

# 데토네이션 파 해석을 위한 탄화수소 연료/산화제의 Induction Parameter Modeling

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## Induction Parameter Modeling of Hydrocarbon Fuel/Oxidizer for Detonation Wave Analysis

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### ABSTRACT

A general procedure of obtaining reliable one-step kinetics model for hydrocarbon mixture from the fully detailed chemistry is described in this study. One-step theoretical formulation of the induction parameter model IPM uses a theoretical reconstruction of the induction time database obtained from a detailed kinetics library. Non-dimensional induction time calculations is compared with that of detailed kinetics. The IPM was latter implemented to fluid dynamics code and applied for the numerical simulation of detonation wave propagation. The numerical results including the numerical smoked-foil record show the all the details of the detonation wave propagation characteristics at the cost around 1/100 of the detailed kinetics calculation.

**Key Words** : Induction Parameter Model (IPM), Detailed Kinetics, Detonation Wave Propagation, Computational Fluid Dynamics,

### 1. Introduction

Accurate numerical simulation of detonation phenomena requires correct information about the chemical induction time for the mixture under consideration. A detailed chemical kinetic mechanism should thus be included in fluid dynamic simulations. In practice, however, such a comprehensive approach may pose serious challenges in computational resource and turn-around time, especially for hydrocarbon mixtures. Computing time for the coupled fluid dynamics and chemical kinetics equations is basically proportional to the number of equations, i.e. number of species conservation equations and fluid dynamics

equations. Evaluation of reaction rate constants, time consuming calculations of exponential functions, takes a computing time proportional to the number of reactions. In addition, an implicit algorithms to overcome the steepness of the chemical kinetics equations takes a computing time proportional to the cubic number of species. Thus the computing time of the coupled fluid dynamics and chemical kinetics equations is at least proportional to the number of species involved. Table 1 is the computing time compared for various fluid dynamics models.

Most comprehensive chemical kinetics library for hydrocarbon mixture would be the GRI Mech-3.0[1] This library involves 53 species in 325 reaction steps in library. Even if a reduced chemical mechanism involving 15 to 20 species is employed to obtain reliable

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results, the computational burden is still enormous.[2] Since comprehensive numerical calculations of detonation waves with detailed chemical kinetics are extremely expensive, a simplified kinetics model based on chemical induction time was often used.[3] The database obtained from detailed kinetics library can be integrated into single or dual parameter model kinetics model over a broad range of flow conditions to determine the chemical induction time. An optimization algorithm such as the least-square method can be used to optimize the results of induction time. The resultant kinetics model is expected to provide much more accurate results than those from a simple ZND approach at the same computational cost. In the present study, general procedure of obtaining one-step kinetic model is developed and implemented to fluid dynamics code to mimic the global detonation physics.

Table 1 Computing time for coupled fluid dynamics and chemical kinetics equations with various kinetics models. The Computing times were obtained with an implicit inviscid fluid dynamics solver model at Pentium III 650MHz processor.

Fluid dynamics/ Kinetics Model	Comuting time $\mu\text{s}/\text{iteration}/\text{node}$
Non-Reacting flow	9.60
Non-Reacting flow + 1 more conservation equation	12.73
Non-Reacting flow + 1 more conservation equation with exponential source term	16.01
5 species and 1 step kinetics for CH <sub>4</sub> /Air	30.53
9 Species and 19 steps kinetics for H <sub>2</sub> /Air	80.40
22 species and 34 steps kinetics for CH <sub>4</sub> /Air	233.06

## 2. Induction Parameter Model

### 2.1 Chemical Kinetics Database

The ignition of cracked JP-7 fuel/oxygen mixture was studied in the present study. The composition of the cracked (gasified) JP-7 fuel was obtained from a GASL internal document submitted to NASA Marshall [4] The major species and their mass fraction are summarized in Table 2.

