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**Coalescence/Dispersion Modeling of High-Intensity
Combustion**

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Abstract

In certain high-intensity continuous combustors, such as pre-mixed, pre-vaporized gas turbine combustors, flame stability and pollutant formation are both controlled by finite-rate complex chemistry and turbulent mixing. The coalescence/dispersion or "Monte Carlo" stochastic model of zero-dimensional continuous combustion due to Curl and to Spielman and Levenspiel has been extended to include complex finite-rate chemistry, by means of a new higher-order, single-step batch reaction kinetics algorithm. Results are presented for premixed and non-premixed H_2 -air combustion, which demonstrate the effects of local temperature inhomogeneities on the mean rates of heat-releasing and pollutant formation reactions.

Introduction

In certain types of high-intensity continuous combustion devices, such as laboratory jet-stirred reactors, automotive exhaust after-reactors or pre-mixed, pre-vaporized gas turbine combustors, flame stability, pollutant production and combustion efficiency are controlled by both finite-rate turbulent mixing and complex chemistry. Unfortunately, almost all modeling techniques in the continuous combustion literature fail to account for the effects of segregation (local inhomogeneity) due to either fuel-air ratio, "age" in the reactor-theoretic sense, or degree of reactedness.⁽¹⁾

Generally speaking, combustion modeling efforts to date stem from one of two fundamentally distinct approaches. The first approach is based on chemical reactor-theoretic or "population balance" models—sometimes called the 'modular' approach—in which the fluid mechanics are simplified to the extent that convective flow and turbulent mixing is represented by inter-connected well-or perfectly-stirred reactors (PSR's) and plug flow reactors (PFR's).⁽²⁾ The second approach is to solve the finite-difference approximated differential equations for conservation of mass, species, momentum and energy, usually simplifying the chemistry to the point where pollutant formation processes cannot be realistically represented.⁽³⁾

What both approaches have lacked to date is the ability to model the effects of β , the rate of turbulent micromixing within the combustor.^(1,4) In the modular approach, β is, by definition, infinite in PSR's, and is infinite for cross-stream mixing and zero for age mixing (axial diffusion) in PFR's. A PSR is an idealization of a region with strong convective recirculation, whereas a PFR is an idealization of a simple stream tube flow.

In finite-difference modeling, it has been necessary to treat turbulent exchange processes as quasi-laminar⁽³⁾; that is, to assume that, within a computational cell, local molecular homogeneity exists, or $\beta \rightarrow \infty$. Some attempts have been made to include moment equations for the probability density function (PDF) of a passive scalar mixture fraction⁽³⁾, which accounts for the effects of finite β , but only with the "flame-sheet" assumption of infinite-rate or equilibrium chemistry. Thus both approaches fail as quantitatively correct models for pollutant production. More sophisticated models have been proposed^(5,6), but have not been demonstrated.

In an actual combustor, recirculating flow is necessary for flame stabilization due to "age mixing"⁽¹⁾, while plug or stream flow is required to allow combustion reactions to progress towards completion within the combustor, and to allow "stream mixing" of secondary air to dilute the burnt gases to a tolerable turbine inlet temperature.

Due to recent advances in computation of stochastic or "Monte Carlo" methods^(7,8), together with improved algorithms for calculating equilibrium and non-equilibrium chemistry^(9,10) it is now possible to introduce finite-rate micromixing into both the PSR (age mixing and, if not premixed, stream mixing) and PFR (cross-stream mixing only) models. In the PSR, this improvement allows assessment of the effects of primary-zone inhomogeneities in fuel-air ratio, temperature, and "age", or degree of reactedness within fluid elements. In the PFR regions, finite-rate mixing of secondary air admission into the post-primary stream may be described, leading eventually to prediction of mixing inhomogeneities on "pattern factor" (a measure of temperature inhomogeneity or "hot spots" at turbine inlet).

The Coalescence/Dispersion (C/D) Model

In the C/D model, the combustor contents are discretized into computational cells or "turbules", which may be regarded (but not too literally) as primitive representations of single-scale turbulent eddies. The mass flow rate through the combustor is then represented by a number flow rate of turbules given by

$$\dot{N} = \dot{m}N/\rho V = N/\tau \quad (1)$$

where ρ is the mean mass density in the combustor, V is the volume, \dot{m} the mass flow rate, N is the number of turbules and τ is the mean residence time in the combustor.

