Journal of Computational Mathematics, Vol.23, No.4, 2005, 337–350.

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.

Mathematics subject classification: 65M06, 80A25, 80M20, 35L65.
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].

* Received January 14, 2004; final revised March 9, 2004.
1) This work was supported by the Major State Research Program of China G1999032803 and the Research Fund for the Doctorial Program of Higher Education.

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.

2. Difference Scheme and Convergence to Weak Solutions

We will use the following fractional step method for the system of equations (1.1), (1.4) and (1.5) with the initial condition (1.6), where the convection and the chemical reaction are split by a three steps procedure, and the solver of the convection part is an upwind scheme.
Step 1.

$$\frac{\tilde{u}_j^n - u_j^n}{\triangle t} + \frac{f(u_j^n) - f(u_{j-1}^n)}{\triangle x} = 0. \tag{2.1}$$

Step 2.

$$z_j^{n+1} = \begin{cases} 0, & \tilde{u}_j^n \geq U_i \\ z_j^n, & \tilde{u}_j^n < U_i. \end{cases} \tag{2.2}$$

Step 3.

$$u_j^{n+1} = \tilde{u}_j^n - q(z_j^{n+1} - z_j^n), \tag{2.3}$$

where $u_j^n = u(j\triangle x, n\triangle t), z_j^n = z(j\triangle x, n\triangle t)$, $\triangle x, \triangle t$ are step sizes, and $\tilde{u}_j^n$ is an intermediate variable.

We first give some estimates for the scheme. We omit most proofs, since they are similar to those in [8]. We assume that u_{0r} is of bounded variation. Let $M = \sup_{x\leq 0} u_{0l}(x)$ and $m = \inf_{x>0} u_{0r}(x)$.

Lemma 2.1. *Assume the following CFL-type condition is satisfied,*

$$\frac{\Delta t}{\Delta x} \leq \frac{q}{\max_{[m,M+2q]} f' \cdot (M + 2q - m)}, \tag{2.4}$$

Then (a). $z_j^n \in [0,1]$ *and* $u_j^n \in [m, M+2q]$;

(b). there is an integer j_0^n *for each* n *such that* $z_j^n = 0, u_j^n \geq U_i$ *for* $j \leq j_0^n$,*and* $z_j^n = 1, u_j^n < U_i$ *for* $j > j_0^n$.

Thus we obtain a sequence $0 = j_0^0 \leq j_0^1 \leq \cdots \leq j_0^n \leq j_0^{n+1} \leq \cdots$. Now we define a subsequence $j_0^0, j_0^{n_1}, j_0^{n_2}, \cdots$, such that $j_0^0 = j_0^1 = \cdots = j_0^{n_1-1}$ and $j_0^{n_1} > j_0^{n_1-1}$. Connecting points $(j_0^{n_k}\Delta x, n_k\Delta t)$ and $(j_0^{n_k+1}\Delta x, n_{k+1}\Delta t)$ by line segments for $k = 0, 1, \cdots$, we obtain a curve, denoted by $x = l_{\Delta x}(t)$.

Lemma 2.2. *The curve* $x = l_{\Delta x}(t)$ *is increasing with respect to* t, *i.e.,* $l'_{\Delta x}(t) > 0$. *Moreover,* $l_{\Delta x}(t)$ *is bounded for all* Δx *and finite* t.

Let $\Delta x, \Delta t \to 0$, then there is a subsequence of $l_{\Delta x}(t)$ converging pointwisely to a curve $\Gamma : x = l(t)$ with $l'(t) \geq 0$ and $l \in BV(0,T)$. Let $\Omega_+ = \{(x,t); x > l(t)\}$ and $\Omega_- = \{(x,t); x < l(t)\}$. We extend u_j^n by constant on $(j\Delta x, (j+1)\Delta x] \times (n\Delta t, (n+1)\Delta t]$, detonated by $u_{\triangle x}$.

Lemma 2.3. $u_{\triangle x}$ *is of bounded variation on* Ω_+.

Proof. Define $Var^+u^n = \sum\limits_{j=j_0^n}^{\infty} \max(u_{j+1}^n - u_j^n, 0)$, $Var^-u^n = \sum\limits_{j=j_0^n}^{\infty} \min(u_{j+1}^n - u_j^n, 0)$m and $Var(u^n) = \sum_{j=j_0^n}^{\infty} |u_{j+1}^n - u_j^n|$. Since $u_{j_0+1}^n - u_{j_0}^n \leq 0$, we have $Var^+u^n = \sum\limits_{j=j_0^n+1}^{\infty} \max(u_{j+1}^n - u_j^n, 0)$. Notice that for $j \geq j_0^n + 1, \tilde{u}_j^{n-1} = u_j^n$, now by the difference scheme we have

$$u_{j+1}^n - u_j^n = u_{j+1}^{n-1} - u_j^{n-1} - r(f(u_{j+1}^{n-1}) - f(u_j^{n-1})) + r(f(u_j^{n-1}) - f(u_{j-1}^{n-1})), \tag{2.5}$$

where $r = \frac{\Delta t}{\Delta x}$. We set $V_j^n = u_{j+1}^n - u_j^n$, $L_j^n = f(u_{j+1}^n) - f(u_j^n)$, then (2.5) is equal to

$$V_j^n = V_j^{n-1} - r(L_j^{n-1} - L_{j-1}^{n-1}). \tag{2.6}$$

Let

$$\delta_j = \begin{cases} 0, & u^n_{j+1} - u^n_j < 0; \\ 1, & u^n_{j+1} - u^n_j \geq 0, \end{cases}$$

and multiply it to the equation (2.6), then sum them up to obtain:

$$\begin{aligned} Var^+u^n = \sum_{j=j_0^n+1}^{\infty} \delta_j V_j^n &= \sum_{j=j_0^n+1}^{\infty} \delta_j V_j^{n-1} - r(\sum_{j=j_0^n+1}^{\infty} \delta_j L_j^{n-1} - \sum_{j=j_0^n+1}^{\infty} \delta_j L_{j-1}^{n-1}) \\ &= \sum_{j=j_0^n+1}^{\infty} (\delta_j V_j^{n-1} + r(\delta_{j+1} - \delta_j) L_j^{n-1}) + r\delta_{j_0^n+1} L_{j_0^n}^{n-1}. \end{aligned} \tag{2.7}$$

