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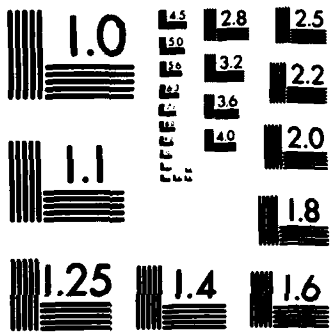


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# BASIC INSTABILITY MECHANISMS IN CHEMICALLY REACTING SUBSONIC AND SUPERSONIC FLOWS

by

Tau-Yi Toong

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Massachusetts Institute of Technology
Cambridge, Massachusetts



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STRACT (Continue on reverse if necessary and identify by block number)
This report summarizes the main results and conclusions obtained in a research program asic instability in chemically reacting subsonic and supersonic flows. Problems studied uded (1) Nonlinear wave-kinetic interactions (2) Sustenance, structure and initiation of ous detonations (3) Sustenance of low-frequency instability in dump combustors (4) Onset nstability in reacting shear flows and (5) Temporal development of turbulence-combustion ractions. Both linear and nonlinear coupling between chemical kinetics and gas dynamics found to play important roles in triggering and sustaining instabilities in these blems. Of special significance were the effects due to non-dimensional activation energy Damköhler's similarity parameters and possible selective amplification within specific quency bands as governed by chemical kinetics. Originator supplied keywords included


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Combustors; Onset of Instability in Reacting Shear Flows; Turbulence-Combustion Interactions.



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This report summarizes the main results and conclusions obtained in a research program on basic instability mechanisms in chemically reacting subsonic and supersonic flows, conducted at the Massachusetts Institute of Technology with the support of the U.S. Air Force Office of Scientific Research under Grant AFOSR-78-3662. Detailed information may be found in the various publications listed in the Bibliography.

The main objective of this program was to study basic mechanisms which play important roles in triggering and sustaining instabilities in chemically reacting flows. Problems studied during this grant period included: (1) Nonlinear wave-kinetic interactions (2) Sustenance, structure and initiation of gaseous detonations (3) Sustenance of low-frequency instability in dump combustors (4) Onset of instability in reacting shear flows and (5) Temporal development of turbulence-combustion interactions. The results obtained are briefly described below.

(1) Nonlinear Wave-Kinetic Interactions

It has now been established both theoretically and experimentally that irreversible exothermic reactions are capable of amplifying pressure disturbances. Earlier theoretical studies [1-4] examined the chemical effects on the propagation of sound waves in spatially homogeneous irreversibly reacting mixtures. These studies were conducted on the basis of a linearized theory of acoustic-kinetic interactions; nevertheless, substantial amplification of the acoustic waves was found possible. This theory was successful in predicting the observed sound amplification rates under quasi-steady conditions when the ratio of the characteristic chemical time to the wave period was large [5,6]. When this ratio was decreased below a critical value, which depended on the reaction kinetic parameters, both theory [1,3,4,8] and experiments [7,8] showed higher amplification rates.

Experimental results [7,8] indicated also that, at high amplification rates, sound waves might develop into weak shocks in rather short time intervals, thereby introducing both hydrodynamic and chemical-kinetic nonlinear effects. Under such conditions, a nonlinear model was necessary for predicting the temporal evolution of the wave amplitudes and structure.

(A) Theoretical Investigation

Nonlinear wave-kinetic interactions were analyzed by examining the propagation of finite-amplitude waves in a gaseous medium undergoing non-equilibrium exothermic reaction [9]. An exact nonlinear wave equation was developed and the various coupling mechanisms were identified.

For weak, nonlinear, high-frequency waves, the exact equation was reduced to an approximate form, which took into account the chemical and transport effects. This equation was numerically integrated to predict the amplification rates of weak shock pulses and changes in their wave forms for different activation energy, thermicity, initial shock strength and pulse duration. The results revealed the following features:

(i) In reacting mixtures of high activation energies (i.e., detonable mixtures), nonlinear wave-kinetic coupling resulted in dramatic increases in amplification rates, even at low shock strengths. These rates were enhanced with increased exothermicity, shock strengths and pulse duration. Furthermore, a minimum pulse duration was required for shock of a given initial amplitude to develop into a stronger shock. These results seemed to indicate that threshold values for shock strength and pulse duration would exist for direct initiation of detonations (cf. Section 2-C).

(ii) Chemical reactions of low activation energies were not capable of sustaining weak shock waves against dissipative losses. The rate of decay of the shock waves increased progressively at higher shock strengths. Moreover, higher exothermicities might enhance attenuation rather than amplification.

