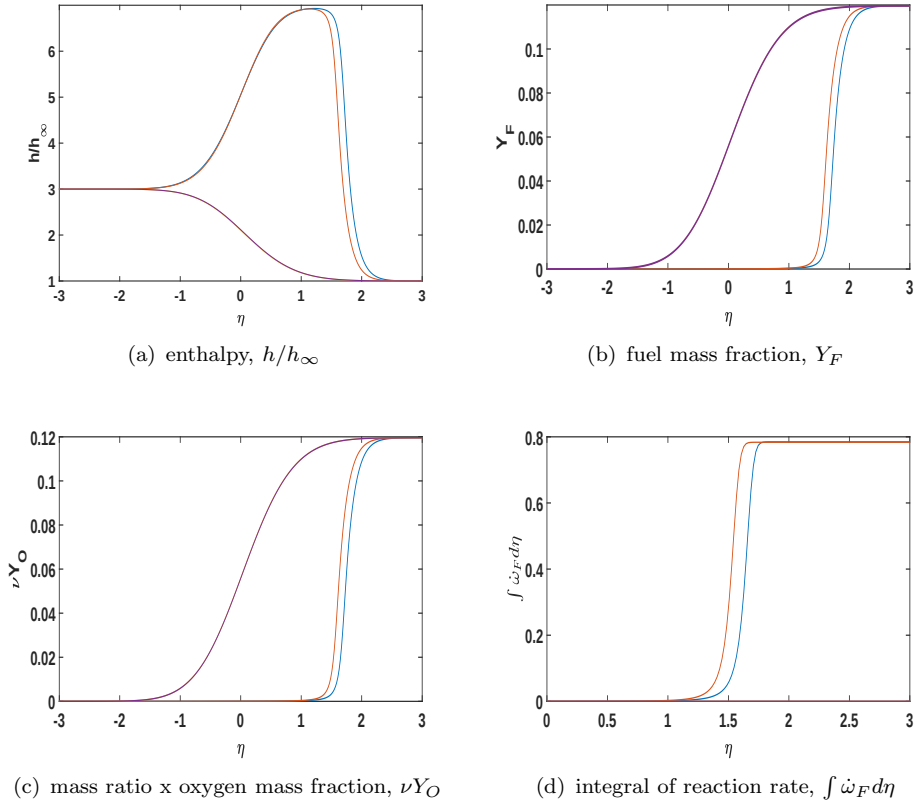


Figure 10.: Scalar properties for premixed flame for premixed flame with varying vorticity near extinction value for Damköhler number. $K = 37.5$, $S_1 = -1.00$, $S_2 = 2.00$. $\omega_\kappa = 1.5$, blue, flame; $\omega_\kappa = 1.0$, red, flame; $\omega_\kappa = 0.5$, purple, no flame; $\omega_\kappa = 0$, dash blue (sometimes covered by purple), no flame.

