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DEPENDENCE OF QUALITATIVE BEHAVIOR OF THE NUMERICAL SOLUTIONS ON THE IGNITION TEMPERATURE FOR A COMBUSTION MODEL *1)

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Abstract

We study the dependence of qualitative behavior of the numerical solutions (obtained by a projective and upwind finite difference scheme) on the ignition temperature for a combustion model problem with general initial condition. Convergence to weak solution is proved under the Courant-Friedrichs-Lewy condition. Some condition on the ignition temperature is given to guarantee the solution containing a strong detonation wave or a weak detonation wave. Finally, we give some numerical examples which show that a strong detonation wave can be transformed to a weak detonation wave under some well-chosen ignition temperature.

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Key words: Detonation wave solutions, Combustion model, Upwind finite difference scheme.

1. Introduction

Fractional step method is frequently applied to the numerical simulation of combustion problems, where the combustion mechanism is split away from the convection process in each time step. Since the rate of chemical reaction is usually much higher than the rate of convection, the combustion step is reduced to a projection, where the rate of chemical reaction is approximated to infinity, that is, the Champmon-Jouguest model.

It is often observed that the results are sensitive to the ignition temperature in the projection method. Sometimes a spurious wave profile, i.e., a weak detonation wave, is generated under a low ignition temperature in the numerical simulation, which is non-physical in many cases (see for example [2], [3], [5]). Therefore a higher ignition temperature is suggested to generate a strong detonation wave. Thus, to determine the ignition temperature becomes a subtle problem.

In [4], A. Majda proposed a qualitative model (so-called Majda's model) to study shock-wave chemistry interactions in combustion theory. This is the starting point for many researches. Then in [2], P. Colella, A. Majda and V. Roytburd studied Euler equations and Majda's model. In particular, for Majda's model, they proved that if one wants to obtain a strong detonation wave, the ignition temperature should be larger than the burnt temperature behind a weak detonation wave traveling at the same speed. In [5], R. B. Pember obtained the same criterion for the Euler equations. A similar behavior was discovered by R. J. Le Veque and H. C. Yee ([3]) for the scalar conservation law with stiff source term.

In [8], the second named author studied this problem for the Riemann problem of the Majda's model. Some sufficient conditions on the ignition temperature were given for the qualitative behavior of the numerical solutions. Some numerical experiments were done in [11]. Recently the second named author obtained some further results in [9].

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In this paper, we extend the results to more general initial data. Moreover, for some technical difficulty reason, we have studied the weak detonation wave only in a weaker sense in [8]. Here we overcome this difficulty and study the weak detonation wave in the natural sense.

Let us briefly give a more precise statement of the problem studied here. The Majda's model for combustion is the following:

$$\frac{\partial(u+qz)}{\partial t}+\frac{\partial f(u)}{\partial x}=0, \tag{1.1}$$

$$\frac{\partial z}{\partial t}=-K\phi(u)z, \tag{1.2}$$

where u is a "lumped variable", representing density, velocity and temperature, $z \in [0,1]$, representing the fraction of unburnt gas, the constant $q>0$, representing the binding energy, the constant $K>0$, representing the rate of chemical reaction, $f \in C^2$, $f'>0, f'' \geq \alpha_0>0$, and

$$\phi(u)=\begin{cases}1, & u>U_i,\\ 0, & u<U_i,\end{cases} \tag{1.3}$$

where U_i is the ignition temperature.

Let $K \to \infty$ formally, then we get $\frac{\partial z}{\partial t} \leq 0$, $\phi(u)z=0$, and if $u<U_i$, then $\frac{\partial z}{\partial t}=0$, therefore (1.2) is replaced by

$$z(x,t)=\begin{cases}0, & \sup\limits_{0\leq\tau\leq t} u(x,\tau)>U_i,\\ z(x,0), & \sup\limits_{0\leq\tau\leq t} u(x,\tau)<U_i.\end{cases} \tag{1.4}$$

$$\frac{\partial z}{\partial t}\leq 0 \tag{1.5}$$

We will study the projective and finite difference method to (1), (4), (5) and the following initial condition:

$$u(x,0)=\begin{cases}u_{0l}(x), & x\leq 0,\\ u_{0r}(x), & x>0\end{cases} \qquad z(x,t)=\begin{cases}0, & x\leq 0,\\ 1, & x>0\end{cases} \tag{1.6}$$

where u_{0l} and u_{0r} are bounded functions and $inf_x u_{0l}(x)-q>U_i>sup_x u_{0r}(x)$.

Notice that (1) can be written as

$$u_t+f(u)_x=Kq\phi(u)z,$$

which falls into the general topic on hyperbolic conservation laws with stiff source terms studied by several authors, among others, including [1] and [7]. It would be interesting to see to what extent our results and methods can be applied there.

Here is an outline of this paper:

In section 2, we prove the convergence of the scheme to a weak solution under the CFL condition. The proof follows in the same line as that in [8]. However there is a major difference (c.f. Lemma 2.3).

In section 3, we prove the existence of a strong detonation wave under a condition on U_i. However this is not a necessary condition for the existence of a strong detonation wave, as demonstrated by the numerical examples in section 5.

In section 4 we prove the existence of a weak detonation wave under another condition on U_i. The key point is to prove that the limit to the discontinuous curve $l(t)$ of u exists.

Finally in section 5, we give some interesting numerical examples. We observe that a strong detonation wave can be transformed to a weak detonation wave.