One- and Two-Dimensional Analysis
on Jet A/Air Two-Phase Detonation

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1. Introduction

Jet A fuel as well as JP8 and JP-10 has been widely used for aviation purposes. A liquid fuel has a higher density and heat value per unit volume than a gaseous fuel. However, liquid fuel must be atomized, vaporized, mixed with air, and ignited within the timescale required during an operation. Inherent to the weight of larger molecules, liquid fuel has a strong tendency of evaporation and ignition.

Aviation fuels, such as Jet A, JP-8 and JP-10, are less volatile than other liquid fuels and have long self-life storage, but are envisioned as operating fuels for liquid-fueled pulse detonation engines (PDE) due to their low volatility. In addition to such low volatility, aviation fuel has a low vapor pressure; hence it tends to have a longer ignition delay time compared with gaseous fuels. Then it is difficult to detonate these fuels directly at the ambient temperature and pressure. Analytical study on Jet/air two-phase detonation has not been carried out much up to now because of its complicate fuel structure

Two-phase detonation studies are not much reported except that by Cheatham and Kailasanath[1-3] who reported the numerical dependence of droplet diameter and evaporation rate on detonation. Kailasanath[4] just recently gave a brief review on two-phase detonation study.

This study will present the numerical 1D and 2D analyses of Jet A fuel by liquid-gas two-phase compressible Euler equations with a chemical reaction mechanism and evaporation model of a two-step Jet A. The present calculation of Jet A detonation is then compared with the experimental data and the equilibrium data using a STANJAN code. The effect of several physical values, such as droplet diameter, pre-vaporization, and fuel concentration, on detonation velocity are discussed.
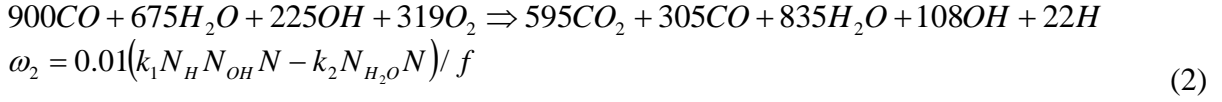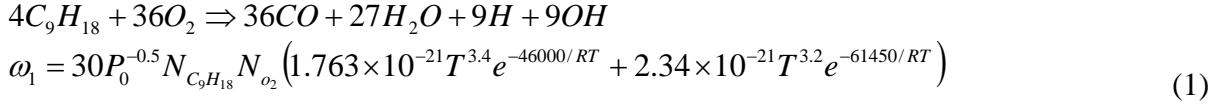
2   Computational method, chemical reaction, and evaporation

1D modified Euler equations are used to the governing equations of Jet A/air mixtures. A time-splitting way is applied because of the inhomogeneous governing system of equations for two-phase system, but otherwise, homogeneous one for single-phase case. For two-phase system the equation system is split into homogeneous partial differential equations and ordinary differential ones. The Godunov-type inter-leaving is used to the PDE part and the same time step is applied to the ODE part. A non-split Godunov-type MUSCL Hancock partial differential solver is applied to the present calculation with a 2nd order accuracy in space and time for the linear advection equation.
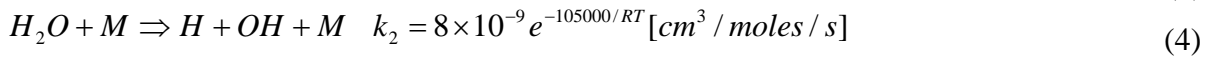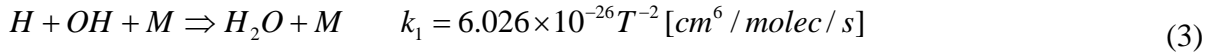
To reduce a computational effect, a simple and inexpensive HLLC Riemann solver is used for the condensed phase as well as the gaseous one. The integration is performed using the high order VODE subroutine from CHEMKIN-II package. The ODE system is solved with the backward differentiating formulae by investigating whether the system equations are stiff.