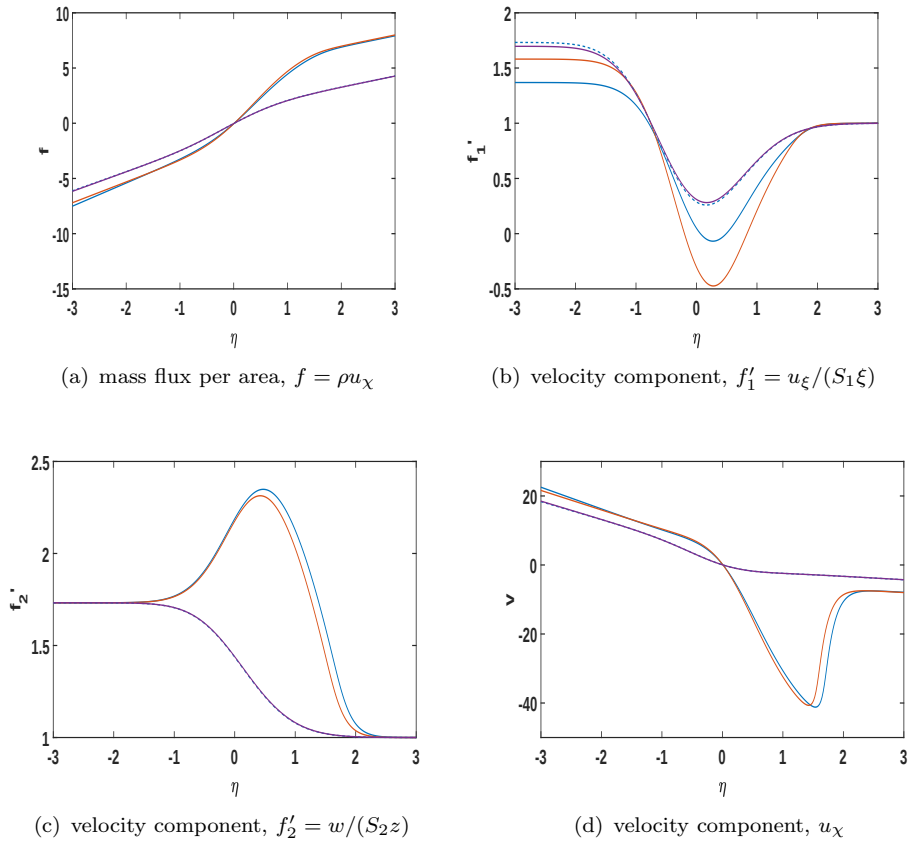


Figure 11.: Velocity behavior for premixed flame with varying vorticity near extinction value for Damköhler number. $K = 37.5$, $S_1 = -1.00$, $S_2 = 2.00$. $\omega_\kappa = 1.5$, blue, flame; $\omega_\kappa = 1.0$, red, flame; $\omega_\kappa = 0.5$, purple, no flame; $\omega_\kappa = 0$, dash blue (sometimes covered by purple), no flame.

3.3 Multi-branched Flamelet Calculations

Recent works have addressed the structure of multi-branched flamelets with a central diffusion flame and one or two premixed flames. The premixed flames can be fuel rich or fuel lean. They might be driven by heat transfer from the stronger diffusion flame. With three flames, the diffusion flame is centered between the two premixed flames and has the highest temperature. See [10, 26, 29] which address three general configurations: a stagnation flow, counterflow imposed on a shear layer, and a rotational flamelet. Here, we examine the multi-flame structure and behavior for the inward-swirling flamelet. Figures 12 and 13 show the computational results for relatively high values of Da . Later, Figures 14 and 15 will address the structure and behavior for values of Da near the flammability limits. The effects of vorticity are especially of interest.

It is sometimes convenient to present the flamelet scalar variables as functions of a conserved scalar instead of as a function of the spatial coordinate. For our simple, one-step kinetics calculations, conserved scalars are formed by defining the Shvab Zel'dovich variables $\alpha \equiv Y_F - \nu Y_O$ and $\beta \equiv h + \nu Y_O \tilde{Q}$ where $\tilde{Q}$ is the fuel heating value normalized by $h^*(\infty)$. Then, Equation (13) yields

$$\begin{aligned}\alpha'' + Pr(S_1 f_1 + S_2 f_2)\alpha' &= 0 \\ \beta'' + Pr(S_1 f_1 + S_2 f_2)\beta' &= 0\end{aligned}\tag{19}$$

In the above relations, the required constants are $S_1, S_2 = 1 - S_1, \rho_{-\infty}, \nu, \tilde{Q}, Pr$. Solutions are coupled to the simultaneous solutions of Equations 11. A normalized conserved scalar Σ varying between the values of 0 and 1 can be formed as shown by Sirignano.

$$\Sigma \equiv \frac{\alpha - \alpha_{-\infty}}{\alpha_{\infty} - \alpha_{-\infty}} = \frac{\beta - \beta_{-\infty}}{\beta_{\infty} - \beta_{-\infty}}\tag{20}$$

The use of plots of scalar variables as a function of Σ are helpful in identifying the location of reaction zones in the flame structure.

