A Numerical Study of Transient Ignition in Opposed-Flow Non-Premixed Combustion using Adaptive Time Integration^{*}

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Introduction

Autoignition of hydrocarbon fuels in air is of great interest in internal combustion application, since it is closely related to the overall performance of diesel engines and the knock problem in spark-ignition engines. It has been recognized that such processes involve complex chemical effects known as the "cool flame" phenomena, as well as fluid dynamic effects such as turbulent mixing and dissipation. The chemical mechanisms for low-temperature hydrocarbon oxidation are fairly well understood [1], and simplified skeletal/reduced mechanisms have been developed [2, 3, 4]. However, much of the chemicalkinetics development and validation have been made in homogeneous systems, and thus do not account for mixture inhomogeneities. A one-dimensional opposed-flow configuration has been commonly used to study the fluid-dynamic effects, which are often characterized by the strain rate. Many of such studies [5, 6, 7], however, deal with identifying ignition limits in a steady context, thereby lacking information of transient ignition history.

Relatively few studies have considered unsteady ignition problems in strained flows. Niioka [8] analyzed a thermal-ignition problem with simple chemistry, demonstrating that ignition delay is more sensitive to strain-rate variation as the system becomes closer to the steady ignition limit. Analogous behavior has been observed in a study considering hydrogen-air system at high temperatures presented elsewhere in this colloquium [9], in which the formal analysis shows that the effect of strain rate is of higher order when the system Damköhler number is sufficiently higher than the critical limit, while more sensitive response was observed near the ignition limit. It is of interest to examine whether the same behavior can be observed in more complex hydrocarbon systems.

Numerical integration of fast transient combustion processes with spatial/temporal stiffness is very difficult due to the associated compressible gas dynamic behavior. From a mathematical standpoint, the standard counterflow formulation with a constant pressure assumption [10, 11] results in a system of high-index differential-algebraic equations (DAE's), such that time-integration methods that implement rigorous error and time-step control can be numerically unstable during periods of rapid change in the solution [12]. Furthermore, for problems with rapid transients, such as ignition, overall solution accuracy demands time-integration methods with adaptive time-step control.

In this study, we present a revised formulation of the opposed-flow problem by incorporating the compressibility effect, thereby reducing the index of the DAE's and ameliorating numerical difficulties. This formulation has been successfully applied to a catalytic ignition problem in stagnation flows [13]. The simulations discussed herein consider ignition in a methane-air mixing layer under various strain-rate conditions. Detailed C_2 chemistry [14] is considered, thus demonstrating the applicability of the numerical method in a relatively complex chemical system. The results include ignition-transient histories and the effects of strain rate on the ignition delay.

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Numerical Method

The governing equations for unsteady axisymmetric (r, x-coordinate) opposed flow are derived based on the finite-separation formulation [10]. With the similarity approximation, u = u(t, x), v/r = V(t, x), T = T(t, x) and $Y_k = Y_k(t, x)$, the conservation equations for mass, axial momentum, radial momentum, energy and species are written as [13]:

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + 2\rho V = \frac{\rho}{p_{tot}}\frac{\partial p}{\partial t} - \frac{\rho}{T}\frac{\partial T}{\partial t} - \rho \bar{W} \sum_{k} \frac{1}{W_{k}}\frac{\partial Y_{k}}{\partial t} + \frac{\partial}{\partial x}(\rho u) + 2\rho V = 0, \tag{1}$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} - 2\mu \frac{\partial V}{\partial x} - \frac{4}{3} \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x}\right) + \frac{4}{3} \frac{\partial}{\partial x} \left(\mu V\right) = 0,$$
(2)

$$\rho \frac{\partial V}{\partial t} + \rho u \frac{\partial V}{\partial x} - \frac{\partial}{\partial x} \left(\mu \frac{\partial V}{\partial x} \right) + \rho V^2 + \Lambda = 0, \quad \text{where} \quad V = \frac{v}{r}, \quad \Lambda = \frac{1}{r} \frac{\partial p}{\partial r}, \tag{3}$$

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p u \frac{\partial T}{\partial x} - \frac{\partial p}{\partial t} - u \frac{\partial p}{\partial x} - \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \rho \left(\sum_k c_{p,k} Y_k V_k \right) \frac{\partial T}{\partial x} + \sum_k h_k W_k \omega_k = 0, \quad (4)$$

$$\rho \frac{\partial Y_k}{\partial t} + \rho u \frac{\partial Y_k}{\partial x} + \frac{\partial}{\partial x} \left(\rho Y_k V_k \right) - W_k \omega_k = 0, k = 1, \cdots, K$$
(5)

where the nomenclature follows that of earlier work [13].