Table 2 Composition of Cracked JP-7 Fuel

Component	H <sub>2</sub>	CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>2</sub> H <sub>4</sub>
mass fraction, $y_i$	0.005	0.383	0.293	0.319
mole fraction, $x_i$	0.052	0.503	0.205	0.240

All the ignition calculations were carried out under constant-volume conditions simulating the process behind the shock of a detonation wave front. The analysis employed the LSODE solver along with the Chemkin-II package [5]. The GRI Mech-3.0 chemical kinetics database for hydrocarbon fuels was used, in which the high-pressure combustion mechanisms was also considered. The oxygen/fuel mole ratio was fixed at 2.0, corresponding to an O/F ratio of 3.75, or an equivalence ratio of 1.23. The initial pressure,  $p_i$ , considered are 0.1, 0.3, 1.0, 3.0, 10, 30, 100, 300 and 1000 bar, and the initial temperature,  $T_i$ , ranges from 900 to 1,800K with an increment of 100K. The corresponding chemical induction time (i.e., ignition delay), defined as the time at which the maximum temperature gradient occurs, are given in Fig. 1.

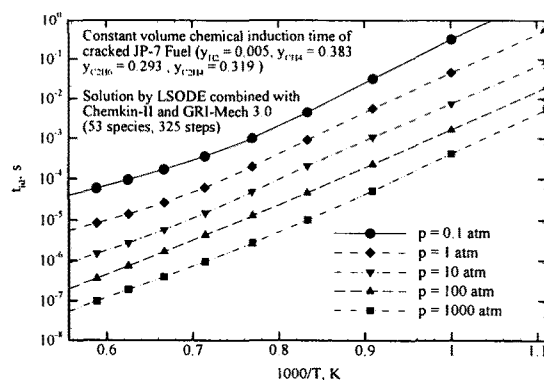


Fig. 1 Effect of initial temperature and pressure on chemical induction time for cracked JP-7 fuel and oxygen mixture

### 2.2 Correlation of Kinetics Database

Results of the induction time database,  $\tau^*$ , obtained above, can be correlated with the initial temperature and pressure through the following functional form.

$$\tau^*(T, p) = \exp(f(T, p)) \quad (1a)$$

where

$$f(T, p) = A^*(p) + \frac{E^*(p)}{T - T^*(p)} \quad (1b)$$

where the coefficients  $A^*$ ,  $E^*$  and  $T^*$  are obtained for each pressure by means of an optimization algorithm such as the least-square method. The Newton iteration method is then used to solve the resulting set of non-linear equations. The same procedure is repeated for the range of pressure under consideration. The pressure dependency of the coefficients can be expressed with a third-order polynomial. The approximation error is typically less than 10%. A higher-order polynomial does not improve the accuracy.

By introducing an induction parameter,  $Z$ , representing the mass fraction of the product, the progress of reaction can be modeled using the following equation.

$$\frac{dZ}{dt} = w(Z) = \frac{1}{\tau(T, p)} \quad (2)$$

Since the induction time,  $\tau^*(T, P)$  is defined as the time instant at which the maximum heat release occurs, we assume that

$$w_{\max} = \frac{1}{\tau^*(T, p)} \quad (3)$$

The induction time data is obtained for a constant-density process. The temperature and pressure can be defined as linear functions of the induction parameter by assuming constant properties and constant volume process.

$$T(z) = T_0 + T_1 Z, \quad p(z) = p_0 + p_1 Z$$

and  $f(T, P) = f(Z)$  (4)

where  $T_0$  and  $p_0$  are the initial temperature and pressure, respectively, and  $T_1$  and  $p_1$  are the differences of temperature and pressure between the burnt and unburnt mixtures.