(B) Experimental Investigation

In order to study the nonlinear wave-kinetic interactions, the amplitudes and structure of weak shocks propagating in hydrogen-chlorine-argon mixtures were examined in a Pyrex tube [7,8]. Planar weak shocks of controlled strengths and widths were generated when a high-voltage capacitor discharged through a solenoid in contact with a thin metallic diaphragm at one end of the reaction tube. The shock examined consisted of a typical N-wave with a steep leading front followed by weaker trailing waves of lower amplitudes and frequencies.

Experiments showed that the leading shock strengths were amplified due to chemical reaction. However, the trailing waves were amplified at much higher rates. Compared with the quasi-steady predictions, the amplification of leading shocks showed good agreement, while that of the trailing waves displayed rates that were much higher, because their corresponding values of the ratio of characteristic chemical time to the wave period were lower and fell into the non-quasi-steady regime. Such behavior agreed with the theory, which predicted stronger acoustic-kinetic interactions as the characteristic acoustic time approached the characteristic chemical time [1,3,4,8].

Except for the frequency effect on the amplification rates described above, no significant nonlinear effect was observed when the Mach number of the leading shocks was approximately 1.05. At shock Mach numbers above 1.2, however, nonlinear wave-kinetic interactions began to play a role in sustaining and amplifying the shocks, despite high dissipative losses at the shock fronts. For high reaction rates, the waves could develop from a decaying N-wave into a rapidly expanding shock pulse.

(2) Sustenance, Structure and Initiation of Gaseous Detonations

The structure, sustenance and stability of gaseous detonations were believed to be the result of complex interactions between chemical kinetics and gas dynamics. These interactions also governed the requirements for their initiation in terms of the power density, energy density and energy-deposition duration or volume [12]. The mechanism which sustained the longitudinal instability of a shock-reaction-zone complex also involved such interactions [13]. Recent studies on the genesis of transverse waves in two-dimensional detonations further showed the importance of these interactions [17].

(A) Longitudinal Instability

The stability of one-dimensional piston-supported shock—reaction-zone complex was examined both numerically and analytically [13]. Numerical calculations were presented for a one-step first-order irreversible reaction, obeying an Arrhenius rate expression. An approximate linearized stability theory was also developed for the case of high activation-energy reactions and the mechanism of instability identified.

The analysis demonstrated that the governing instability mechanism was a non-acoustic one. The sequence of events was as follows: Pressure waves perturbed the shock front and generated irreversible temperature fluctuations. The latter, in turn, were carried by and interacted with the reacting flow, thereby inducing a fluctuating energy-source field. This energy-source field then generated the pressure waves which led to shock perturbations and thereby the temperature fluctuations, thus completing the cycle.

The low- and high-frequency modes previously reported by Fickett and his co-workers were two of the unstable resonance modes of this oscillatory system. However, the present theory was capable of predicting all the succeeding modes. Oscillation periods and amplification (or attenuation) rates were obtained and the results agreed well with the findings of both the numerical calculations and the exact linearized stability analysis reported in the literature. The predicted periods agreed also well with those observed in blunt-body flow experiments.

For high activation energies or low degrees of overdrive, the numerical solutions showed that a one-dimensional shock—reaction-zone complex underwent periodic pressure oscillations around its steady-state value.

As the activation energy was increased or the overdrive decreased, the onset of these oscillations was enhanced dramatically and both their amplitude and period increased. For detonable mixtures with high activation energies and at no overdrive, the pressure underwent excursions as large as 300% of its steady-state value with a period of $\sim$ 20 characteristic reaction time (defined as the time required for a particle to react fully).

(B) Genesis of Transverse Waves

Results of a linearized theory developed for the case of high activation-energy reactions [17] showed that the mechanism responsible for the one-dimensional longitudinal instability (cf. Section 2-A) was also responsible for the two-dimensional instability. Stability limits as well as amplification (or attenuation) rates and oscillation periods were obtained for different transverse wave numbers at different degrees of overdrive. The amplification rates were found to decrease and become negative for larger wave numbers or for larger degrees of overdrive. In other words, transverse waves did not develop in very narrow channels or in highly overdriven detonations because of attenuation. Moreover, it was shown that for the most unstable wavelength, the oscillation period was almost equal to that of the one-dimensional oscillation, as was also observed in the numerical simulations.