Micromixing, or mixing between turbulent eddies at the micro-scale level, is simulated by consideration of Corrsin's time constant for decay of a concentration fluctuation in an isotropic turbulent field, β .^(1,4) Defining I_m as the ratio of mixing frequency β to feed frequency (τ^{-1}), pairs of turbules within the combustor are allowed to simply average their properties, with one such "coalescence and dispersion" pair interaction

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allowed per time interval ($\tau/I_m N$). Pairs are chosen by random selection so that there is no bias with respect to turbule age, thus representing a perfectly-stirred reactor with non-zero segregation.⁽¹⁾ During the time interval between C/D events, all turbules undergo adiabatic batch reaction, using either an infinite rate (equilibrium) assumption or a chemical kinetic mechanism and rate data, as desired. Whenever a feed time interval (τ/N) has elapsed, one turbule is selected at random to be removed from the assembly, and is replaced by a fresh feed turbule.

The assembly of turbules is initialized by assuming a homogeneous PSR distribution of mole numbers and corresponding temperatures.⁽⁹⁾ The C/D simulation is allowed to run for three to five equivalent residence times, until the ensemble statistics (mean and variance of properties) are observed to stabilize. Finally, ensemble averages and other statistics are obtained to represent the properties of interest at combustor exit.

Summary of Computational Methods

Mixing-limited, Non-premixed Combustion

For non-premixed combustion of gaseous fuel and oxidizer, equilibrium or infinite-rate chemistry is assumed: "if it mixes, it burns". Since age-mixing occurs as well as stream-mixing in a non-premixed PSR, it is assumed that no reaction occurs unless a "hot" turbule (previously reacted to adiabatic equilibrium) mixes with a "cold" turbule (feed turbules of fuel or air, or unreacted mixtures of fuel and air). Thus the only attributes or properties required are the fuel mixture fraction f (the fraction of molecules within a turbule which entered via the fuel feed stream, whether reacted or not) and the "hot" or "cold" attribute (unity or zero degree of reaction, respectively). Adiabatic chemical equilibrium composition and temperature are pre-calculated over the range of mixture fractions zero to unity (all air to all fuel, respectively) using a modified version of the Gibbs function minimization scheme of Gordon and McBride, as described in Reference (9). Mean and standard deviation (rms) values are obtained from the ensemble of equal-mass turbules using the elementary moment equations of descriptive statistics. For example, for temperature,

$$\langle T \rangle \equiv \frac{1}{N} \sum_{i=1}^N T_i \quad (2)$$

and

$$T_{rms} \equiv \left[\frac{1}{N} \sum_{i=1}^N (T_i - \langle T \rangle)^2 \right]^{1/2} \quad (3)$$

Premixed Combustion with Finite-rate Chemistry

For finite-rate gaseous chemistry, either premixed or non-premixed, it was found necessary to develop a new algorithm for integration of the coupled, non-linear, first-order ordinary differential equations describing the variation in composition and temperature with elapsed time within a constant-pressure, adiabatic batch reactor (turbule). The required characteristics for this

algorithm were:

- (a) Speed. The large numbers of species (15-30) and turbules (presently 20, eventually up to 500) requires the fastest possible speed of execution.
- (b) Stability. The infinity of initial conditions, equivalence ratio and chemical time scales resulting from random selection procedures requires an extremely robust algorithm, preferably with automatic stepsize variation.
- (c) Accuracy. This is relatively unimportant, consistent with the crude assumptions on which the entire scheme is predicated. Further, accumulated roundoff errors leading to violation of atom conservation tend to be "flushed away" by the replacement of outflowing turbules with the steady inflow of reactants of prescribed stoichiometry.

An algorithm was developed which meets all of the above criteria, and is described in detail in Reference (10). Briefly, it is a single-step second-to sixth order implicit "exponential-fitting" method (very stable and reasonably accurate) which uses the mixed partial first derivatives or Jacobian matrix both for accuracy (analogous to cubic spline methods) and for convergence (by a modified Newton-Raphson scheme). The step size is automatically adjusted by first attempting to use the entire time elapsed since the turbule was last "updated". Next, by comparing the zero-iterate value of the Newton-Raphson corrections against empirically prescribed bounds on incremental changes in values of the dependent variables (for example, only $\pm 20^\circ\text{C}$ is permitted in a single time step), the stepsize is modified accordingly. The resulting efficiency leads to acceptably short execution times.

Applications

Mixing-limited Combustion of Non-premixed Hydrogen and Air in a Jet-stirred Reactor

A Longwell jet-stirred reactor, such as that described in Reference (11) and illustrated in Fig. 1, may be thought of as an idealization of a highly loaded gas turbine combustor primary zone. For this reactor, the mixing parameter may be estimated to be about $I_m = 10$, with $I_m = 50$ being a practical upper bound.⁽⁴⁾

Conditions chosen for the C/D simulation are summarized in Table I. Partial results of the C/D simulation for conditions of Table I are given in Figures 2 and 3. In Figure 2, it may be seen that for poor mixing (low I_m), the ensemble mean temperature is low, and the rms or standard deviation of temperature is high. As $I_m \rightarrow 0$, a condition of complete segregation (no mixing) is approached, for which no reaction is possible, so that $\langle T \rangle$ must approach the inlet value of 300 K. As $I_m \rightarrow \infty$, a homogeneous PSR condition is approached. Since infinite-rate chemistry has been assumed, "perfect" mixing corresponds to homogeneous chemical equilibrium.