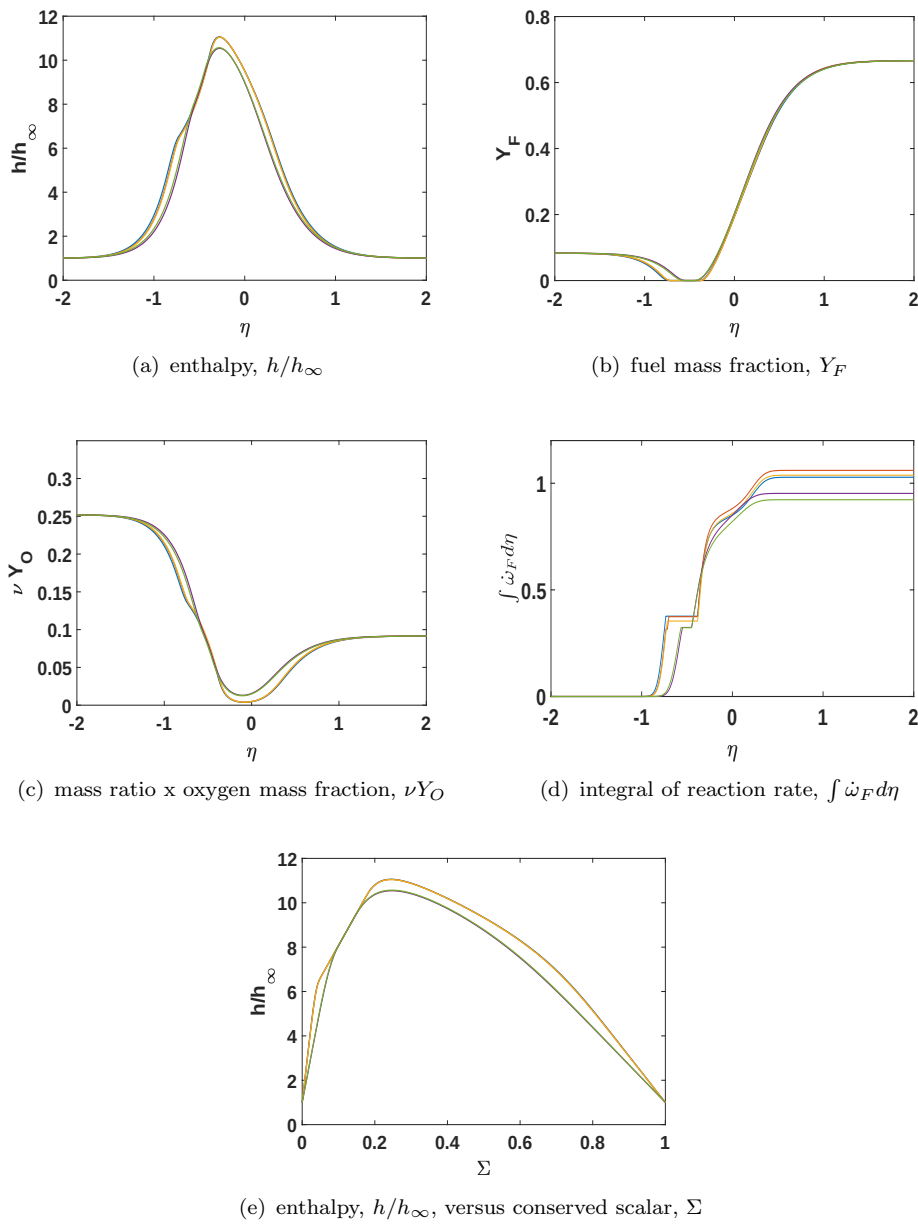


Figure 12.: Scalar properties for multibranched flame with varying Damköhler number and vorticity. $S_1 = -1.00$, $S_2 = 2.00$. $K = 1.00$: $\omega_\kappa = 1.0$, blue; $\omega_\kappa = 0.50$, red; $\omega_\kappa = 0$, orange. $K = 0.300$: $\omega_\kappa = 1.0$, green; $\omega_\kappa = 0$, purple.

