Numerical Analysis of Solid Propellant Ignition
~ Numerical Formulation Assessment~

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Keywords: Propulsion, Solid Propellant Ignition

Abstract

For a simple one-dimensional ignition problem a mathematical model is described to investigate the difficulties in numerical simulations. Some computation results are obtained and comparison is made with analytical solution. Discussions are made on topics such as 1) coordinate transformation, 2) gas-phase and solid-phase analysis; (divergence form of the governing system, a finite-volume discretization, implicit time integration, upwind split flux, spatial accuracy improvement are described. Mass, reagent mass, and energy conservations are solved.), and 3) method to determine quantities on the burning surface (matching). Results obtained for small values of the non-dimensional pressure show a steady-combustion and good agreement with the analytical solution. Numerical instability appeared for larger values of the pressure, discussion on the cause of the problem is made. This effort is a part of a study of flame spread phenomena on solid propellant surface.

Introduction

The phenomenon of flame spread is seen during the ignition period. (Fig.1) To understand flame spread over solid propellant is very important to promote advanced solid propulsion, and further more it will deepen the understanding of the ignition, erosive burning, and unsteady combustion, and so on. It is at the same time very difficult since it is essentially multi-dimensional and unsteady phenomenon.

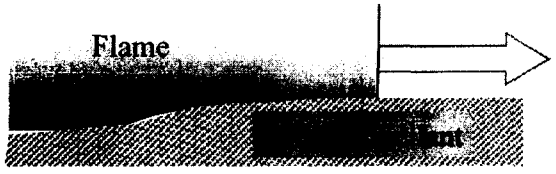


Fig. 1 Flame Spread

A system of governing equations and its non-dimensional form are prepared to describe a mathematical model of two-dimensional unsteady combustion of solid propellant in order to investigate flame spread. While this effort is in progress, we need to consider several things to overcome before we perform a real flame spread simulation. There are various challenging aspects, mainly related to the essential multi-dimensionality and unsteadiness of the flame spread phenomena. Other difficulties are in the numerical procedures of dealing with the phase-interface. There are basically two types of methods for it, namely, "fitting" and "capturing" (Fig.2).

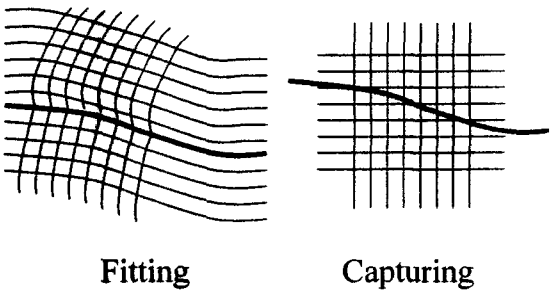


Fig. 2 Types of methods of interface handling

Before studying multi-dimensional problems, it is necessary to check numerical method in one-dimensional problem where some theoretical solutions and analysis exist. A flame spread problem can be a problem of ignition when it is reduced to one-dimension (Fig. 3). In this report, for a simple one-dimensional ignition problem, a numerical model for "fitting" is described to investigate the difficulties in numerical simulations.

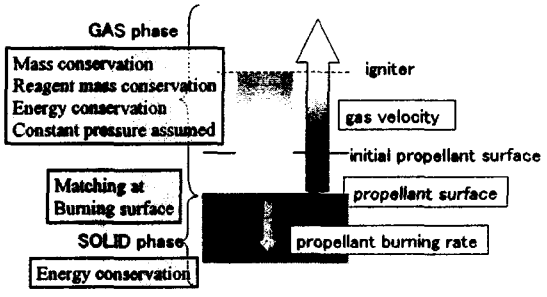
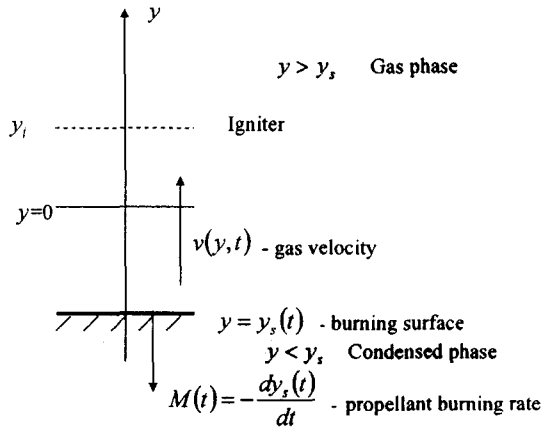