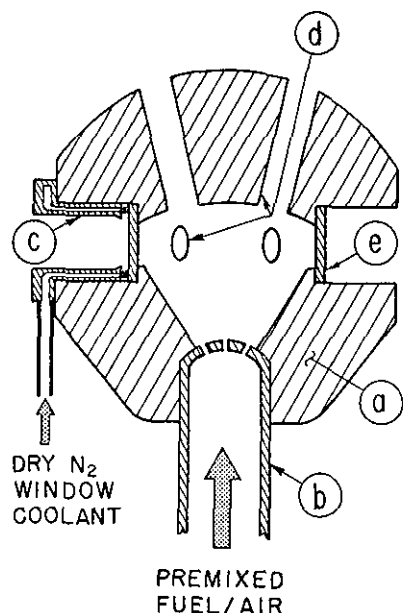


Figure 1. Jet-stirred reactor with optical access. Details: (a) zirconia reactor wall; (b) reactant feed tube with feed jets; (c) spring-loaded window holder; (d) exhaust ports; and (e) sapphire window.

Table I. Conditions for C/D Simulation of Mixing-limited Combustion of Non-premixed Hydrogen and Air in a Jet-stirred Reactor.

| | |
|-----------------------------|---|
| Fuel: | Gaseous H_2 at 300 K |
| Oxidizer: | Air at 300 K |
| Fuel-air equivalence ratio: | 0.25 (fuel lean) |
| Reactor Pressure: | 100 kPa (1 bar) |
| Reactor Loading: | $500 \text{ kg m}^{-3} \text{ bar}^{-2} \text{ s}^{-1}$ |
| Residence Time: | 3-6 ms |

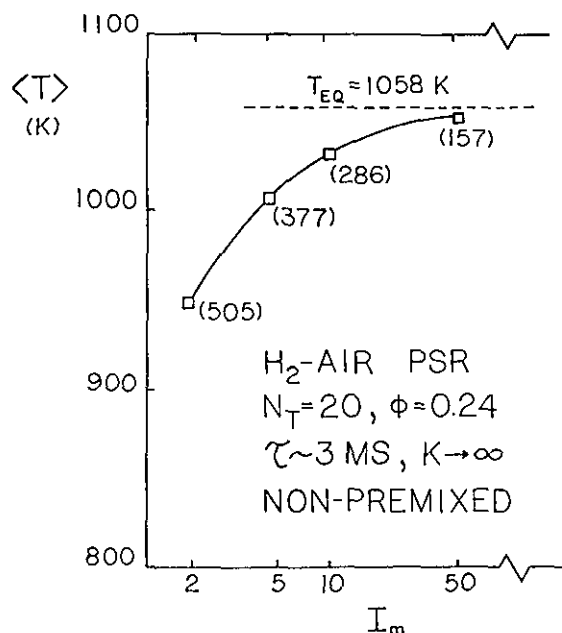


Figure 2. Variation of ensemble-mean temperature with mixing parameter, for conditions of Table I.

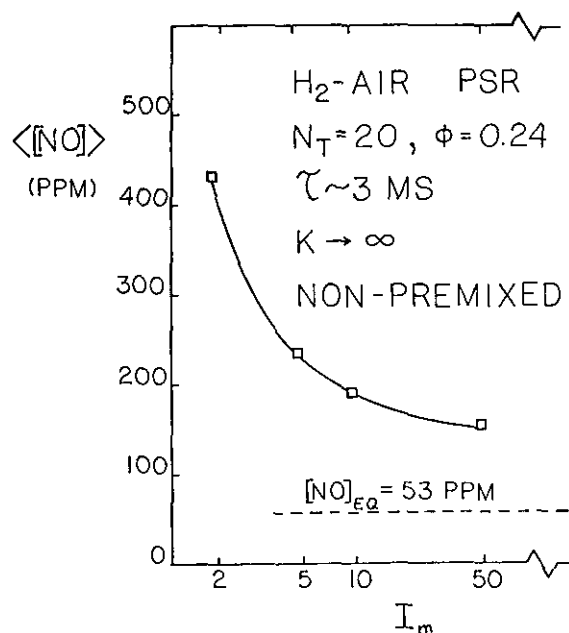


Figure 3. Variation of ensemble-mean NO concentration with mixing parameter, for conditions of Table I.