Numerical simulations of two-dimensional detonations in channels of different widths were also conducted. It was observed that (i) transverse waves did not develop in channels whose widths were smaller than or of the order of the characteristic reaction length, in spite of the presence of longitudinal waves (ii) a critical channel width existed beyond which a transverse wave developed (iii) as the channel became wider and up till a second critical width, the transverse wave persisted while its oscillation period became longer (iv) beyond that second critical channel width, new transverse waves were formed, with their wavelengths equal to the wavelength corresponding to the second critical value. Moreover, at and beyond that critical value, the oscillation period attained a constant value, identical to that of the one-dimensional oscillation. These results demonstrated the existence of a most unstable wavelength which would persist further on and govern the cell size in wide channels.

### (C) Direct Initiation of Gaseous Detonations

A simple theoretical model was developed to determine the correlation between the critical energy and power of an igniter required for direct initiation of detonations and to predict their respective threshold values [12]. The model comprised a constant-velocity piston which was set in motion at time $t = 0$. The resulting constant-velocity shock wave heated up the explosive mixture and triggered the chemical reaction. It was shown that for direct initiation, the piston should remain in motion for a time interval, at least, equal to the induction time. The predictions based on this simple model were in good qualitative and quantitative agreement with the experimental findings, reported in the literature on cylindrical detonations.

(3) Sustenance of Low-Frequency Instability in Dump Combustors

One major problem related to the use of dump combustors in propulsion devices is to eliminate the low-frequency oscillations which cannot be damped by ordinary acoustic liners. In order to study the governing mechanism, an instability model was postulated which asserted that a coupling occurred between two processes, one located in the combustion zone and the other at the choked nozzle [10,11,16]. Pressure disturbances were produced as entropy waves convected through the nozzle and entropy waves were generated as the pressure disturbances perturbed the combustion zone. An approximate linearized stability theory was developed for the case of near blow-off (which corresponded to maximum rumble). Both oscillation frequencies and amplification rates were obtained.

The theory was used in conjunction with the experimental data obtained at the Aero Propulsion Laboratory, AF Wright Aeronautical Laboratories, to analyze the effect of combustor-to-inlet area ratio, nozzle-to-combustor area ratio, inlet stagnation temperature, presence of a flameholder, mode of fuel injection, fuel-air ratio and combustor size on stability. Both frequency calculations and stability analysis agreed well with the experimental measurements and observations.

As the combustor diameter increased for a given inlet area, the flow tended to be more stable with accompanying increase in the combustion efficiency. The amplification rates were smaller at lower fuel-air ratio, suggesting possible domination of high-frequency instability under such conditions as observed in the APL experiments. Theory also showed that the flow was more stable at higher inlet stagnation temperatures, smaller nozzle-to-combustor area ratios (although reverse trend was also predicted for some conditions), larger combustor diameters and with a flameholder. Similar trends were observed for uniform injection of fuel-air mixture.

(4) Onset of Instability in Reacting Shear Flows

Despite the importance of turbulence in enhancing combustion efficiency and reducing pollutant emissions, the exact nature of its role is not completely understood, thus making full utilization of its effects difficult. One promising way to achieve detailed physical understanding of the turbulence-combustion interactions involved is to study the temporal development of the turbulent characteristics from laminar combustion. One such problem was examined by studying the growth of Tollmien-Schlichting disturbance waves in a reacting shear layer [14,15]. Analysis showed that the growth rates of these waves depended on the order, the thermicity, and the activation energy of the Arrhenius-type chemical reaction as well as the disturbance wavelengths and Damköhler's similarity parameters. In the case of quasi-steady situation, the chemical effect was represented by the product of Damköhler's third similarity parameter and the non-dimensional activation energy. Also, the chemical effect was smaller for longer wavelength. In other words, the effects of chemical kinetics were different for eddies of different sizes. Regardless of the wavelengths, however, exothermic reaction increased the growth rates.

The quasi-steady assumption was valid when the characteristic chemical time was long compared with the characteristic flow time. However, the unsteady effects became important as the reaction rate increased or as the shear-layer thickness decreased for a given maximum mean velocity or as the maximum mean velocity increased for a given shear-layer thickness.

Analysis showed also that when these unsteady effects were present the normal-mode disturbances could no longer exist. The disturbances must take on a more general form. However, it is believed that the trend of increased disturbance growth rates for exothermic reactions is still valid for unsteady flow situations.