Fig. 3 One-dimensional ignition problem

One-dimensional Ignition Problem

In the relating paper[1] a mathematical formulation will be given for one-dimensional ignition problem shown in Fig.4.



time $0 \le t < \infty$

space coordinate $-\infty < y < \infty$

Fig. 4 Dimensional description of one-dimensional ignition problem

The functions $T_c(y,t)$ - condensed phase temperature, $T(y,t)$ - gas phase temperature, $Y(y,t)$ - reagent mass fraction in the gas phase, $v(y,t)$ - gas velocity, and $M(t) = -\frac{dy_s}{dt}$ - propellant burning rate should be found using the governing equations for the condensed phase and the gas phase. The detailed description of the governing equations and their non-dimensionalization shall be presented in Ref.1.

The normalized space and time coordinate system (η,τ) is transformed to the coordinate moving with the burning surface

$$\begin{cases} \tau' = \tau \\ \eta' = \eta - \eta_s(\tau) \end{cases}$$

$$\begin{cases} \left.\frac{\partial}{\partial \tau}\right|_{\eta} = \left.\frac{\partial}{\partial \tau'}\right|_{\eta'} + \mu \left.\frac{\partial}{\partial \eta'}\right|_{\tau'} \\ \left.\frac{\partial}{\partial \eta}\right|_{\tau} = \left.\frac{\partial}{\partial \eta'}\right|_{\tau'} \end{cases}$$

where $\mu(\tau) = -\frac{d\eta_s}{d\tau}$ is the propellant burning rate.

Condensed phase : $-\infty < \eta \le \eta_s(\tau)$

$$\frac{\partial \theta_c}{\partial \tau} = \frac{\partial^2 \theta_c}{\partial \eta^2}$$

Gas phase : $\eta_s(\tau) \le \eta < \infty$

$$\sigma \frac{\partial}{\partial \tau}\left(\frac{1}{\theta}\right) + \frac{\partial}{\partial \eta}\left(\frac{u}{\theta}\right) = 0, \qquad \frac{\rho_g}{(\rho_g)_r} = \frac{z}{\theta}$$

$$\sigma \frac{\partial \theta}{\partial \tau} + u \frac{\partial \theta}{\partial \eta} = b^2 \theta \frac{\partial}{\partial \eta}\left(\theta \frac{\partial \theta}{\partial \eta}\right) + q_g W(Y,\theta)$$

$$\sigma \frac{\partial Y}{\partial \tau} + u \frac{\partial Y}{\partial \eta} = b^2 \theta \frac{\partial}{\partial \eta}\left(\theta \frac{\partial Y}{\partial \eta}\right) - W(Y,\theta)$$

$$z = Const.$$

where

$$W(Y,\theta) = 0, \quad \theta < \theta_a + \varepsilon$$

$$W(Y,\theta) = k_g Y \exp\left[\varepsilon_g\left(\frac{1}{\theta_h} - \frac{1}{\theta}\right)\right]; \quad \theta > \theta_a + \varepsilon$$

The normalized functions are $\theta_c(\eta,\tau)$ - condensed phase temperature, $\theta(\eta,\tau)$ - gas phase temperature, $Y(\eta,\tau)$ - reagent mass fraction in the gas phase, and $u(\eta,\tau)$ - gas velocity. It is assumed that the pressure z is constant.