Based on mathematical intuition, let the reaction rate  $w$  be defined as

$$w(Z) = \frac{C}{f'(Z)} \exp(-f(Z)) \quad (5)$$

Since the maximum value of  $w$  should be equal to  $w_{\max}$  defined in Eq. (3), we may find the coefficient  $C$  from the derivative of  $w(z)$ . By assuming  $A^*$ ,  $E^*$  and  $T^*$  are locally constant, and by taking the Taylor series approximation of  $f(z)$  to second order, the coefficient  $C$  is approximated as

$$C = -\frac{4T_1}{E^*} \quad (6)$$

Finally, the induction parameter model (IPM) equation is summarized as

$$\frac{dZ}{dt} = w(Z) = C \frac{(T - T^*(p))}{E^*(p)T_1} \exp\left(-A^*(p) - \frac{E^*(p)}{T - T^*(p)}\right) \quad (7)$$

where  $A^*$ ,  $E^*$  and  $T^*$  are obtained from the curve fit of the detailed kinetics data. The coefficient  $C$  may be varied with local flow conditions, since  $E^*$  in Eq. (6) is a function of pressure.

By assuming a constant-volume process, the induction time is obtained from the IPM for the same temperature and pressure ranges used for the detailed kinetics calculations. The computed value of the coefficient,  $C$ , is slightly less than 1.0 for most of the conditions and becomes greater than 1.5 at high pressures where the induction time is under-predicted. Since the present model is based on the curve-fitted data and some approximation are already included in the IPM, the constant in Eq. (6) can be adjusted to 1.0 to improve the overall accuracy. The induction time is re-calculated using this new constant.

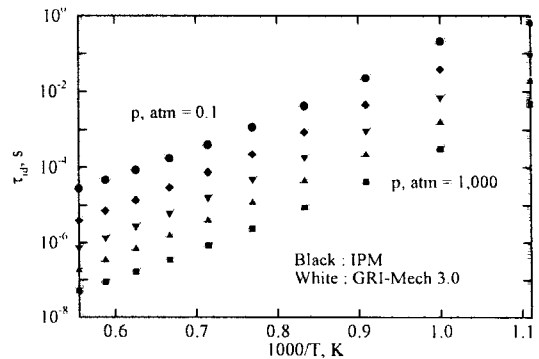


Fig. 2 Comparison of induction time between detailed kinetics scheme and IPM with  $C = 1.0$ .

Fig. 2 shows the result with  $C = 1.0$ , compared with the detailed kinetics data. Remarkably good agreement is obtained between the detailed kinetics and the IPM results. The logarithmic-scale error of the induction time is less than 1% for most of the conditions except at very low pressures or temperatures. Fig. 3 shows the temperature profiles compared with the detailed kinetics

results for several temperature and pressure conditions. Note the burnt gas temperature is taken from the CEA result and thus leads to an exact agreement.[6] In addition to a slight disagreement of the induction time, the IPM result shows an early temperature rise due to the mathematical characteristics of Eq. (7). The deviation, however, appears to be modest, and fairly good agreement is achieved.

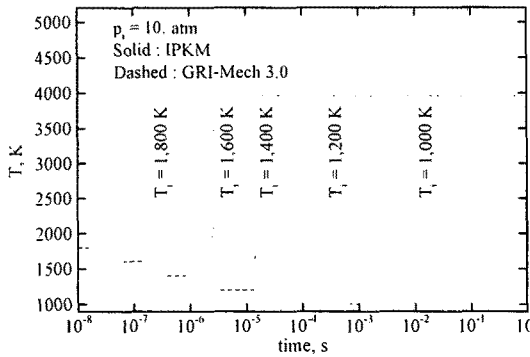


Fig. 3 Comparison of temperature evolution for various initial temperature at  $p_1 = 10$  atm.

### 2.3 Implementation to Fluid Dynamics Equations

The IPM is incorporated into a compressible flow solver for simulating detonation wave dynamics. The coupled governing equations in two-dimension are arranged in a vector form as follows.