(5) Temporal Development of Turbulence-Combustion Interactions

Several important questions which remain unresolved in the study of turbulent combustion are related to turbulence-combustion interactions — whether they exist or not, what is their nature and what are the governing mechanisms. Our study on premixed methane-air V-flames stabilized behind a cylindrical flameholder demonstrated the presence of significant interactions within the flame brush in different characteristic frequency bands. But the governing mechanisms are still not clear. The main objective of this research program* is to determine and elucidate the governing mechanisms by examining the temporal development of spectral changes within the flame brush as a quasi-laminar flame propagates into the wake region of a neighboring cylinder.

Detailed spectral changes in the structure of disturbed and undisturbed flames were examined by measuring instantaneous temperatures within the flame brush by the use of frequency-compensated, 25 μm-diameter, Pt/Pt-10% Rh

*This research is being continued with the support of the U.S. Air Force Office of Scientific Research under Grant AFOSR-83-0373.

thermocouples. Low-pass (20 Hz) signals showed the presence of low-frequency flame movement relative to the thermocouple for both cases. The significant difference due to the presence of the disturbance wake, however, was in the high-frequency fluctuations — the amplitudes of the high-frequency fluctuations in the disturbed flame (somewhat similar to those in a turbulent flame in the presence of grid-generated turbulence) were much larger than those in the undisturbed flame. This observation seemed to imply that the turbulence-combustion interactions were greatly enhanced due to the turbulence in the wake of the neighboring cylinder, thus leading to the development of the turbulent structure within the disturbed flame brush.

Such development of the turbulent structure was also noted in a comparison of the spectral density distributions of mean-square temperature fluctuations for the disturbed and the undisturbed flame at a fixed distance from the flameholder. An increase of nearly two orders of magnitude was observed in the spectral densities within the higher-frequency region for the disturbed flame, despite almost equal values in the lower-frequency region (< 10 Hz). This comparison clearly showed a significant increase in the intensities of the smaller eddies (or eddies of higher frequencies) which would lead to an increase in the turbulent-flame-propagation speeds through augmentation of transport rates of energy and mass and of effective chemical reaction rates within the flame structure.

Across the flame brush from the unburned to the burned region, there was a large variation in the spectral densities of mean-square temperature fluctuations for both the disturbed and the undisturbed flames. They were the lowest in the burned region and the highest inside the flame brush at a position where the gradient of the apparent mean temperature was near maximum and the reaction rate the highest. This observation seemed to imply the important role of the chemical reaction rate in determining the turbulent structure of a flame.

Selective amplification within certain frequency bands was also noted in the spectral density distributions. It is quite likely that the turbulence-combustion interactions are due to the coupling between chemical kinetics and gas dynamics, which would result in the observed spatial variation across the flame brush and frequency-dependence as inferred from our previous instability studies in reacting flows*.

Spectral density distributions of mean-square temperature fluctuations (at a position within the flame brush where the all-pass RMS temperature fluctuations were the maximum) were compared at different distances from the flameholder for both the disturbed and the undisturbed flames. Near the flameholder (3 mm downstream of its axis) the spectral densities were rather low at all frequencies. However, they seemed to attain some fully-developed values 35 mm downstream and beyond, more than two-orders-of-magnitude increase over the values upstream. This observation implied that the turbulent structure depended on interactions of <u>rate</u> processes, presumably due to the coupling between chemical kinetics and turbulence.

Spectral density distributions of mean-square temperature fluctuations were also compared with those of mean-square velocity fluctuations measured

*Toong, T.Y., Combustion Dynamics — The Dynamics of Chemically Reacting Fluids, Ch. 10, McGraw-Hill, New York, NY, 1983.

under corresponding cold-flow conditions 3 mm downstream of the flameholder. Some similarities were noted, although additional peaks in the spectral densities of mean-square temperature fluctuations were found to occur in several frequency bands. Whether these additional peaks are due to selective amplification through coupling between chemical kinetics and turbulence is still under investigation.

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12. Abouseif, G. E. and Toong, T. Y., "On Direct Initiation of Gaseous Detonations", Combustion and Flame, 45, 39-46, 1982.

13. Abouseif, G. E. and Toong, T. Y., "Theory of Unstable One-Dimensional Detonations", Combustion and Flame, 45, 67-94, 1982.

14. Greiner, M., "Onset of Instability in a Chemically Reacting Laminar Shear Layer", S.M. Thesis, Department of Mechanical Engineering, M.I.T., May 1982.

15. Tangborn, A. V., "The Influence of Chemical Reaction on an Unstable Perfect-Gas Laminar Shear Layer", S.M. Thesis, Department of Mechanical Engineering, M.I.T., May 1983.