Let $a = \delta_j V_j^{n-1} + r(\delta_{j+1} - \delta_j)L_j^{n-1}$, then there are four cases:

i). $\delta_j = \delta_{j+1} = 1$, then $a = V_j^{n-1}$.

ii). $\delta_j = \delta_{j+1} = 0$, then $a = 0 \leq \max(V_j^{n-1}, 0)$.

iii). $\delta_j = 1, \delta_{j+1} = 0$, then $a = (1 - r(f'(\xi_j))V_j^{n-1} \leq V_j^{n-1}$.

iv). $\delta_j = 0, \delta_{j+1} = 1$, then $a = rL_j^{n-1} = r(f'(\xi_j))V_j^{n-1} \leq V_j^{n-1}$, where ξ_j is a mean value.

We get $Var^+u^n \leq \sum\limits_{j=j_0}^{\infty} \max(V_j^{n-1}, 0) + r\delta_{j_0^n+1} L_{j_0^n}^{n-1}$. Notice that $L_{j_0^n}^{n-1} < 0$, thus $Var^+u^n \leq \sum\limits_{j=j_0}^{\infty} \max(V_j^{n-1}, 0) \leq Var^+u^{n-1}$.

Repeat this procedure, we get $Var^+u^n \leq Var^+u_{n-1} \leq \cdots \leq Var^+u^0$. Since $u_{0r}(x)$ is of bounded variation, there exists a constant C such that $Var^+u^0 \leq C$. Then $Var^+u^n \leq C$. By $Var^+u^n + Var^-u^n = \sum\limits_{j=j_0^n} (u_{j+1}^n - u_j^n) = u(+\infty) - u(j_0^n)$, Var^-u^n is bounded. Since $Var(u^n) = Var^+u^n - Var^-u^n$, thus $Var(u^n)$ is bounded. On the other hand, by the estimate of $Var(u^n)$ and the equation (2.1), we can estimate the variation of $u_{\Delta x}$ with respect to t. The proof for that $u_{\Delta x}$ being of bounded variation on Ω_+ is thus complete.

By the precedent lemma, $u_{\Delta x}$ is bounded in BV on Ω_+. There is a subsequence converging in L^1 and the limit is of bounded variation. Let the limit be $u(x,t)$. On Ω_-, $u_{\Delta x}$ is bounded in L^∞. There is a subsequence weakly converging in $L^p, p > 1$. However for $j < j_0^n$, u_j^n is the discrete solution of the conservation law:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

Applying the result of compensated compactness we know it also converges to u strongly in L^1.

Theorem 2.1. *The limit u, z is the weak solution to (1), (4), (5) and (6).*

3. Convergence to Strong Detonation Waves

This section is parallel to section 3 of [8]. Most proofs there work here with slight modifications, so we will omit most details, but just give some outlines.

Set $u_1 = \inf_{x\leq 0} u_{0l}(x)$,$u_2 = \sup_{x>0} u_{0r}(x)$. We define

$$s_1 = \frac{f(u_1) - f(u_2)}{u_1 - u_2 - q}.$$

By the assumption of f,there exist some U_{CJ} with $u_{CJ} > u_2 + q$ such that

$$f'(u_{CJ}) = \frac{f(u_{CJ}) - f(u_2)}{u_{CJ} - u_2 - q}.$$

For any $s \in (f'(u_{CJ}), \infty)$, there are two values of u corresponding to s. Let them be $u_l^* \geq u_{l^*}$ and we will always assume that $s_1 \geq f'(u_{CJ})$ and $u_1 = u_l^*$ later on. Obviously, $u_2+q < u_{l^*} < u_1$. In this section , we will assume $U_i \in [u_{l^*} - q, u_l^*)$.

First we will consider Ω_+. For a point (x_0, t_0), we denote the downward characteristic line starting from (x_0, t_0) by $C(x_0, t_0)$, whose equation is given by $x = g(t; x_0, t_0)$.

Lemma 3.1. *For any $(x_0, t_0) \in \Omega_+$, we have $l(t) \leq g(t; x_0, t_0)$ for all $0 \leq t \leq t_0$, i.e. the characteristic line $C(x_0, t_0)$ does not intersect Γ transversely.*

Proof. There are two cases:

(i) $C(x_0, t_0)$ has no intersection with the curve $x = l(t)$. In this case, the conclusion is obvious.

(ii) $C(x_0, t_0)$ intersects with $x = l(t)$. Denoted by $(l(t_1), t_1)$ which is an intersection point with t_1 maximal. Let $g(t) = \max\{l(t); g(t; x_0, t_0), g(t; l(\tau), \tau), \forall \tau \leq t_1\}$ and $v(t) = u(g(t) + 0, t)$. We first show that $v(t) \equiv u(g(0) + 0, 0)$. Let $S = \{t \in (0, t_0) | g(t) = l(t)\}$. We need the following two affirmations:

Claim 1: $Meas(S) = 0$.

Claim 2: v is continuous and has bounded variation.

With these, we can conclude the proof as follows: $v(t) = \int_0^t v'(s)ds + u(g(0) + 0, 0)$. Note that if $t \notin S$, then $g(t)$ is the equation of a characteristic line, so $v(t)$ is constant, i.e. $v'(t) = 0$. This gives that $v(t) = \int_S v'(s)ds + u(g(0)+0, 0) = u(g(0)+0, 0)$ since $Meas(S) = 0$. Therefore the equation $x = g(t)$ defines a characteristic line, which intersects with line $x > 0, t = 0$, so $l(t) \leq g(t; x_0, t_0)$.

The proof of Claim 1 is the same as the proof of Lemma 3.1 [Yin].