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \\ \rho Z \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho e + p)u \\ \rho Zu \end{bmatrix} + \frac{\partial}{\partial y} \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho e + p)v \\ \rho Zv \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (3)$$

where

$$e = \frac{R(Z)}{\gamma(Z)-1} T + \frac{1}{2}(u^2 + v^2) - Zq \quad \text{and} \quad p = \rho R(Z)T. \quad (4)$$

Ideal gas assumption is used in this formulation, but the specific heat ratio and the gas constant are considered as functions of the induction parameter. The fluid dynamics equations are discretized by means of Roe's Riemann solver with a third-order variable extrapolation method and a TVD limiter. Both a fourth-order Runge-Kutta method and a

second-order implicit method are used for temporal discretization.[7,8] The implicit method, however, is much more preferred, not only because of its larger time step, but also the earlier triggering of unstable motions. In the implicit code, the chemical source term is treated fully implicitly, and sub-iterations are employed to reduce the numerical errors arising from implicit approximations.

## 3. Detonation Wave Propagation

### 3.1 One-Dimensional Detonation Wave

In the present study of the detonation wave propagation through a cracked JP-7 fuel/oxygen mixture of an equivalence ratio of 1.23 was considered with a preconditioned state of 1 MPa and 400 K. The Chapman-Jouguet (C-J) detonation properties, calculated using the CEA code [6], were used as an initial condition for both the unburned and burned states of the gas mixture. The theoretical C-J detonation properties obtained from the CEA code are  $p/p_1 = 26.884$ ,  $T/T_1 = 10.672$ ,  $\rho/\rho_1 = 1.8384$ , and  $V_{CJ} = 2580.1$  m/s. The gas properties, including the amount of heat release, were determined by solving the Rankine-Hugoniot relation with the C-J constraint. They are  $v_b = 1.1484$ ,  $v_u = 1.2992$ ,  $R_u = 293.23$  J/kgK,  $R_b = 401.79$  J/kgK, and  $q = 1.0422107$  J/kg.

A series of one-dimensional numerical simulations were first carried out to determine the grid size required to resolve the detonation wave dynamics in a cracked JP-7 fuel/oxygen mixture. Fig. 4 shows the one-dimensional detonation wave propagation for two different numerical grids. Both grids show good agreement in the overall characteristics such as the wave locations. The von Neumann spike is well resolved with a dense grid, but not with a coarse grid, although the resolution is thought to be not sufficient to capture all of the detailed physics inside the spike. The pressure drops behind the spike to the C-J condition and then expands to satisfy the closed end condition. The calculated C-J pressure in Fig. 4 is 26.8 MPa, which agrees quite well with the theoretical C-J value obtained from the CEA Code. The speed of the detonation wave propagation, estimated by the

locations of the wave front, is 2580.3 m/s, is also in good agreement with the theoretical result.

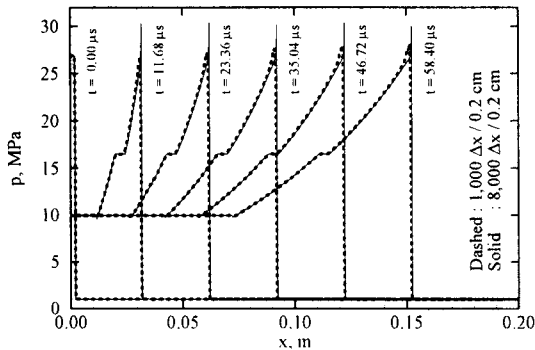


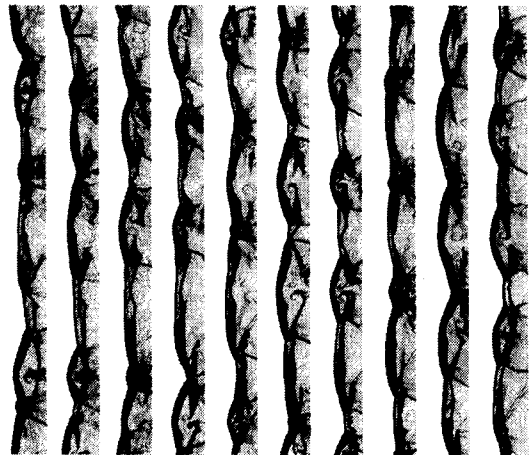
Fig. 4 Temporal evolution of detonation wave propagation with different numerical grid.

