TECHNICAL NOTE

# Solution of the autoclave discharge problem by the Lax-Wendroff method

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This paper considers the problem of calculating the discharge arising from the collapse of the safety disc in an autoclave system. The autoclave is approximated by an equivalent system consisting of a high-pressure reservoir and a discharge pipe with a diaphragm and nozzle. Solutions to the problem are calculated using the Lax-Wendroff method. These solutions are compared with ones obtained from analytical methods and with a solution obtained by practical measurement.

**Keywords:** *autoclave system; Lax-Wendroff method*

## Introduction

In many processing plants, chemical reactions are carried out in closed vessels in which the pressure increases as the reaction continues. If the chemical reaction goes out of control, unacceptably high levels of pressure may arise, and to avoid this situation the vessels are connected to a discharge pipe fitted internally with a safety disc. On collapse of the safety disc, a rapid discharge from the autoclave takes place through the discharge pipe. At the end of the discharge pipe, there is usually a deflector plate. The effect of the deflector plate is to contain the discharge to some extent, but this placement will have the undesirable effect, in general, of producing a reflected shock wave. The estimation of the transients during the discharge is thus of great interest.

It is of both theoretical and practical interest to construct a mathematical model of this system that will predict these transients and so serve as a useful tool in the design of an autoclave system. Here the model of an autoclave system is assumed to consist of a reservoir maintained at constant pressure and a discharge pipe with diaphragm and nozzle as shown in Figure 1. The diaphragm corresponds to the autoclave's safety disc, which collapses when a predetermined safety pressure is exceeded. The deflector plate at the end of the discharge pipe may be approximated by an equivalent nozzle. The calculation of the transients is achieved here by the Lax-Wendroff method[1] because of its simplicity, accuracy, speed, and robustness.

Other accounts and solutions of the problem may be found in Woods,[2] Woods and Thornton,[3] Woods and Owen,[4] and Baltas.[5] In this paper, the Lax-Wendroff method is used to calculate the numerical solution from the data supplied by Baltas. This numerical solution is then compared with the solution Baltas obtained by practical measurement.

For convenience, the data taken from the Baltas paper is summarized here.

| | |
|---|---|
| Length of discharge pipe | 9.212 m |
| Diaphragm position from the reservoir | 4.606 m |
| Transducer position from the reservoir | 5.923 m |
| Nozzle to pipe area ratio ($\psi$) | 0.4444 |

The atmospheric pressure was measured as $p_1 = 1.02187$ bar, and the high/low pressure ratio was taken as $p_4/p_1 = 7.0722$.
The temperature of the system, initially, was measured as $T = 291.45°K$.

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From these values, the following initial variable values for the autoclave may be calculated to four significant figures, using the notation shown in Figure 2:

$\rho_1 = 1.222 \quad p_1 = 0.1022.10^6 \quad a_1 = 342.2$

$\rho_4 = 8.640 \quad p_4 = 0.7227.10^6 \quad a_4 = 342.2$

## Governing equations

### Conservation form

During the discharge, the flow values are governed by the continuity, momentum, and energy equations of unsteady gas flow. These equations may be written in the conservation form:

$$\frac{\partial V}{\partial t} + \frac{\partial G(V)}{\partial x} = B \tag{1}$$

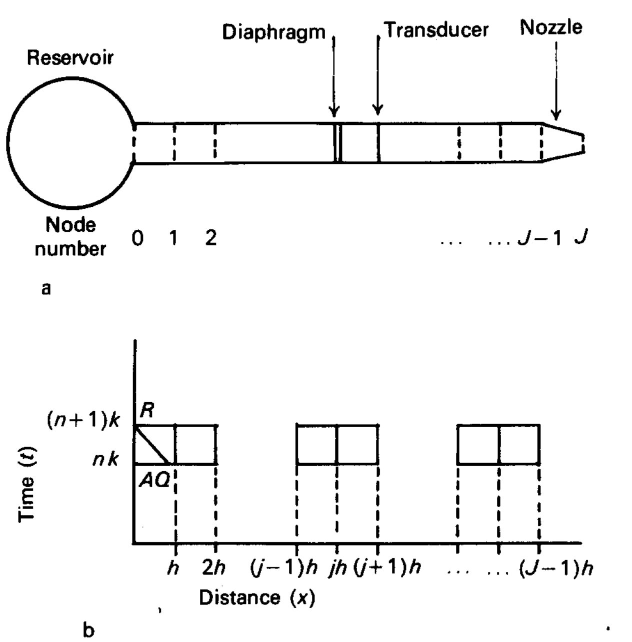


*Figure 1* (a) Autoclave representation; (b) computational grid for pipe of length $x=(J-1)h$