Proof of Claim 2: We define a curve $\Gamma^\epsilon : x = l(t) + \epsilon$, $\Gamma^\epsilon \in \Omega_+$. From each point on it we can construct $C(x, t)$. Similar to $g(t), v(t)$ we have $g^\epsilon(t)$ and $v^\epsilon(t)$. For each point $(g^\epsilon(t), t)$, we have a download characteristic line $C(g^\epsilon(t), t)$.$(g^\epsilon(t), t) \in \Omega_+$, then $u \equiv u(g^\epsilon(t), t)$ on $C(g^\epsilon(t), t)$. For $u(g^\epsilon(t), t)$ is bounded variation, we have two not decreasing monotone functions $w_1^\epsilon, w_2^\epsilon$ such that $v^\epsilon(t) = w_1^\epsilon(g^\epsilon(t), t) - w_2^\epsilon(g^\epsilon(t), t)$. $g^\epsilon(t)$ is monotone increasing by $(g^\epsilon)'(t) > 0$, $\Rightarrow w_1^\epsilon(g^\epsilon(t), t), w_2^\epsilon(g^\epsilon(t), t)$ are monotone increasing respect to x. By the construction of $v^\epsilon(t)$ and $g^\epsilon(t)$,$v^\epsilon(t) \to v(t)$, $g^\epsilon(t) \to g(t)$. So we have $v(t) = w_1(g(t), t) - w_2(g(t), t)$ as $\epsilon \to 0$.For w_1, w_2 are also not decreasing monotone functions , $v(t)$ is bounded variation , then $\frac{dv}{dt}$ exists. For the continuity of $v(t)$, we have

$$
\begin{aligned}
v(t) &= \int_0^t v'(\tau)d\tau + u(g(0) + 0, 0) \\
&= \int_S v'(\tau)d\tau + u(g(0)+), 0) \equiv u(g(0) + 0, 0),
\end{aligned}
$$

which finishes the proof of our claim 2. This completes the proof of Lemma 3.1.

Now we turn to consider Ω_-. Let

$$
f^*(v) = \frac{f(v) - f(u_2)}{v - u_2 - q}.
$$

First we prove the following simple lemma.

Lemma 3.2. *For any $u \in [u_{l*}, v]$ with $v \geq u_l^*$, we have $f^*(u) \leq f^*(v)$.*

Proof. The derivative of f^* is $(f^*)'(v) = \frac{f'(v)(v-u_2-q)-(f(v)-f(u_2))}{(v-u_2-q)^2}$. Set $F(v) = f'(v)(v - u_2 - q) - (f(v) - f(u_2))$, then we have $F'(v) = f''(v)(v - u_2 - q)$, so $F(v)$ is an increasing function if and only if $v \geq u_2 + q$. By the definition of u_{CJ}, we know that $F(u_{CJ}) = 0$. Then $F(v) \geq 0$ for $v > u_{CJ}$ and $F(v) < 0$ for $v \in [u_2 + q, u_{CJ})$, i.e. $f^*(v)$ is increasing (resp. decreasing) for $v \in [u_{CJ}, u_l^*]$ (resp. $v \in [u_2 + q, u_{CJ})$). So $\max_{v\in[u_{l^*}, u_{CJ}]} f^*(v) = f^*(u_{l^*})$ (for $u_{l^*} > u_2 + q$), and $\max_{v\in[u_{CJ}, u_l^*]} f^*(v) = f^*(u_l^*)$. Thus if $v \geq u_l^*$, then $f^*(v) \geq f^*(u)$ for $u \in [u_{CJ}, v]$ and $f^*(v) \geq f^*(u_l^*) = f^*(u_{l^*}) \geq f(u)$ for $u \in [u_{l^*}, u_{CJ}]$, which concludes the proof.

Theorem 3.1. *If $\Delta x, \Delta t$ satisfy the CFL condition (10) and $U_i \in [u_{l*} - q, u_l^*)$, then as $\Delta x, \Delta t \to 0$, the difference scheme converges to a weak solution to (1), (4), (5) and (6) with a strong detonation wave.*

Proof. By using the precedent lemma, an argument in [8] (Lemma 3.2) shows that if $u \in [u_{l^*}, v]$ on a neighborhood of Γ, where $v \geq u_l^*$, then $l'(t) \leq f^*(v)$ for all t. Now we define $\bar{u}$ such that $f'(\bar{u}) = f^*(u_l^*)$, then $u_{CJ} < \bar{u} < u_l^*$. Let L be the half-line $\{t = 0, x < 0\}$. Then above observation implies (see Lemma 3.3 [Yin]) that the downward characteristic line $C(x,t)$ intersects L (resp. Γ) if and only if $u(x,t) > \bar{u}$ (resp. $u(x,t) \leq \bar{u}$).

Since $f' > 0$, $C(x_0, t_0)$ intersects $\{t = 0, x < 0\}$ for all $x_0 < 0, t_0 > 0$, which implies $g(t; x_0, t_0) < l(t)$. Let $s(t) = \sup\{x; x = g(t; x_0, t_0) < l(t), \forall t\}$, then $s(0) = 0$. Now a similar argument as that in the proof of Lemma 3.4 [8] gives $s(t) = l(t)$ for all t. Thus for any $(x,t) \in \Omega_-$, the characteristic line $C(x,t)$ intersects the half-line L. So for all $t \in [0, t_0]$, we have $g(t; x_0, t_0) < l(t)$. By Lemma 3.1, this implies that the solution contains a strong detonation wave.

4. Convergence to Weak Detonation Waves

In this section, we define $s_2 = \dfrac{f(M) - f(u_2)}{M - u_2 + q}$, then similarly we get $\bar{u}_{CJ}, \bar{u}_{l*}$ and $\bar{u}_l^*$. We will assume $M = \bar{u}_l^*$ and $U_i < \bar{u}_{l*} - q$. Furthermore, we will always assume the following CFL condition:

$$\frac{\Delta x}{\Delta t} \geq \max\left(f'(M), \frac{f(M) - f(\bar{u}_{l*} - q)}{M - \bar{u}_{l*}}\right). \tag{4.1}$$

Following the proof of Lemma 2.4[Yin],we get $U_i + q \leq u_j^n \leq M$ for $j \leq j_0^n$ and $m \leq u_j^n < U_i$ for $j > j_0^n$.