2.1 Reaction model for Jet A

Although Jet A is composed by $C_{12}H_{23}$, but this time C_9H_{18} is used in stead to represent a Jet A fuel. A four-step chemical reaction model is used for a reaction of hydrocarbon. The four-step mechanism is as follows:

$$4C_9H_{18} + 36O_2 \Rightarrow 36CO + 27H_2O + 9H + 9OH$$
$$\omega_1 = 30P_0^{-0.5}N_{C_9H_{18}}N_{o_2}\left(1.763\times10^{-21}T^{3.4}e^{-46000/RT} + 2.34\times10^{-21}T^{3.2}e^{-61450/RT}\right) \tag{1}$$

$$900CO + 675H_2O + 225OH + 319O_2 \Rightarrow 595CO_2 + 305CO + 835H_2O + 108OH + 22H$$
$$\omega_2 = 0.01\left(k_1 N_H N_{OH} N - k_2 N_{H_2O} N\right)/f \tag{2}$$

where $f = 9/4$.

$$H + OH + M \Rightarrow H_2O + M \qquad k_1 = 6.026\times10^{-26}T^{-2}\,[cm^6/molec/s] \tag{3}$$
$$H_2O + M \Rightarrow H + OH + M \quad k_2 = 8\times10^{-9}e^{-105000/RT}\,[cm^3/moles/s] \tag{4}$$

Equations (1) and (2) are the overall equations and Equations (3) and (4) are radical recombination and its backward step.

2.2 Evaporation model for droplets

Two-phase flow case needs an evaporation model   In this study a simplified combustion law of the d^2-type is applied. The mass transfer factor is shown as:

$$\Delta c = \frac{3\phi_l \rho_l}{\tau}(1 + 0.276\sqrt{Re}) \tag{5}$$

Where ϕ_l is the condensed phase volume fraction, ρ_l the material density, τ the characteristic combustion time, and Re the Reynolds number. τ is related to the particle life time and can be expressed as:

$$\tau = K_r d_0^2 \tag{6}$$

and d_0 is an initial particle diameter and K_r is the burning rate constant, which is expressed as: initial particle diameter and K_r is the burning rate constant, which is expressed as:

$$K_r = \frac{\rho_l C_{pg}}{8\lambda \ln(1+B)} \tag{7}$$

In Eq.(7) C_{pg} is the specific heat of the gas, λ the thermal conductivity, and B the transfer number. The mass transfer number **B** is proportional to the amount of Jet A in the mixture and droplet diameter. Eq. (5) is not a function of the Weber number since it is more or less about 10 or less in the present case, which implies that a majority of the droplet would not break up.

3   Results and discussion

One- and two-dimensional Jet A/air two-phase detonations are studied numerically using Euler equations with a Jet A/air four-step reaction mechanism and evaporation model. In this extended abstract two-dimensional gas-phase Jet A/air detonation is simulated to compare with the detonation velocity calculated using the numerical program of the STANJAN code. In the full paper one- and two-dimensional two-phase detonation will be simulated and will be discussed their properties.

3.1 Jet A/air detonation velocity

The velocity of two-dimensional Jet A vapor/air detonation is calculated by two ways to compare; one by STANJAN equilibrium code and another by the present two-phase code. Figure 1 shows the detonation velocity comparing between STANJAN equilibrium one and the present original two-phase detonation code together with JP10/air case. The data point of detonation velocity for Jet A by the original code is only one, but is compared with the STANJAN equilibrium data and JP10 data. The Jet A detonation velocity is a little over-driven value, but its difference with the equilibrium data is about 6 %.
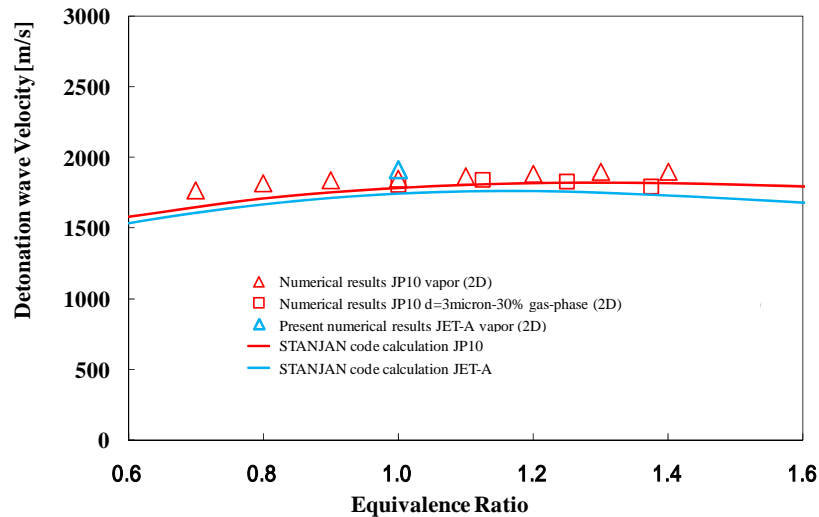