The boundary conditions are

$$\eta \to -\infty : \theta_c = \theta_a$$

$$\eta \to \infty : \frac{\partial \theta}{\partial \eta} = 0, \quad \frac{\partial Y}{\partial \eta} = 0.$$

The matching conditions at the burning surface are

Temperature continuity : $\theta_c = \theta$

Heat balance : $\frac{\partial \theta_c}{\partial \eta} = b\theta \frac{\partial \theta}{\partial \eta} - q_s \mu(\tau)$

Mass balance : $b\theta\mu(\tau) = \sigma\mu(\tau) + u$

Reagent balance : $b\theta\mu(\tau) = \sigma Y\mu(\tau) + uY - b^2\theta^2 \frac{\partial Y}{\partial \eta}$

Evaporation condition : $Y = \frac{1}{z}\exp\left[\varepsilon_s\left(1 - \frac{1}{\theta}\right)\right]$

The initial conditions are

$$\eta_s(0) = 0, \quad \theta_c(\eta,0) = \theta_a, \quad \theta(\eta,0) = \theta_a,$$
$$Y(\eta,0) = Y_a, \quad u(\eta,0) = 0, \quad \mu(0) = 0$$

where $Y_a = \frac{1}{z}\exp\left[\varepsilon_s\left(1 - \frac{1}{\theta_a}\right)\right]$.

Ignition boundary condition at $\eta = \eta_i$; $0 \le \tau \le \tau_i$ can be written as below.

$$\left.\frac{\partial \theta}{\partial \eta}\right|_{\eta_i^-} - \left.\frac{\partial \theta}{\partial \eta}\right|_{\eta_i^+} = q(\tau)$$

$$q(\tau) = \begin{cases} q & \text{at} \quad 0 \le \tau \le \tau_i \\ 0 & \text{at} \quad \tau > \tau_i \end{cases}$$

Numerical Procedure

Gas Phase

It is convenient to employ the divergence form when we construct a finite-volume discretization.

$$\frac{\partial \mathbf{q}}{\partial \tau'} + \frac{\partial}{\partial \eta'}(\mathbf{f} - \mathbf{f}_v) = \mathbf{S}, \quad 0 \le \eta' < \infty \qquad (1)$$

$$\mathbf{q} = \begin{bmatrix} \theta \\ \sigma Y/\theta \\ \sigma \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} (u+\sigma\mu)/\theta \\ (u+\sigma\mu)Y/\theta \\ u+\sigma\mu \end{bmatrix},$$

$$\mathbf{f}_v = \begin{bmatrix} 0 \\ b^2\theta\,\partial Y/\partial\eta' \\ b^2\theta\,\partial\theta/\partial\eta' \end{bmatrix},\quad \mathbf{S} = \begin{bmatrix} 0 \\ -W(Y,\theta)/\theta \\ q_g W(Y,\theta)/\theta \end{bmatrix}$$

Divide the η'-domain, $0 \le \eta' \le \eta'_{\max}$, into finite volume (length) cells. Say the total number of cell boundaries is N_g. We have $(N_g - 1)$ cells over the domain. Each cell has width of $\Delta\eta'_i$. The values of $\Delta\eta'_i$ for $i = 1, \cdots, N_g - 1$ may vary. The value of $\eta'_{\max}$ should be large enough for the far field boundary condition can be applied. The cell widths are given in the present calculation as $\Delta\eta'_i = \Delta\eta'_1(1+\alpha)^{i-1}$, where α is small positive constant determined from the condition, $\eta'_{\max} = \sum_{i=1}^{N_g-1} \Delta\eta'_i$. The smallest cell width $\Delta\eta'_1$ occurs adjacent to the burning surface. The location of the interface of consecutive cells, i-th and $(i+1)$-th is denoted as $\eta'_{i+1/2}$.