Lemma 4.1. *If*

$$u_2 < U_i \leq m + qf^{'}(m) \cdot \begin{cases} \frac{\Delta t}{\Delta x}, & for \frac{\Delta t}{\Delta x} \geq \frac{1}{2f^*}, \\ \frac{1}{f^*} - \frac{\Delta t}{\Delta x}, & for \frac{\Delta t}{\Delta x} < \frac{1}{2f^*}, \end{cases} \tag{4.2}$$

then

$$l^{'}_{\triangle x}(t) \geq f^*, \tag{4.3}$$

where $f^* > f'(M)$. Furthermore, we have $l^{'}(t) \geq f^*$ for all $t > 0$.

The proof can be found in [Yin] (see Lemma 4.1 and 4.2 *loc. cit.*). First we consider the region Ω_+. Notice that $u(x,t) \leq U_i$ in Ω_+, and $f'(U_i) < f^* \leq l'(t)$, $f'(u) < l'$, thus $C(x,t)$ intersects $t = 0, x > 0$ in Ω_+.

Now we consider Ω_-. We define $w(t)$, such that

$$\frac{f(w(t)) - f(u(l(t) + 0, t)}{w(t) - u(l(t) + 0, t) - q} = l^{'}(t), \quad and\ w(t) \in (m + q, \bar{u}_{l*}). \tag{4.4}$$

and we define $H(u,t) = ul^{'}(t) - f(u)$. Notice that u is of bounded variation on Ω_+, so $u(l(t)+0,t)$ exists. Our utmost aim (also the main difficulty) is to prove the existence of $u(l(t) - 0, t)$. We will prove some properties of the solution given by Theorem 2.1.

Let $\Gamma_\epsilon = \Gamma - \epsilon := \{x = l(t) - \epsilon\}$ with $\epsilon > 0$, $\Gamma_1 = \Gamma \cup \{t = 0, x \leq 0\}$, $\Omega_-^\epsilon = \{(x,t); x < l(t) - \epsilon, t > 0\}$.

Lemma 4.2. *On Ω_-, the solution u given by Theorem 2.1 satisfies*

$$\iint\limits_{\Omega_-} (u\psi_t + f(u)\psi_x)dxdt + \int\limits_{t=0} u_{0l}(x)\psi(x,0)dx + \int\limits_{\Gamma} \psi H(w,t)dt = 0, \tag{4.5}$$

for any function $\psi \in C_0^1(\Omega_- \cup \Gamma_1)$. Furthermore the solution satisfies the following Oleinik entropy condition: there exists a constant $E > 0$, such that for any $a > 0$ and for any $(x,t) \in \Omega_-$, we have

$$\frac{u(x,t) - u(x-a,t)}{a} < \frac{E}{t - a(x)}, \tag{4.6}$$

where $a(x) = l^{-1}(x)$ if $x > 0$, and $a(x) = 0$ if $x \le 0$.

Proof. Since u satisfies the conservation law in Ω_ϵ, we have

$$0 = \iint\limits_{\Omega_\epsilon} (u\psi_t + f(u)\psi_x)dxdt + \int_{t=0,x<0} u_{0l}(x)\psi(x,0)dx + \int_{\Gamma_\epsilon} \psi(ul' - f(u))dt, \tag{4.7}$$

for any function $\psi \in C_0^1(\Omega_- \cup \Gamma_1)$. Let $\epsilon \to 0$, we get

$$\iint\limits_{\Omega_-} (u\psi_t + f(u)\psi_x)dxdt + \int\limits_{t=0} u_{0l}(x)dx + \int\limits_{\Gamma} \psi H(w,t)dt = 0. \tag{4.8}$$

Here we have used Lemma 4.5 ([8], the proof) to obtain that $lim_{\epsilon\to 0}\int_{\Gamma_\epsilon} \psi(ul' - f(u))dt = \int\limits_{\Gamma} \psi H(w,t)dt$.

Now we need to verify the Oleinick entropy condition for the solution u. Consider the region $\Omega(t_0) = \{(x,t)|x < l(t_0), t > t_0\}$ for $t_0 > 0$. On this region, recall that u is the (bounded) limit of numerical solutions using the upwind scheme, thus u satisfies the following Oleinick entropy condition: there exists a constant $E > 0$, such that for any $a > 0$ and for any $(x,t) \in \Omega(t_0)$, we have

$$\frac{u(x,t) - u(x-a,t)}{a} < \frac{E}{t - t_0},$$

which implies (4.6), since t_0 is arbitrary.

Our next lemma says that the entropy solution is unique.

Lemma 4.3. *The entropy solution to problem (4.5) is unique.*

Proof. Let u, v be two solutions. we need to show $u = v$, which is equivalent to show that

$$\iint\limits_{\Omega_-} (u - v)\psi dxdt = 0 \tag{4.9}$$

for every $\psi \in C_0^1(\Omega_- \cup \Gamma_1)$.

Recall that u and v satisfied (4.5). Subtract them to obtain

$$\iint\limits_{\Omega_-} ((u-v)\psi_t + (f(u) - f(v))\psi_x)dxdt = 0 \tag{4.10}$$

or

$$\iint\limits_{\Omega_-} (u-v)(\psi_t + \frac{f(u) - f(v)}{u - v}\psi_x)dxdt. \tag{4.11}$$

Recall that the solution satisfies the Oleinik Entropy condition (Lemma 4.2). The remain proof of uniqueness is similar to that of Theorem 16.10 in [6].

Now we will consider problem (4.12, 4.13). Our strategy is to firstly prove that there exists a solution to (4.12, 4.13) having some nice properties, then we prove in fact the solution coincides with the solution given by Theorem 2.1, which will show that the solution u in Theorem 2.1 enjoys also these nice properties. These properties will make the pointwise Rankine-Hugniot condition available, which is a key ingredient to our proof of the main theorem of this section.