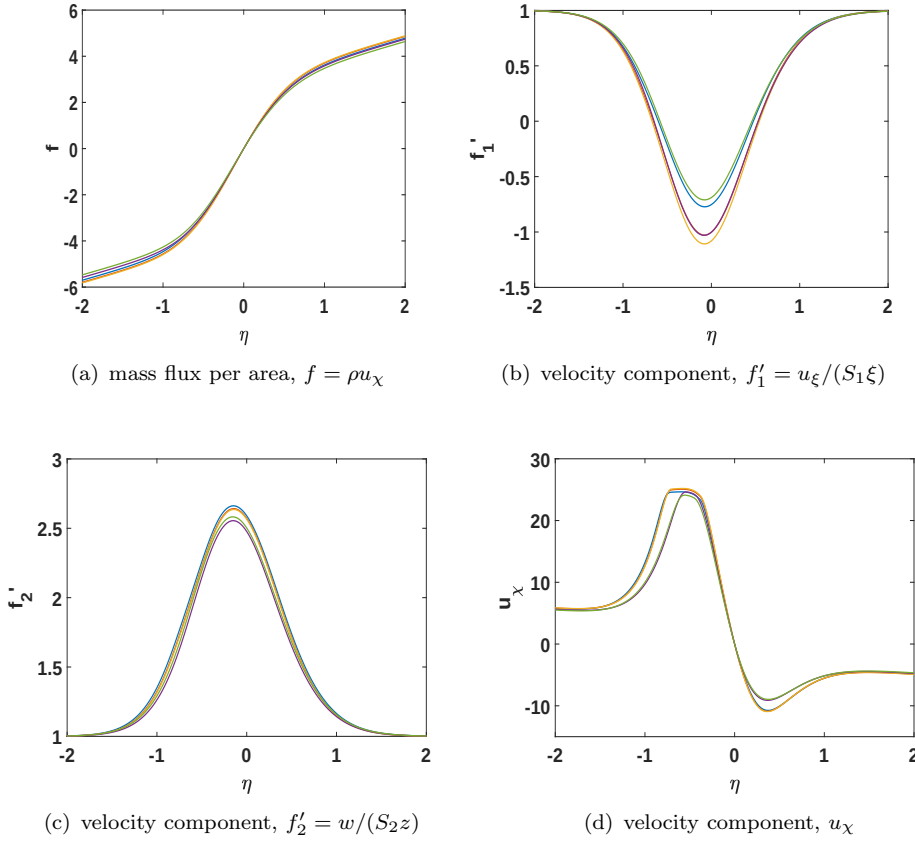


Figure 13.: Velocity behavior for multibranch flame with varying Damköhler number and vorticity. $S_1 = -1.00$, $S_2 = 2.00$. $K = 1.00$: $\omega_\kappa = 1.0$, blue ; $\omega_\kappa = 0.50$, red ; $\omega_\kappa = 0$, orange. $K = 0.300$: $\omega_\kappa = 1.0$, green; $\omega_\kappa = 0$, purple.

In Figures 14 and 15, results are shown for a configuration with a fuel-rich mixture at $\eta = \infty$ and a fuel-lean situation at $\eta = -\infty$. The fuel-rich mixture exists with $Y_F = 2/3$ and $Y_O = 1/3$ flows inward on one side of the swirling flame and a fuel-lean mixture with $Y_F = 1/12$ and $Y_O = 11/12$ flows inward from the other side.

For a sufficiently high value of Da , a strong diffusion flame and a weak, fuel-rich premixed can co-exist without a rotational flow. See the case with $K = 0.180$ and $\omega_\kappa = 0$ in the figures. The weak premixed flame is indicated by the region of negative second derivative for enthalpy on the right-side of Figure 14e. (A negative second derivative also exists on the right-side of Figure 14a but is more difficult to detect.) In Figure 14d, the diffusion flame contributes to the region with the largest first derivative (the reaction rate which is the integrand) while the premixed flame contributes in the region where the first derivative is still positive but smaller. The existence of multiple flames is also indicated by consumption of oxygen to the right of the diffusion flame in 14c. The weak premixed flame is driven by heat diffusion from the strong diffusion flame. More information about these multi-flame structures are provided by [29].

For the reduced values of Damköhler number Da , rotation is needed to produce a flame. For example, as the same figures show with $K = 0.170$, a strong flame appears with $\omega_\kappa = 0.75$ but there is no flame development possible with $\omega_\kappa \leq 0.5$. Similarly, for still smaller Da , even greater rotational rate is needed; for $K = 0.160$, $\omega_\kappa = 1.50$ produces a strong flame, while for $\omega_\kappa \leq 1.00$, no flame is sustained with any vorticity value.