The main distinction of the present formulation compared to that with incompressible approximation is that the hydrodynamic pressure, p, is now included as a dependent variable, and the equation of state is modified as

$$\rho = p_{\text{tot}} W/RT, \quad p_{\text{tot}} = p_{\text{ref}} + p, \tag{6}$$

where p_{ref} is the constant reference pressure. Introducing the variable p requires an additional equation (axial momentum) to be considered, and it allows for a compressible relaxation of the flow field arising from the fast flow transients, thereby alleviating numerical difficulties caused by the high index.

The radial pressure curvature, $\Lambda(t)$, appears as an eigenfunction of the system, which behaves as an index-two variable. Because the system is in a special form called Hessenberg index-two, an additional, and necessary, reduction of the system to index-one can be achieved by the substitution $\Lambda = \partial \phi / \partial t$, with arbitrary choice of the initial condition for ϕ [12, 13].

Equations (1) - (5) are subject to the boundary conditions:

$$x = 0: u = u_0(t), V = 0, T = T_0(t), Y_k = Y_{k,0}(t),$$
(7)

$$x = L : u = u_L(t), V = 0, T = T_L(t), Y_k = Y_{k,L}(t), p = 0.$$
(8)

Time integration of the DAE system is accomplished as a method-of-lines approach, using DASSL [15], which is an implicit, variable-order method with adaptive time-step control. The spatial differencing employs a staggered grid, with the axial velocities represented on the control-volume faces and all other variables at the nodes. To achieve stability, numerical damping in the form $\sigma(\Delta x)\partial^2 p/\partial x^2$ is added to the continuity equation (1), where a sufficiently small value of σ is chosen to ensure that the solution is not affected by the damping term.

Results and Discussion

As a test of the numerical method, we consider the ignition problem in a pure methane against hot air under constant pre-ignition strain rates, using GRI v1.2 as the chemical mechanism. The inlet separation is fixed at 1 cm and the pressure is at 1 atm. The fuel-side temperature is held at 300K and the hot-air temperature is at 1400K, which is the main ignition heat source. Under this condition, the steady ignition limit is found to be at $\chi_{st} = 17.3 \ s^{-1}$, which occurs at $u_0 = u_L = 2.2 \ m/s$, where $\chi_{st} = 2\alpha (\partial \xi / \partial x)_{st}^2$ is the scalar dissipation rate at the stoichiometric condition, ξ the mixture fraction based on the formula by Bilger [17], and $\alpha = \lambda / \rho c_p$ the thermal diffusivity. It has been shown that χ_{st} better represents the flow residence time scale than the strain rate in unsteady flows with fast time scales [16]. For each transient calculation, a steady solution is obtained with the identical boundary conditions by suppressing all reaction rates and used as the initial condition. The effects of strain rates on ignition are studied by computing solutions for various values of χ_{st} that are in ignitable states ($\chi_{st} < 17.3$). Figure 1 illustrates a typical evolution history of temperature and OH profiles through the ignition event. During a very short period of time (B to E), the ignition kernel develops and propagates into the location at which diffusion flame is established. The temporal evolution of the spatial maximum values for temperature and a few intermediate species are further shown in Fig. 2. The temporal change of some minor intermediates such as HCO, which correlates closely with heat release [18], exhibits a very fast transient response. The adaptive, stiff time integrator employed in this study permits large time steps throughout most of the calculation, while accurately capturing the abrupt transients when necessary.

From Fig. 2, the ignition delay can be defined as the time at which the steep temperature rise occurs. The variation of the ignition delay for a range of scalar dissipation rate is shown in Fig. 3. It is clearly seen that, as the characteristic flow time is reduced to approach the steady ignition limit, the ignition delay becomes more sensitive to the variations in the strain rate. The result is consistent with those observed in hydrogen-air mixtures [9].