Consider the following initial value problem:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \qquad -\infty < x < l(t), t > 0, \tag{4.12}$$

$$u(x,0) = u_{0l}(x), x \le 0, \qquad u(l(t),t) = w(t). \tag{4.13}$$

Convention: from now on till to Lemma 4.6, we still denote by u a solution (we will construct it numerically) to the problem (4.12, 4.13), by abusing the notation. However, this should not make any confusion. In fact, we will prove that this solution coincides with the solution u in Theorem 2.1 (restricted to Ω_-).

Lemma 4.4. *Suppose that the functions w and u_{0l} are of bounded variation. Then there exists an entropy solution u for problem (4.12) (4.13) such that the limit $u(l(t)-0,t)$ exists in L^1.*

Proof. Notice that we have $l'(t) \ge f^* > f'(M)$, and the slope of the characteristic line $C(x,t)$ is $f'(u(x,t))$. The slope of Γ is greater than $f'(w)$ almost everywhere. This means that in our problem (4.12, 4.13), condition $u(l(t),t) = w(t)$ is not a boundary condition, but an initial condition. We use then the up-wind difference scheme to obtain an approximate solution (which is still denoted by u_j^n).

Let Δx, Δt satisfy $f'(M) \le \Delta x/\Delta t \le f^*$. For any $j \in \mathbb{N}$, we denote by w_j the value of w at the intersection point of Γ and the line $x = j\Delta x$. We give the value of the nearest grid point on the line $x = j\Delta x$ to Γ by u_j^*.

For any $n \in \mathbb{N}$, let $m_n = max_k \,\{k|(k\Delta x, n\Delta t) \in \Omega_-\}$, then $m_{n+1} > m_n$. By our discussions above, for any $m_n < k \le m_{n+1}$, we have $u_k^{n+1} = w_k$. In particular, $u_{m_n}^n = w_{m_n}$.

Let $\Omega_j^n = u_{j+1}^n - u_j^n$, $z_j^n = u_j^{n+1} - u_j^n$. By the conservation law, we have

$$u_j^{n+1} = u_j^n + r(f(u_{j-1}^n) - f(u_j^n)), \tag{4.14}$$

subtract (4.14) for $j+1, j$, we have

$$\Omega_j^{n+1} = (1 - rf^{'}(\xi_j))\Omega_j^n + rf^{'}(\xi_{j-1})\Omega_{j-1}^n,$$

where ξ_{j-1} is a mean value. Sum them up from $-\infty$ to m_n, we get

$$\sum_{j=-\infty}^{m_n-1} |\Omega_j^{n+1}| \le \sum_{j=-\infty}^{m_n-1} |\Omega_j^n| - rf^{'}(\xi_{m_n-1})|\Omega_{m_n-1}^n|.$$

Notice that

$$\begin{aligned}\Omega_{m_n}^{n+1} &= u_{m_n+1}^{n+1} - u_{m_n}^{n+1} = w_{m_n+1} - u_{m_n}^n + r(f(u_{m_n}^n) - f(u_{m_n-1}^n)) \\ &= (w_{m_n+1} - w_{m_n}) + rf'(\xi_{m_n-1})\Omega_{m_n-1}^n,\end{aligned}$$

thus

$$\sum_{j=-\infty}^{m_n} |\Omega_j^{n+1}| \le \sum_{j=-\infty}^{m_n-1} |\Omega_j^n| + |w_{m_n+1} - w_{m_n}|,$$

which gives the following estimation:

$$\sum_{j=-\infty}^{m_{n+1}} |\Omega_j^{n+1}| \leq \sum_{j=-\infty}^{m_n-1} |\Omega_j^n| + \sum_{k=m_n}^{m_{n+1}-1} |w_{k+1} - w_k|$$

Now using an argument of induction, we get $Var(u^{n+1}) \leq Var(u_{0l}) + Var(w)$, which shows by hypothesis that $Var(u^{n+1}) < \infty$.

Next we consider z_j^n. Substract (4.14) for $n, n+1$, we get

$$\begin{aligned} z_j^n &= (1 - rf'(\xi_j))z_j^{n-1} + rf'(\xi_{j-1})z_{j-1}^{n-1}, \; for \; j \leq m_{n-1}. \\ \sum_{j=-\infty}^{m_{n-1}} |z_j^n| &\leq \sum_{j=-\infty}^{m_{n-1}} |z_j^{n-1}| - rf'(\xi_{m_{n-1}-1})|z_{m_{n-1}-1}^{n-1}|. \end{aligned}$$

Notice that for $m_{n-1} + 1 \leq j \leq m_n$, we have

$$|z_j^n| = |u_j^{n+1} - u_j^n| = rf'(\xi_{j-1})|u_j^n - u_{j-1}^n| \leq |w_j - w_{j-1}|.$$

Thus we have the following estimate:

$$\begin{aligned} \sum_{j=-\infty}^{m_n} |z_j^n| &\leq \sum_{j=-\infty}^{m_{n-1}} |z_j^{n-1}| - rf'(\xi_{m_{n-1}-1})|z_{m_{n-1}-1}^{n-1}| + \textstyle\sum_{k=m_{n-1}+1}^{m_n} |w_k - w_{k-1}| \\ &\leq \sum_{j=-\infty}^{m_{n-1}} |z_j^{n-1}| + \textstyle\sum_{k=m_{n-1}+1}^{m_n} |w_k - w_{k-1}|. \end{aligned}$$

By induction, we obtain $\sum_{j=-\infty}^{m_n} |z_j^n| \leq \sum_{j=-\infty}^{0} |z_j^0| + \; Var(w)$. From $z_j^0 = u_j^1 - u_j^0 = rf'(\xi_{j-1})(u_{j-1}^0 - u_j^0)$, we have $|z_j^0| \leq |\Omega_{j-1}^0|$, and finally

$$\sum_{j=-\infty}^{m} |z_j^n| \leq \sum_{j=-\infty}^{0} |\Omega_j^0| + Var(w). \tag{4.15}$$

The rest of the proof is similar to that of Theorem 3.1 in [10].