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17. Abouseif, G. E. and Toong, T. Y., "Theory of Unstable Two-Dimensional Detonations: Genesis of the Transverse Waves", in preparation.

# APPENDIX I

(1) Professional Personnel

Professor T. Y. Toong, Principal Investigator

Dr. G. E. Abouseif, Co-Investigator

Mr. M. Greiner, Research Assistant

Mr. J. A. Keklak, Research Assistant

Mr. A. V. Tangborn, Research Assistant

(2) Advanced Degrees Awarded

(i) G. E. Abouseif Ph.D. Department of Aeronautics and Astronautics, M.I.T., January 1979
"Wave-Kinetic Interactions in Non-Equilibrium Reactions"

(ii) J. A. Keklak S.M. Department of Mechanical Engineering, M.I.T., January 1982
"A Low-Frequency Instability Mechanism in a Coaxial Dump Combustor"

(iii) M. Greiner S.M. Department of Mechanical Engineering, M.I.T., May 1982
"Onset of Instability in a Chemically Reacting Laminar Shear Layer"

(iv) A. V. Tangborn S.M. Department of Mechanical Engineering, M.I.T., May 1983
"The Influence of Chemical Reaction on an Unstable Perfect-Gas Laminar Shear Layer"

(3) Interactions

(A) Spoken Papers and Other Presentations

See Appendix II

(B) Major Expressions of Interest

Many requests for our papers have been received.

Appreciable interest in our research accomplishments has been expressed by Drs. Roger Strehlow and Harold Barthel of the University of Illinois, Dr. J. H. S. Lee of the McGill University, Dr. A. K. Oppenheim of the University of California, Berkeley, Dr. F. J. Weinberg of the Imperial College, Dr. J. Ross of the Massachusetts Institute of Technology, Dr. R. G. Gilbert of the University of Sydney, Dr. W. Strahle of Georgia Tech and Dr. J. F. Clarke of the Cranfield Institute of Technology, as related to their work on detonation wave structure, direct initiation of gaseous detonations, blast wave theory, unconfined fuel-air explosions, chemical kinetics, wave-kinetic interactions, combustion-generated noise, etc. Dr. F. D. Stull of the AF Wright Aeronautical Laboratories and Dr. N. Slagg of the Picatinny Arsenal have also expressed interest in our work on low-frequency instability in dump combustors and direct initiation of detonations.

# APPENDIX II

## Spoken Papers and Other Presentations

1. A report on technical progress and future plans on "Basic Instability Mechanisms in Chemically Reacting Subsonic and Supersonic Flows", by G. E. Abouseif at the 1978 AFOSR Contractor's Meeting on Air-Breathing Combustion Dynamics and Kinetics, Dayton, OH, October 11, 1978.
2. A report on technical progress and future plans on "Basic Instability Mechanisms in Chemically Reacting Subsonic and Supersonic Flows", by T. Y. Toong at the AFOSR Contractor's Meeting on Unconfined Fuel-Air Explosions (FAE) and Other Combustion/Explosion Related Research at Fort Walton Beach, FL, January 24, 1979.
3. A paper on "Nonlinear Wave-Kinetic Interactions in Irreversibly Reacting Media" presented by T. Y. Toong at the Seventh International Colloquium on Gasdynamics of Explosions and Reactive Systems, University of Göttingen, Göttingen, Germany, August 20, 1979.
4. A report on technical progress and future plans on "Basic Instability Mechanisms in Chemically Reacting Subsonic and Supersonic Flows", by G. E. Abouseif at the 1979 Contractor's Meeting on Air-Breathing Combustion Dynamics and Kinetics, Alexandria, VA, January 29, 1980.

5. A report on technical progress and future plans on "Basic Instability Mechanisms in Chemically Reacting Subsonic and Supersonic Flows" by T. Y. Toong at the 1981 AFOSR Contractor's Meeting on Air-Breathing Combustion Dynamics and Explosion Research, Clearwater, FL, November 17, 1981.
6. A report on technical progress and future plans on "Basic Instability Mechanisms in Chemically Reacting Subsonic and Supersonic Flows" by T. Y. Toong at the 1982 AFOSR Contractor's Meeting on Air-Breathing Combustion Dynamics Research, Clearwater, FL, November 2, 1982.
7. A report on technical progress and future plans on "Basic Instability Mechanisms in Chemically Reacting Subsonic and Supersonic Flows" by T. Y. Toong at the 1983 AFOSR Contractor's Meeting on Air-Breathing Combustion Dynamics Research, Scottsdale, AZ, September 22, 1983.

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