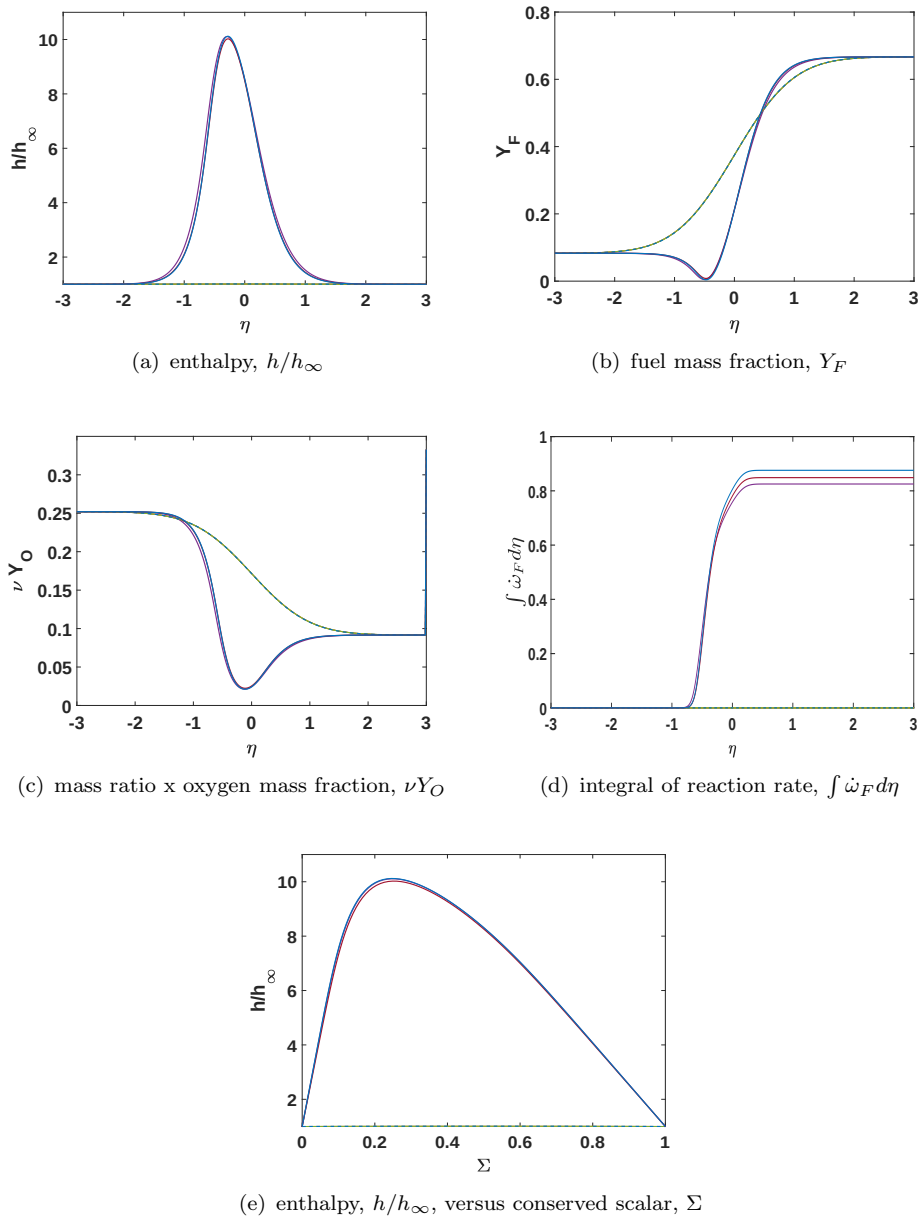


Figure 14.: Scalar properties for multibranched flame with varying vorticity. $S_1 = -1.00$, $S_2 = 2.00$. Cases with a strong flame: $K = 0.180$, $\omega_\kappa = 0$, solid blue; $K = 0.170$, $\omega_\kappa = 0.75$, red; $K = 0.160$, $\omega_\kappa = 1.50$, purple. Other curves show no flame (extinction) and all fall on the dashed blue line: $K = 0.170$, $\omega_\kappa = 0.50$; $K = 0.160$, $\omega_\kappa = 1.00$.

Figure 15b indicates that a strong flame will cause flow reversal in the ξ direction due to gas expansion.