Now our next step is to remove the condition that w and u_{0l} are of bounded variation in the precedent lemma. To do this, we first prove that the solution to problem (4.12), (4.13) depends continuously on the initial condition (4.13). More precisely, we have the following lemma.

Lemma 4.5. *Let u, v be two entropy solutions to problem (4.12) with (possibly different) initial conditions. Then for any $x_0 < 0$ and for any $T > 0$, there exists a constant $0 \leq c < 1$ such that:*

$$\begin{aligned} &\int_{x_0}^{0} |u(x,0) - v(x,0)| dx + (1+c) \int_{\Gamma_0} |u - v| d\gamma \\ &\qquad \geq \int_{l(T)+x_0}^{l(T)} |u(x,T) - v(x,T)| dx + (1-c) \int_{\Gamma_{x_0}} |u - v| d\gamma, \end{aligned}$$

where for any z, Γ_z denotes the curve $x = l(t) + z, 0 \leq t \leq T$, and the integral $\int_{\Gamma_z} d\gamma$ is the curve integral over Γ_z.

Proof. First a standard argument (see for example the proof of Theorem 2.4 Chapter III [**?**]) will give the following

$$\iint_K \{|u(x,t) - v(x,t)| \frac{\partial \phi}{\partial t} + sign(u(x,t) - v(x,t))(f(u(x,t)) - f(v(x,t))) \frac{\partial \phi}{\partial x}\} dxdt \geq 0,$$

for any $\phi \geq 0$ in $C_0^1(K)$, where K is the region $\{(x,t)|l(t)+x_0 < x < l(t), 0 < t < T\}$.

Let $\omega \geq 0$ be a function in $C_0^\infty(-1,1)$ such that $\int_{-\infty}^{+\infty} \omega(x)dx = 1$. We define $\omega_h(x) = \frac{1}{h}\omega(\frac{x}{h})$ for $h > 0$. Then $\omega_h(x) = 0$ if $|x| \geq h$. Let $\alpha_h(x) = \int_{-\infty}^{x} \omega_h(y)dy$, then $\alpha_h(x) = 1$ if $x \geq h$.

For any $\epsilon > 0$, we define the following functions:

$$\psi_1(x,t) = 1 - \alpha_\epsilon(-t+\epsilon), \quad \psi_2(x,t) = 1 - \alpha_\epsilon(t - T + \epsilon),$$
$$\psi_3(x,t) = 1 - \alpha_\epsilon(l(t) + x_0 - x + \epsilon), \quad \psi_4(x,t) = 1 - \alpha_\epsilon(x - l(t) + \epsilon).$$

Let $\phi_\epsilon(x,t) = \prod_{i=1}^4 \psi_i(x,t)$. Then *supp* $\phi_\epsilon \subset K$ and $\lim\limits_{\epsilon\to 0+} \phi_\epsilon(x,t) = 1$ for any $(x,t) \in K$.

Replace ϕ by ϕ_ϵ in the above inequality, then take $\epsilon \to 0+$, we obtain

$$\begin{aligned}\int_{x_0}^{0} |u(x,0) - v(x,0)|dx + \int_{\Gamma_0} |u-v|(1 - \frac{F(x,t)}{l'(t)})d\gamma \\ \geq \int_{l(T)+x_0}^{l(T)} |u(x,T) - v(x,T)|dx + \int_{\Gamma_{x_0}} |u-v|(1 - \frac{F(x,t)}{l'(t)})d\gamma,\end{aligned}$$

where $F(x,t) = sign(u-v)\frac{f(u)-f(v)}{u-v}$.

By Lemma 4.1, $0 \leq \frac{|F(x,t)|}{l'(t)} \leq c < 1$ for some constant c. Then the precedent inequality gives that

$$\begin{aligned}\int_{x_0}^{0} |u(x,0) - v(x,0)|dx + (1+c)\int_{\Gamma_0} |u-v|d\gamma \\ \geq \int_{l(T)+x_0}^{l(T)} |u(x,T) - v(x,T)|dx + (1-c)\int_{\Gamma_{x_0}} |u-v|d\gamma,\end{aligned}$$

which completes the proof.

As a corollary, we see that the solution to problem (4.12) is unique if condition (4.13) is fixed. We should point out that in the proof (also in the proof of Lemma 4.4), the condition $l'(t) > f'(M)$ is essential.

Now we consider the general case, i.e. w (resp. u_{0l}) is not necessarily of bounded variation, but bounded and measurable. Then we can take a sequence $w^{(k)}$ (resp. $u_{0l}^{(k)}$) of functions of bounded variation on $l(t)$ (resp. on $t = 0, x \leq 0$) which converges to w in L^1. Let $u^{(k)}$ be the solution to problem (4.12) corresponding to the conditions $u_{0l}^{(k)}$ and $w^{(k)}$. Then by the precedent lemma, $u^{(k)}$ converges to u in L^1. Furthermore, we have

$$\begin{aligned}\int_{x_0}^{0} |u_{0l}^{(k)} - u_{0l}^{(l)}|dx + (1+c)\int_{\Gamma_0} |w^{(k)} - w^{(l)}|d\gamma \\ \geq \int_{l(T)+x_0}^{l(T)} |u^{(k)}(x,T) - u^{(l)}(x,T)|dx + (1-c)\int_{\Gamma_{x_0}} |u^{(k)} - u^{(l)}|d\gamma,\end{aligned}$$

for any k, l and any $x_0 < 0$. Now take k, l goes to infinity, then the above inequality shows that $u^{(k)}(l(t)+x_0,t)$ converges uniformly with respect to x_0 to $u(l(t)+x_0,t)$ in $L^1(\Gamma_{x_0})$. Thus when x_0 goes to 0, $u(l(t)+x_0,t)$ goes to w, which shows that $u(l(t)-0,t)$ exists in L^1, which proves the following:

Lemma 4.6. *If w is bounded and measurable, then there exists an entropy solution u for problem (4.12) (4.13) such that the limit $u(l(t)-0,t)$ exists in L^1.*

Now we come to the main result of this section.