Many ignition models in turbulent reacting flows are based on the concept that ignition occurs instantaneously when the local scalar dissipation rate at the ignition kernel falls below the steady ignition limit. This is based on the assumption that the flow field variation is sufficiently slower than the ignition delay. However, the result in Fig. 3 suggests that this assumption may not hold, since ignition delay is a strong function of the flow field *near* the onset of ignition. Further study is needed to better understand this issue.

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References

- [1] Westbrook, C. K. and Dryer, F. L., Prog. Energy Combust Sci., 10, 1 (1984).
- [2] Hu, H. and Keck, J. C., SAE Paper No. 872110 (1987).

[3] Cowart, J. S., Keck, J. C., Heywood, J. B., Westbrook, C. K. and Pitz, W. J., Twenty-Third Symposium (International) on Combustion, The Combustion Institute, pp. 1055-1062 (1990).

[4] Müller, U. C., Peters, N. and Liñán, A., Twenty-Fourth Symposium (International) on Combustion, pp. 777-784 (1992).

- [5] Darabiha, N. and Candel, S., Combust. Sci. Tech., 86, 67 (1992).
- [6] Balakrishnan G., Smooke, M. D. and Williams, F. A., Combust. Flame, 102, 329 (1995).
- [7] Kreutz, T. G. and Law, C. K., Combust. Flame, 104, 157 (1996).

[8] Niioka, T., Eighteenth Symposium (International) on Combustion, The Combustion Institute, pp. 1807-1813 (1981).

[9] Mellado, D. J., Sánchez, A. L., Kim, J. S. and Im, H. G., "High-Temperature Radical Growth in the Hydrogen-Oxygen Counterflow Mixing Layer," in 17th International Colloquium on the Dynamics of Explosions and Reactive Systems, Heidelberg, Germany (1999).

[10] Kee, R. J., Miller, J. A., Evans, G. H. and Dixon-Lewis, G., Twenty-Second Symposium (International) on Combustion, The Combustion Institute, pp. 1479-1494 (1988).

[11] Lutz, A. E., Kee, R. J., Grcar, J. F. and Rupley, F. M., "OPPDIF: A Fortran Program for Computing Opposed-flow Diffusion Flames," *Sandia Report* SAND96-8243, May 1996.

[12] Brenan, K. E., Campbell, S. L. and Petzold, L. R., Numerical Solution of Initial-Value Problems in Differential Algebraic Equations, 2nd ed., SIAM, Philadelphia, PA (1996). [13] Raja, L. L., Kee, R. J. and Petzold, L. R., Twenty-Seventh Symposium (International) on Combustion, The Combustion Institute, in press (1998).

[14] Frenklach, M., Wang, H., Goldenberg, M., Smith, G. P., Golden, D. M., Bowman, C. T., Hanson, R. K., Gardiner, W. C. and Lissianski, V. "GRI-Mech—An Optimized Detailed Chemical Reaction Mechanism for Methane Combustion," *GRI Report* No. GRI-95/0058, November 1, 1995.

[15] Petzold, L. R. "A Description of DASSL: A Differential/Algebraic System Solver," Sandia Report SAND82-8637, Sept. 1982.

[16] Im, H. G., Chen, J. H. and Chen, J. Y., Combust. Flame, in press (1999).

[17] Bilger, R. W., Twenty-Second Symposium (International) on Combustion, The Combustion Institute, pp. 475-488 (1988).

[18] Najm, H. N., Paul, P. H., Mueller, C. J. and Wyckoff, P. S., Combust. Flame, 113, 312 (1998).





Figure 1: Evolution of temperature and OH profiles during ignition for $u_0 = 1 \text{ m/sec}$ or $\chi_{\text{st}} = 7.06$.

Figure 2: Transient evolution of the spatial maximum temperature, OH and HCO mole fractions for $u_0 = 1$ m/sec or $\chi_{st} = 7.06$.



Figure 3: Ignition delay as a function of the scalar dissipation rate, demonstrating the sensitive response near the steady ignition limit.