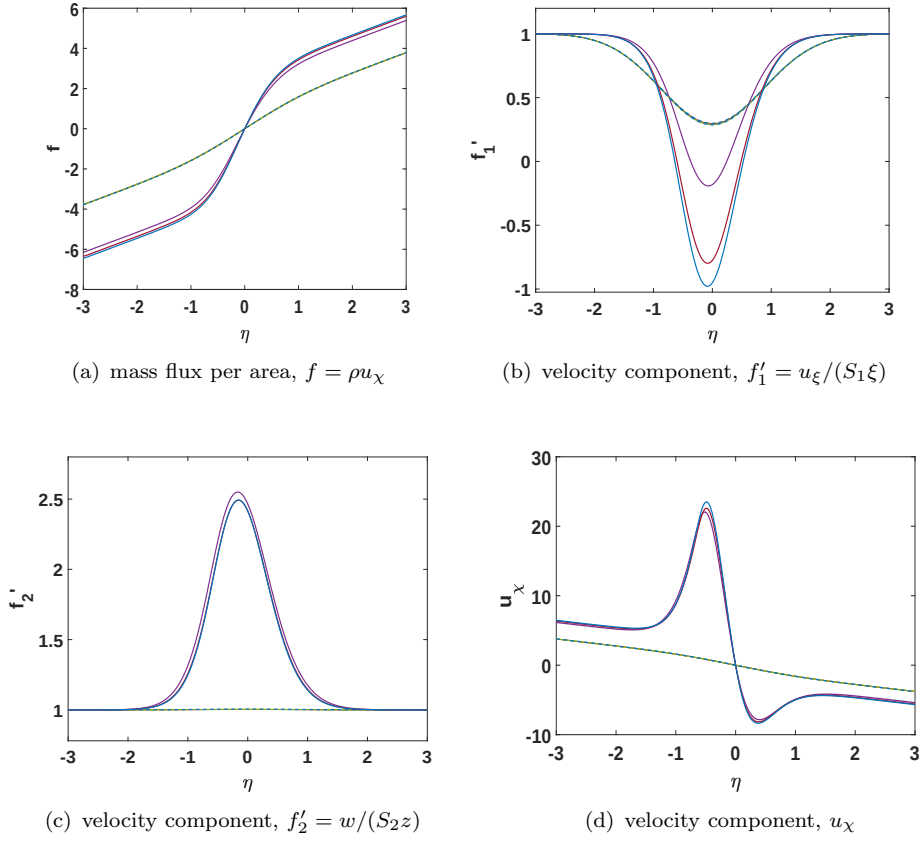


Figure 15.: Velocity behavior with varying vorticity for multibranched flame. $S_1 = -1.00$; $S_2 = 2.00$. Cases with a strong flame: $K = 0.180$, $\omega_\kappa = 0$, solid blue; $K = 0.170$, $\omega_\kappa = 0.75$, red; $K = 0.160$, $\omega_\kappa = 1.50$, purple. Other curves show no flame (extinction) and all fall on the dashed blue line: $K = 0.170$, $\omega_\kappa = 0.50$; $K = 0.160$, $\omega_\kappa = 1.00$.

4. Conclusions

A new flamelet model is developed to treat a range of flame structures in a steady, stretched, three-dimensional vortex. Non-premixed flames, premixed flames, and multi-branched flames are addressed through a unified theory. The creation of a contrived parameter such as a progress variable is avoided. Four nondimensional parameters are controlling: the imposed, normalized compressive strain rate S_1 ; the imposed, normalized vorticity ω_κ ; the Damköhler number Da ; and the Prandtl number Pr which equals the Schmidt number Sc here. The effects of these quantities are shown in the computational results. While this new theory is established for multi-step oxidation chemistry, a simple example of one-step, propane-oxygen kinetics is considered.

The effects of the inward swirl inherent to the stretched vortex are shown to have significant effects, especially in modifying the flammability limits. Variable density is shown to have a critical role since the centrifugal force created through the vorticity has impact in that case.

For any of the flame structures, the increased vorticity can move the flammability limit to lower Da values. Higher Da (for proper ambient mixtures) makes multi-branched flames more likely. Heat from the diffusion flame can drive the premixed flames. The distribution of the normal compressive strain between the directions for incoming swirling flow can affect the results. The variation of Pr within the expected range can have some effect on the flammability limit.

For future studies, several issues are important. The computations should be extended to cases with detailed chemical kinetics, detailed transport models, and improved equations of state. Coupling of the flamelet model should be made with a RANS or LES analysis for a practical, reacting, mixing, shear flow. Direct numerical simulations of reacting flows that give improved correlations of resolved-scale velocity gradients with the smallest-scale velocity gradients would be helpful.

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Declaration of Interests.

The author reports no conflict of interest.

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