Theorem 4.1. *If (4.1), (15) hold, then the discontinuity* Γ *of the weak solution* u, z *is a weak detonation wave, which satisfies the Rankine-Hugoniot condition:*

$$l'(t) = \frac{f(u(l(t)-0,t)) - f(u(l(t)+0,t))}{u(l(t)-0,t) - u(l(t)+0,t) - q},$$

and $l'(t) \geq f'(u(l(t)-0,t)) \geq f'(u(l(t)+0,t))$ *almost everywhere.*

Proof. It is easy to see that the weak solution to (4.12) (4.13) satisfies the condition (4.5). By Lemma 4.3, it is the solution provided by Theorem 2.1. Now Lemma 4.6 implies that for the solution u to the problem (1), (4), (5) and (6), the limit $u(l(t)-0,t)$ exists. Thus the limit of the solution u to the curve Γ exists from both sides, so the solution u satisfies the pointwise Rankine-Hugoniot condition. Now by Lemma 4.1 and the discussions on the region Ω_+, the solution u contains a weak detonation wave.

Remark 4.1. In [Yin], the second named author has proved a similar result for the Riemann problem, but in a weaker sense. The main difficulty there is that we did not know how to prove the existence of the limit $lim_{\epsilon \to 0+} u(l(t)-\epsilon,t)$, which made unavailable the pointwise Rankine-Hugoniot condition.

5. Numerical Examples

Example 1. Let u, z be two functions which satisfy

$$\frac{\partial(u+qz)}{\partial t} + \frac{\partial}{\partial x}(\frac{u^2}{2}) = 0,$$

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

with $q = 0.5$, $u_{0l}(x) = 8.0$ and

$$u_{0r}(x) = \begin{cases} 1.5, & x \in (0,20] \\ x/2 - 8.5, & x \in (20,22] \\ 2.5, & \text{else.} \end{cases}$$

As easily seen, we have the following results: $u_1 = 8, u_2 = 2.5, u_{CJ} = (6+\sqrt{11})/2, \bar{u}_{CJ} = (4+\sqrt{7})/2, u_{l*} = (10-\sqrt{5})/2, u_l^* = (10+\sqrt{5})/2, \bar{u}_l^* = (10+\sqrt{29})/2$ and $\bar{u}_{l*} = (10-\sqrt{29})/2$. Let $u_3 = 1.5$.

Fig.1, Fig.2 and Fig.3 are the numerical results of our upwind scheme with the ignition temperature $U_i = 2.6$, but at different time.

In Fig.1, we take $t = 2$, then we find just one discontinuity. The speed there is $s = 5.1458$, which is equal to $(f(u_1) - f(u_3))/(u_1 - u_3 - q)$, thus it is a strong detonation wave. Recall that by our Theorem 3.1, if the ignition temperature U_i is in $[u_{l*} - q, u_l^*)$, then our upwind scheme leads to a strong detonation wave. In Fig. 1, U_i is not in $[u_{l*} - q, u_l^*)$, however we still obtain a strong detonation wave, which gives an example to show that our conditions in Theorem 3.1 are only sufficient, but not necessary.

In Fig.3, we take $t = 15$, then we find the speed at the right discontinuity is $s = 12.1525$ which equals to $(f(a) - f(u_2))/(a - u_2 - q)$., which is a weak detonation wave, where $a = 3$ is the value of the second horizontal line in Fig.3. At the left side of this weak detonation wave, there is a shock wave. An interesting phenomena appears here: we observe that a strong detonation wave (at $t = 2$) is transformed to a weak detonation wave (at $t = 15$).

In fact the weak detonation wave can be explained as follows: when U_i is slightly bigger than 2.5 (the precise meaning of "slightly" will be made clear later), then by Theorem 4.1 there is a weak detonation wave followed by a shock wave. In fact, this weak detonation wave can be regarded as the weak detonation wave appeared in the Riemann problem with initial values $u_l = 8$ and $u_r = 2.5$ (see [8] for a theoretical support and [11] for a numerical support).