Fig. 1 Jet A/air detonation velocity to the equivalence ratio.

3.2 Maximum pressure records of Jet A/air gas-phase detonation

Figure 2 is the maximum pressure traces of Jet A/air gas-phase detonation. The cell structures are quite smaller than the JP10/air cases. It seems that the Jet A fuel is more energetic than the JP10 fuel.
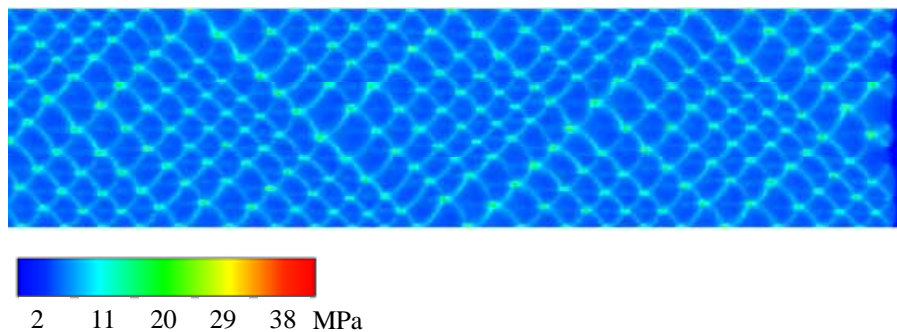

Fig.2 Maximum pressure trajectories of Jet A/air gas-phase detonation

3.3 Gas-phase temperature profiles of Jet A/air detonation

Figure 3 shows the gas-phase temperature profiles of Jet A/air detonation. The cell size of Jet A/air detonation is smaller than that of JP10/air detonation.
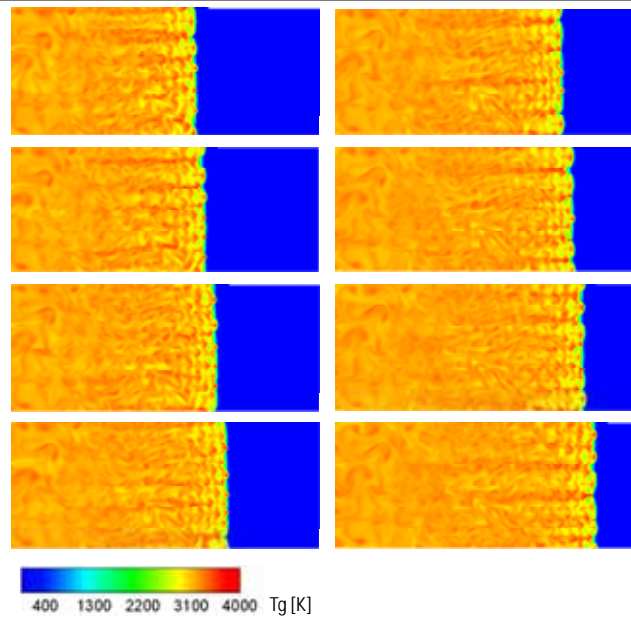
Fig. 3 the gas-phase temperature profiles of Jet A/air detonation.

4 Summery

There are few data for Jet A/air or Jet A/O2 detonations. The present extended abstract shows the detail numerical analysis of Jet A/air comparing with the equilibrium data and JP10/air data. Since this abstract provides only gaseous detonation cases, the cell size of Jet A/air detonation is quite small, but the two-phase detonation case will give us a larger cell or non-detonation case. The data will give us the important information for detonation devises such as two-phase PDE.

Acknowledgement

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