In order to get algebraic equations from the partial differential equations, we apply the finite-volume method. First, we integrate the governing equations, Eq.(1) over the i-th cell.

$$\int_{\eta'_{i-1/2}}^{\eta'_{i+1/2}} \frac{\partial \mathbf{q}}{\partial \tau'} d\eta' + \int_{\eta'_{i-1/2}}^{\eta'_{i+1/2}} \frac{\partial(\mathbf{f} - \mathbf{f}_v)}{\partial \eta'} d\eta' = \int_{\eta'_{i-1/2}}^{\eta'_{i+1/2}} \mathbf{S}\, d\eta'$$

Define cell-averaged quantities such as

$$\bar{\mathbf{q}}_i \equiv \frac{\int_{\eta'_{i-1/2}}^{\eta'_{i+1/2}} \mathbf{q}\, d\eta'}{\Delta\eta'_i}, \text{and} \quad \bar{\mathbf{S}}_i \equiv \frac{\int_{\eta'_{i-1/2}}^{\eta'_{i+1/2}} \mathbf{S}\, d\eta'}{\Delta\eta'_i}.$$

Then we get ordinary differential equations for the i-cell.

$$\frac{d\bar{\mathbf{q}}_i}{d\tau'} \Delta\eta'_i = -(\mathbf{f}_{i+1/2} - \mathbf{f}_{i-1/2}) + (\mathbf{f}_{v\,i+1/2} - \mathbf{f}_{v\,i-1/2}) + \bar{\mathbf{S}}_i \Delta\eta'_i$$

where $\mathbf{f}_{i+1/2}$ denotes values of $\mathbf{f}$ at the cell interface location $\eta'_{i+1/2}$. This equation is solved at each cell by time dependent fashion. An implicit time integration scheme is employed.

$$\left[\mathbf{I} + \frac{\Delta\tau'^n}{\Delta\eta'_i}\left\{D_{q'}\left(\frac{\partial \mathbf{f}}{\partial \mathbf{q}}\right)_i^n - D_{q'}\left(\frac{\partial \mathbf{f}_v}{\partial \mathbf{q}}\right)_i^n - \left(\frac{\partial \mathbf{S}}{\partial \mathbf{q}}\right)_i^n \Delta\eta'_i\right\}\right]\Delta\bar{\mathbf{q}}_i^n \qquad (2)$$
$$= \frac{\Delta\tau'^n}{\Delta\eta'_i}\left[-(\mathbf{f}_{i+1/2} - \mathbf{f}_{i-1/2}) + (\mathbf{f}_{v\,i+1/2} - \mathbf{f}_{v\,i-1/2}) + \bar{\mathbf{S}}_i \Delta\eta'_i\right]^n$$

We know that σ is constant and, if we write $\Delta\bar{\mathbf{q}} = \left[\Delta\bar{q}^{(1)} \quad \Delta\bar{q}^{(2)} \quad \Delta\bar{q}^{(3)}\right]^T$, $\Delta\bar{q}^{(3)} \equiv 0$. So, we can reduce the coefficient matrices to (2×2) size. The reduced matrices can be written as follows.

$$\frac{\partial \mathbf{f}^{\pm}}{\partial \mathbf{q}} = \frac{\mu + (u/\sigma) \pm |\mu + (u/\sigma)|}{2}\mathbf{I}, \quad \left|\frac{\partial \mathbf{f}}{\partial \mathbf{q}}\right| = \left|\mu + \frac{u}{\sigma}\right|\mathbf{I},$$

$$\frac{\partial \mathbf{g}}{\partial \mathbf{q}} = \begin{bmatrix} 0 & 0 \\ -\dfrac{2Y\theta^2}{\sigma} & \dfrac{\theta^2}{\sigma} \end{bmatrix}, \quad \frac{\partial \mathbf{h}}{\partial \mathbf{q}} = \begin{bmatrix} 0 & 0 \\ -\dfrac{\theta^2}{\sigma} & 0 \end{bmatrix},$$

$$\frac{\partial \mathbf{S}}{\partial \mathbf{q}} = \frac{W(Y,\theta)}{\sigma\theta Y}\begin{bmatrix} 0 & 0 \\ \varepsilon_g Y & -\theta \end{bmatrix}.$$