A quasi-stationary wave simulation was then conducted by assuming the incoming flow at the C-J detonation speed in order to avoid the numerical difficulties arising from the simulation of a propagating wave, for which a large number of grid points or even an adaptive grid clustering at the wave front are required. The results showed that about 100 grid points with a grid size less than 0.1mm were necessary to resolve the detonation wave front dynamics under realistic operation conditions.

Based on the one-dimensional study, the two-dimensional structure of the detonation wave was investigated in detail. The computational zone measures 20 mm in length and 30 mm in height. The C-J properties and a flow speed of 2590.1 m/s (greater than the C-J speed by 10 m/s) were employed as the initial condition for all the computational cells except for the inflow boundary, which was specified based on the unburned mixture condition. Periodic boundary conditions were used for the lower and upper boundaries. The exit condition was assumed to be supersonic. A total of 500 grid points were distributed along the flow direction, of which 400 grid points with a size of 25 nm were evenly distributed around the detonation wave. 600 grid points with a uniform size of 50 nm were used in the transverse direction. A physical time step of  $7.87 \times 10^{-12}$  s was used based on

the CFL number of 1.0, and a maximum of four sub-iterations were used within each time step.

Fig. 5 shows a series of numerical Schlieren images i.e., (plots of the density gradient field). The temporal evolution of the detonation wave front and the ensuing cellular structure are clearly observed. The detailed structure of the detonation wave front was captured well, including the formation of the transverse waves and vortex generation. One important characteristic of the cracked JP-7/oxygen mixture under consideration is that the cell structure is quite irregular. The cell width varies from 5 to 10 mm.



← Direction of the Detonation Wave Propagation

Fig. 5 Numerical Schlieren images showing the temporal evolution of the detonation wave front and the cellular structure.

Fig. 6 shows the time histories of the shock location and the post-shock pressure along the middle line of the computational domain. The data analysis of the detonation wave front dynamics is rather complex due to the existence of several modes of unsteady motions. The peak pressure behind the shock wave, that may corresponds to the von Neumann peak, oscillates within the range between 35 and 100 MPa, and the frequency of the dominant wave motion is around 100 MHz. This irregular oscillation is also observed from the history of the leading shock wave location. The averaged speed of the wave propagation is estimated to 30 m/s relative to the inflow

speed. Thus the detonation wave propagation speed estimated from the two-dimensional simulation is 40 m/s higher than the theoretical C-J detonation speed of 2580.1 m/s.

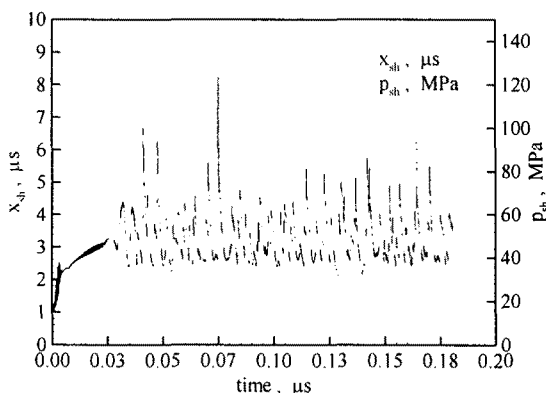


Fig. 6 Time history of shock wave location at the middle of the computational domain and the pressure behind the shock wave.

#### 4. Conclusions

A general procedure of obtaining reliable one-step kinetics model for hydrocarbon mixture is devised in the present study. One-step theoretical formulation of the IPM based on the induction time database of the detailed kinetics library produces a remarkable reproduction of the detailed kinetics results at a significantly reduced cost.

The IPM was implemented to the fluid dynamics code and applied for one- and two-dimensional the detonation wave propagation simulation. The numerical results shows a all the details of the detonation wave propagation characteristics at the cost around 1/100 of the detailed kinetics calculation.

#### Acknowledgements

This work is sponsored by NASA Marshal Flight Center with the Grant No. NAG8-187

under supervision of Mr. B. Bullard.. The first author was also supported by the Post-doctoral Fellowship Program of Korea Science & Engineering Foundation (KOSEF).

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