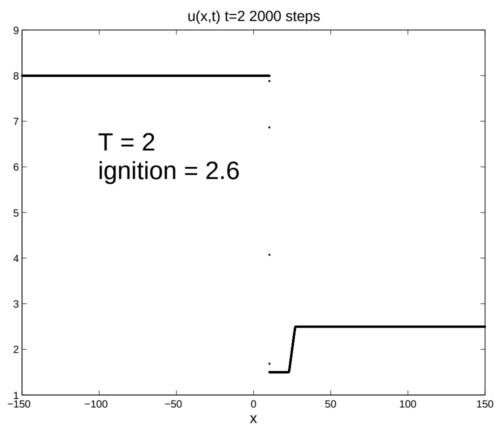

Fig.1 $U_i = 2.6, t = 2$

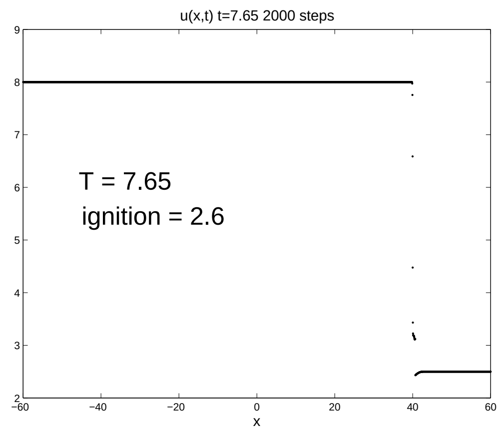

Fig.2 $U_i = 2.6, t = 7.65$

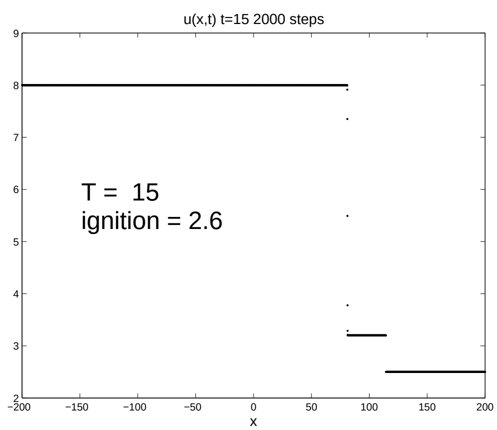

Fig.3 U_i = 2.6, t= 15

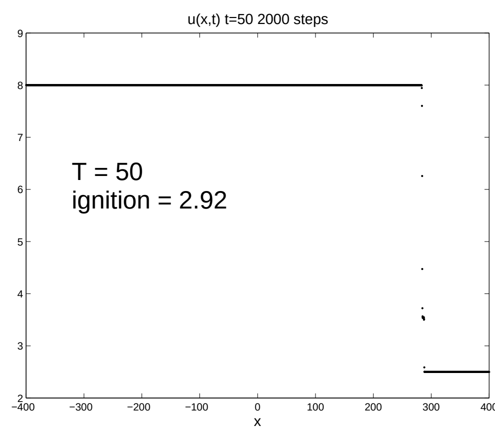

Fig.4 $U_i = 2.92, t = 50$

In Fig. 2, we take $t = 7.65$, then we are in the phrase of this transformation from a strong detonation wave to a weak one.

Then one may wonder if such a transformation happens for all U_i. Interestingly this is not the case. By some numerical experience, we find that if $2.5 < U_i < c$, then such a transition happens, and when $U_i > c$, there is only one strong detonation wave, and there is no such a transition, where c is a constant between 2.92 and 2.93. Fig. 4 and Fig. 5 are illustrations of this observation: when $U_i = 2.92$, there exists such a transition, but there is none if $U_i = 2.93$.

However, for the moment we don't know how to determine the exact value of c. Some estimates of such a jump can be given based on our Theorem 4.1, but as we stated before, our Theorem 4.1 gives just a sufficient condition, but not a necessary condition. An optimal estimate of a such jump would require more insight.

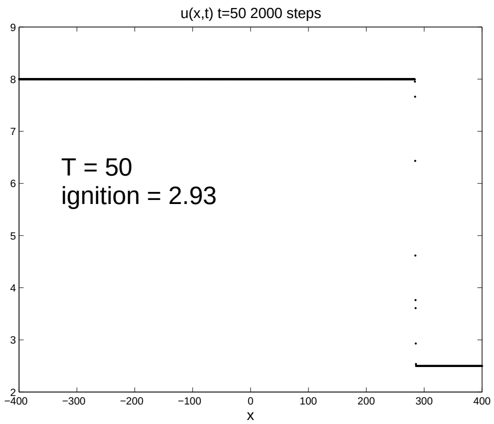

Fig. 5 $U_i = 2.93$, t=50

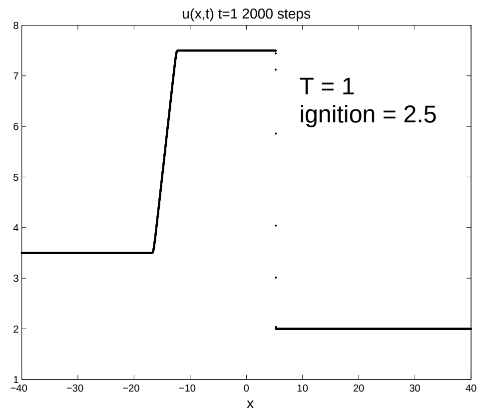

Fig. 6 $t = 1$ $U_i = 2.5$

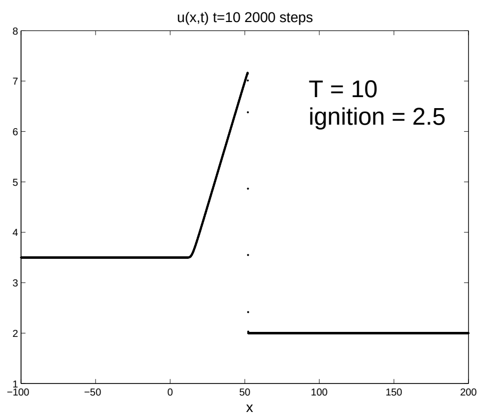

Fig. 7 $t = 10, U_i = 2.5$

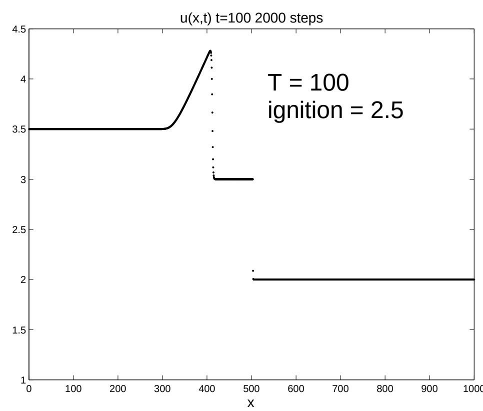

Fig. 8 $t = 100$ $U_i = 2.5$

Example 2. Finally we consider the same equation with initial condition: $u_{or} = 2$ and

$$u_{0l}(x) = \begin{cases} 7.5, & x \in [-20, 0] \\ 3.5, & x \in (-\infty, -20) \end{cases}$$

We have done numerical simulation for $U_i = 2.5$. Fig. 6, Fig. 7 and Fig. 8 are the results corresponding respectively to $t = 1, 10, 100$.

We observe that when $t = 1$, there is a strong detonation wave and a central rarefaction wave, and when $t = 100$, this strong detonation wave is transformed to be a weak detonation wave. When $t = 10$, the picture shows that this is still a strong detonation wave, but it is in the phrase of transition.

Acknowledgments. We want to thank the referee for the suggestions, which has greatly improved the presentation of this paper.

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