The equations for both ends, simply explicit boundary conditions are applied, namely,

$$\Delta\bar{q}^{(i)}\big|_0^n = \Delta\bar{q}^{(i)}\big|_{N_g}^n = 0$$

The mass conservation equation creates tri-diagonal system and can be solved efficiently, if gas velocities are given.

The flux-term of right-hand side can be calculated using upwind flux-splitting. The left-side and right-side values at the cell-interface are re-constructed from cell-averaged quantities. If we apply linear distribution within each cell, then 2nd-order scheme is obtained. If we apply parabolic distribution within each cell, then 3rd-order scheme is obtained.

To preserve the monotonic nature of the solution, it is sometimes necessary to apply a limiter function in the high-order reconstruction of cell-interface values. That is we should not introduce artificial local extrema by the above extrapolation procedure.

Similarly the reagent mass conservation equation can be solved.

The energy equation can be written, using mass conservation equation, at every time period as below.

$$-f^{(3)}\big|_{i+1/2} + f^{(3)}\big|_{i-1/2} + f_v^{(3)}\big|_{i+1/2} - f_v^{(3)}\big|_{i-1/2} + \bar{S}^{(3)}\big|_i \Delta\eta'_i = 0$$

Therefore, after θ_i^{n+1} and Y_i^{n+1} are determined for $i = 1, \ldots, N_g - 1$, the gas velocity $u_{i+1/2}^{n+1}$ can be obtained by the following equation.

$$u_{i+1/2}^{n+1} = u_{i-1/2}^{n+1} + \frac{b^2}{2}\left(\frac{\theta_{i+1}^{n+1^2} - \theta_i^{n+1^2}}{\Delta\eta_{i+1/2}} - \frac{\theta_i^{n+1^2} - \theta_{i-1}^{n+1^2}}{\Delta\eta_{i-1/2}}\right) + \frac{q_g W\left(Y_i^{n+1}, \theta_i^{n+1}\right)\Delta\eta'_i}{\theta_i^{n+1}}$$

This equation determines the value of gas velocity u at each cell interface by space-marching fashion, if we can specify the gas velocity at the burning surface, namely $u_{1/2}^{n+1}$. We denote it as u_0.

Next, therefore, how the burning surface values are determined at each time period is described.

Burning-surface values

We assume that variation of the temperatures in both adjacent cells to the burning surface can be well-approximated by linear function because the cell spacing at the burning surface is small enough for the approximation. θ_0 is the burning surface temperature and Y_0 can be evaluated by this temperature.

From the definition of cell-averaged quantities, we have

$$a_c \Delta\eta'_{c N_c-1} + a_g \Delta\eta'_1 + 2\bar{\theta}_{c N_c-1} = 2\bar{\theta}_1$$

From matching conditions

$$a_c = b\theta_0 a_g - \mu q_s \quad \mu = \frac{2bz\{-\exp(\varepsilon_s) + \exp(\varepsilon_s/\theta_0)\bar{Y}_1 z\}}{\{\exp(\varepsilon_s) - \exp(\varepsilon_s/\theta_0)z\}\Delta\eta_1}$$

From above three equations, we obtain the following relation.

$$b\Delta\eta'_{c N_c-1}\theta_0^2 + \theta_0\left[\frac{bq_s(\bar{Y}_1 - 1)z\Delta\eta'_{c N_c-1}}{\exp\left\{\varepsilon_s\left(1-\frac{1}{\theta_0}\right)\right\} - z} + \Delta\eta'_1 - b\Delta\eta'_{c N_c-1}(q_s + \bar{\theta}_1)\right] - \Delta\eta'_1\bar{\theta}_{c N_c-1} = 0$$

By solving the above equation numerically we can determine the value of θ_0. From θ_0, all the rest variables at the burning surface are determined. The values of gradients at the burning surface are specified in the solution process of the governing equations.

