NUMERICAL COMPUTATION OF FLOW FIELD WITH DEFLAGRATION AND DETONATION*1)

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I. Introduction

The problems involving combustion are increasingly important, and are attracting more and more attention. The task for the computational mathematicians is to compute accurately the flow fields with combustion waves. The transition from deflagration to detonation is an important problem in the combustion phenomenon. Because the velocity and the strength of detonation are much larger than those of deflagration, detonation is much more dangerous than deflagration. [1] has computed the flow fields generated by accelerated flames using the floating-shockfitting method. [2] has also computed such problems using the random choice method and showed how to determine the transition from deflagration to detonation by numerical methods. In this paper the singularity-separating method (S. S. M. for short) is used to compute the whole flow fields with transition to detonation. The comparison between the results of the random choice method (R. C. M. for short) and our method is presented. Because there are many complicated interactions between different discontinuity lines, such a combustion problem is a good choice for testing numerical methods. The solution obtained by S. S. M. has the second order accuracy not only in the smooth regions but also in the regions near the discontinuity lines.

II. Formulation of the Problem

The system of nonlinear gas dynamics is

$$\begin{cases} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0, \\ \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0, \\ \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + \gamma p \frac{\partial u}{\partial x} = 0. \end{cases}$$
(1)

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Throughout this paper, the subscript 1 refers to burned gas and the subscript 0 unburned gas, V stands for the velocity of the reacting front, Q for the energy released by unit gas in the process of reaction, γ for ratio of specific heats, ρ , u, p and c for the density, gas velocity, pressure and sound velocity respectively. The relations of combustion wave in the polytropic gas are

$$\rho_0(u_0-V)=\rho_1(u_1-V), \qquad (2)$$

$$\rho_0(u_0-V)^2+p_0=\rho_1(u_1-V)^2+p_1, \qquad (3)$$

$$\frac{1}{\gamma_0-1}\frac{p_0}{\rho_0}-\frac{1}{\gamma_1-1}\frac{p_1}{\rho_1}+Q-\frac{1}{2}\left(\frac{1}{\rho_0}-\frac{1}{\rho_1}\right)(p_0+p_1). \tag{4}$$

From the above formulae the following formulae for the strong detonation, the C-J detonation and the weak deflagration can be obtained. The relations of the strong detonation are

$$V = \frac{\rho_1 u_1 - \rho_0 u_0}{\rho_1 - \rho_0},\tag{5}$$

$$\rho_{1} = \rho_{0} \frac{\frac{\gamma_{1}+1}{\gamma_{1}-1} \frac{p_{1}}{p_{0}} + 1}{\frac{\gamma_{0}+1}{\gamma_{0}-1} + \frac{p_{1}}{p_{0}} + 2Q \frac{\rho_{0}}{p_{0}}},$$
(6)

and

$$u_1 = u_0 \pm \psi(p_1; p_0, \rho_0)$$
 (7)

Here, the upper sign stands for the first family of waves and the lower sign for the second family, and

$$\psi(p_1; p_0, \rho_0) = \sqrt{\frac{(p_1 - p_0)(\frac{2}{\gamma_1 - 1} p_1 - \frac{2}{\gamma_0 - 1} p_0 - 2\rho_0 Q)}{\rho_0(\frac{\gamma_1 + 1}{\gamma_1 - 1} p_1 + p_0)}}.$$
 (8)

The relations of the C-J detonation are

$$M_{0}^{*} = \pm \left(\sqrt{\frac{\gamma_{1}-1}{2}} \left[(\gamma_{1}+1) \frac{Q}{c_{0}^{2}} + \frac{\gamma_{1}+\gamma_{0}}{\gamma_{0}(\gamma_{0}-1)} \right] + \sqrt{\frac{\gamma_{1}+1}{2}} \left[(\gamma_{1}-1) \frac{Q}{c_{0}^{2}} - \frac{\gamma_{0}-\gamma_{1}}{\gamma_{0}(\gamma_{0}-1)} \right] \right), \tag{9}$$

$$p_{J} = p_{0} + p_{0} \frac{\gamma_{0}}{\gamma_{1} + 1} \left(M_{0}^{*2} - \frac{\gamma_{1}}{\gamma_{0}} \right), \tag{10}$$

$$u_{J} = u_{0} + c_{0} \frac{1}{\gamma_{1} + 1} \left(M_{0}^{*} - \frac{\gamma}{\gamma_{0} M_{0}^{*}} \right),$$
 (11)

$$\rho_{J} = \rho_{0} / \left(1 - \frac{1}{\gamma_{1} + 1} \left(1 - \frac{\gamma_{1}}{\gamma_{0} M_{0}^{*2}} \right) \right). \tag{12}$$

Because there are two characteristic lines entering a weak deflagration front in one side and only one in the other side, there must be one more condition for determining a weak deflagration. The following formula for the velocity of weak deflagration is used in our computation (see [2])

$$V = u_0 + K \left(\frac{p_0}{\rho_0}\right)^{\hat{q}}, \qquad (13)$$

where the constants K and \hat{Q} are determined by experiments. Suppose that

$$M_0 = \frac{K}{\sqrt{\gamma_0}} \left(\frac{p_0}{\rho_0}\right)^{\hat{Q} - \frac{1}{2}} \tag{14}$$