In Figure 3, the effect of inhomogeneity of fuel-air ratio on NO formation may be clearly seen. In contrast to the well-known dependence of NO concentration on temperature in homogeneous mixtures—either at equilibrium or chemically rate-controlled—the ensemble mean value of NO increases as $\langle T \rangle$ decreases, due to the concomitant increase in T_{rms} . That is, poorer mixing leads to the existence of "hot spots", or turbules of near-stoichiometric fuel-air ratio, where NO concentration is high.

Premixed, Finite-rate Combustion of Hydrogen and Air in a Jet-stirred Reactor

The effects of inhomogeneities in age and degree of reactedness are demonstrated in this first attempt to include finite-rate chemical kinetics with complex chemistry, using the simplified mechanism for H_2 /air combustion given in Table II. Conditions for this simulation were similar to Table I, except that fuel-air equivalence ratio was increased to 0.5. The resulting mean residence time was ca. 5 ms.

The simulation was calculated for five mean residence times, a sufficient time for the ensemble statistics to stabilize. The most interesting result is the predicted contact index⁽¹⁾ for the individual reactions in Table II.

Table II Mechanism, Activation Temperatures and Calculated Contact Indexes for Mixing Limited Combustion of Premixed Hydrogen and Air in a Jet-Stirred Reactor.

$P = 1 \text{ bar}$, $I_m = 10$, $\phi = 0.5$, inlet $T = 300 \text{ K}$;

$\langle T \rangle = 1112 \text{ K}$, $T_{\text{RMS}} = 252^\circ\text{C}$;

$T_{\text{EQ}} = 1643 \text{ K}$, $T_{\text{PSR}} = 1233 \text{ K}$.

| Reaction | T_f/T_b | X_f/X_b |
|--|---------------|-----------------|
| 1. $\text{H}_2 + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ | 16.5 0.5 | 1.3 0.9 |
| 2. $\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$ | 9.4 7.3 | 0.5 1.1 |
| 3. $\text{H}_2\text{O} + \text{O} \rightleftharpoons \text{OH} + \text{OH}$ | 18.1 1.0 | 2.1 1.1 |
| 4. $\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$ | 19.9 4.8 | 2.0 0.5 |
| 5. $\text{N} + \text{O}_2 \rightleftharpoons \text{NO} + \text{O}$ | 6.3 41.4 | 1.0 7.1 |
| 6. $\text{N}_2 + \text{O} \rightleftharpoons \text{N} + \text{NO}$ | 75.5 0.3 | 64.6 1.1 |
| 7. $\text{NO} + \text{M} \rightleftharpoons \text{N} + \text{O} + \text{M}$ | 149.0 -6.1 | 13,840.0 0.9 |
| 8. $\text{H} + \text{H} + \text{M} \rightleftharpoons \text{H}_2 + \text{M}$ | 0.0 101.3 | 1.1 8.6 |
| 9. $\text{O} + \text{O} + \text{M} \rightleftharpoons \text{O}_2 + \text{M}$ | 0.3 115.5 | 1.0 894.1 |
| 10. $\text{H} + \text{OH} + \text{M} \rightleftharpoons \text{H}_2\text{O} + \text{M}$ | 0.0 111.2 | 0.8 1,059.0 |
| 11. $\text{H}_2 + \text{O}_2 \rightleftharpoons \text{OH} + \text{OH}$ | 43.0 25.0 | 1.6 3.4 |

The "contact index" X_j for an individual reaction is defined as the ratio of ensemble-mean reaction rate to the apparent rate based on ensemble-mean properties:

$$X_j \equiv \frac{\langle r_j(\{\sigma_k\}; T) \rangle}{r_j(\langle \{\sigma_k\} \rangle; \langle T \rangle)}, \quad k = 1, \text{NS} \quad (4)$$

where σ_k are the mole numbers of NS species present (9 in the present case), and where r_j represents the usual modified Arrhenius expression for homogeneous, gas phase reaction rate^(1,9):

$$r_j \equiv 10^{B_j} T^{N_j} \exp(-T_j/T) \prod_{i=1}^{\text{NS}} (\rho \sigma_i)^{\alpha'_{ik}} \quad (5)$$

The calculated values of contact index for each forward and reverse reaction are given in Table II. As would be expected, the reactions with highest activation temperatures T_j (and therefore those most sensitive to temperature) show the greatest deviation of X_j from unity.

Discussion and Conclusions

The preliminary results reported here are very encouraging for the use of coalescence/dispersion modeling for prediction of pollutant formation and eventually flame stabilization in high-intensity continuous combustors. Extensions of the concept to flows lacking the strong convective recirculation characteristic of the present system are possible (1), and such work is presently in progress.

An additional benefit of C/D modeling that has not been explored here is the potential ability to predict realistic combustor stability or blowout maps, as well as transient behavior. However, the variation of I_m with combustion temperature during transients would have to be calculated.⁽¹²⁾

Acknowledgements

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