Solid-Phase

The temperature of the solid propellant is solved using similar numerical procedure. The flux term (temperature at cell interface) in the right-hand side is evaluated similarly with the gas-mass conservation equation. The boundary conditions are implied explicitly.

Results

Parameter values

The following values are used for the constants;

$\theta_a = 0.7$, $q_s = 1.43$, $q_g = 4.12$, $\varepsilon_s = 12.8$, $\varepsilon_g = 33.9$, $\sigma_r = 10^{-4}$, $b = 10^{-1}$, $\varepsilon = 10^{-2}$

As regards to igniter parameters, they should be chosen so that only to ignite the propellant. For example, $\eta_i = 10$, $q = 1$ and τ_i should be large enough for ignition. At $\tau \to \infty$ the burning regime is steady-state one with $\mu = Const$.

Results obtained for small values of the non-dimensional pressure, $z = 1$, show a steady-combustion. In Fig.5, the temperature distribution in steady state is shown. The time history of the values at the burning surface is shown in Fig.6.

As is discussed in Ref.1, in the approximation of an infinitely thin gas-phase reaction zone, the non-dimensional burning rate in the steady-state regime is $\mu = 1$. Calculations that were naturally carried out without the assumption of infinitely thin reaction zone showed that μ to a high accuracy does not depend on pressure. However, the value of μ depends on the activation energy of the gas-phase reaction. For $\varepsilon_g = 33.9$, the value $\mu = 0.856$ has been obtained. This value is in good agreement with the present unsteady computational results.

For other pressure values, present solution showed numerical instability. Detailed analyses for the stability problem will be given in Ref.1

Summary

In order to investigate numerical problems in solving flame spread, one-dimensional ignition problem is considered as a test bed. It is found that the present numerical model can give basically correct values of the burning surface speed, but at the same time have shown difficulties as regards to the numerical instability. Further improvement is necessary.

References

1) Novozhilov, B and Shimada, T., "Numerical Analysis of Solid Propellant Ignition, will be presented in the 24th ISTS, 2004.

Acknowledgement

One of the authors (B. Novozhilov) would like to express his gratitude to the Russian Foundation of Basic Research for partial financial support of this work (grant 02-03-32077).

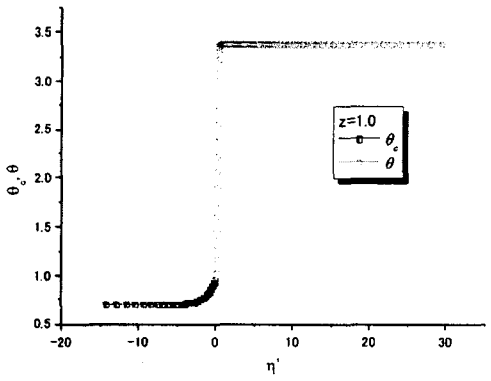


Fig.5 Temperature Distribution in Steady State, z=1.0

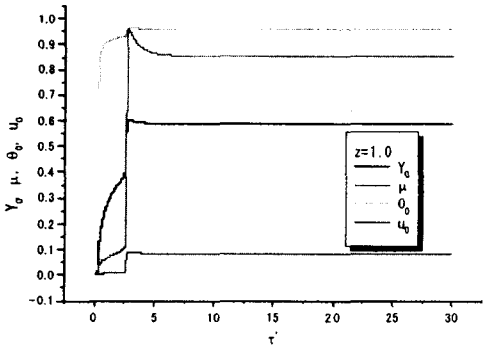


Fig.6 Time History of values at the burning surface, z=1.0