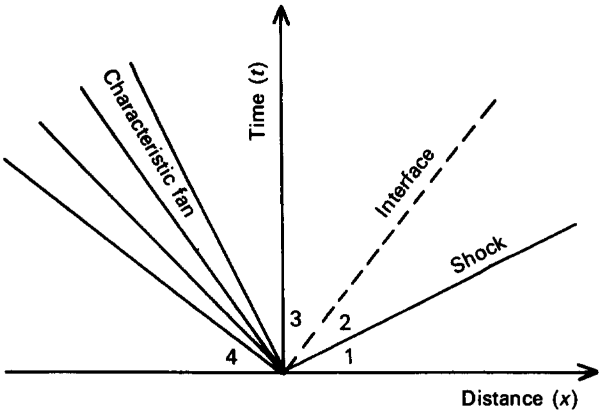


*Figure 2* Position-diagram for shock-tube problem

where

$$V=\begin{bmatrix}\rho\\ m\\ e\end{bmatrix}\qquad G(V)=\begin{bmatrix}m\\ p+m^2/\rho\\ (e+p)m/\rho\end{bmatrix}\qquad B=\begin{bmatrix}0\\ -\rho\phi\\ \rho q\end{bmatrix}$$

and the wall friction term is defined by

$$\phi=\frac{4f}{D}\cdot\frac{u}{2}|u| \tag{2}$$

The value of the wall friction term, unclear in transient flow involving shocklike discontinuities, was taken as zero in all the calculations in this paper. The heat transfer rate term, $q$, was also taken as zero.

### Quasilinear form

The quasilinear form of these equations is

$$\frac{\partial W}{\partial t}+A\frac{\partial W}{\partial x}=C \tag{3}$$

where

$$W=\begin{bmatrix}\rho\\ u\\ p\end{bmatrix}\quad A=\begin{bmatrix}u & \rho & 0\\ 0 & u & \dfrac{1}{\rho}\\ 0 & \gamma p & u\end{bmatrix}\quad C=\begin{bmatrix}0\\ -\phi\\ (\gamma-1)\rho(q+u\phi)\end{bmatrix}$$

The characteristics, and characteristic relations along the characteristics, can be obtained from these quasilinear equations and written in the following form:[6]

$$\alpha a\pm\frac{\gamma-1}{2}\,du=\frac{\gamma-1}{2}\,\alpha\,dt+\frac{a}{a_a}\,\alpha a_a \tag{4}$$

where

$$\alpha=(\gamma-1)\frac{q}{a}\mp\phi\left(1\mp(\gamma-2)\frac{u}{a}\right)$$

on the $C^{(1)}$, $C^{(2)}$ characteristics, $dx/dt=u\pm a$, and

$$\alpha a_a=\frac{1}{2}\frac{a_a}{\rho a^2}\beta\,dt \tag{5}$$

where

$$\beta=(\gamma-1)p(q+u\phi)$$

on the $C$ characteristic, $dx/dt=u$.

## Analytical solution

This section obtains the theoretical solutions for the initial and final flow values of the autoclave system.

### Incident wave solution

A shock tube is considered with the gas initially in the state

$$u=0\qquad p=p_1\qquad \rho=\rho_1$$

for $x>0$, on the low-pressure side of the diaphragm, and

$$u=0\qquad p=p_4>p_1\qquad \rho=\rho_4$$

for $x<0$, on the high-pressure side of the diaphragm. The governing equations with these initial values form a Riemann initial value problem. For Riemann problems, it is possible to obtain an exact analytical solution for the incident wave. The structure of the solution may be illustrated in the position-diagram of Figure 2, which shows that a shock and interface wave travel toward the nozzle, and a rarefaction wave travels toward the reservoir. Once reflections from the pipe ends have occurred, exact analytical solutions are not available, in general, until the arrival of the steady discharge state.

A convenient method for obtaining this solution is outlined in Whitham.[7] The procedure is to obtain a nonlinear equation in terms of the shock strength parameter, $z$, defined by $z=(p_2-p_1)/p_1$, using the notation of Figure 2. The problem may be viewed as the combination of two piston problems, with the interface acting effectively as a piston. From a manipulation of the Rankine-Hugoniot equations holding across the shock wave in front of the interface, and the characteristic equations governing the flow behind the interface, the following nonlinear equation may be obtained:

$$\frac{z}{\gamma\left(1+\dfrac{\gamma+1}{2\gamma}z\right)^{1/2}}=\frac{2}{(\gamma-1)}\frac{a_4}{a_1}\left\{1-\left[\frac{p_1}{p_4}(1+z)\right]^{\gamma-1/2\gamma}\right\} \tag{6}$$

This equation can be solved for the shock parameter, $z$, by a numerical method, for example, the method of bisection. Once the magnitude of this shock strength parameter has been

## Notation

- $a$ Speed of sound
- $a_a$ Speed of sound after isentropic change of state to reference pressure $p_{ref}$
- $D$ Pipe diameter
- $e$ Total energy per unit volume
- $f$ Friction factor
- $m$ Momentum per unit volume
- $p$ Pressure
- $q$ Heat transfer rate per unit mass
- $t$ Time
- $T$ Temperature
- $u$ Particle velocity
- $x$ Distance
- $\gamma$ Ratio of specific heats ($\gamma=1.4$)
- $\rho$ Density
- $\psi$ Nozzle to pipe area ratio

*Subscript/superscript*

$U_j^n\equiv U(jh,nk)\equiv U(x,t)$

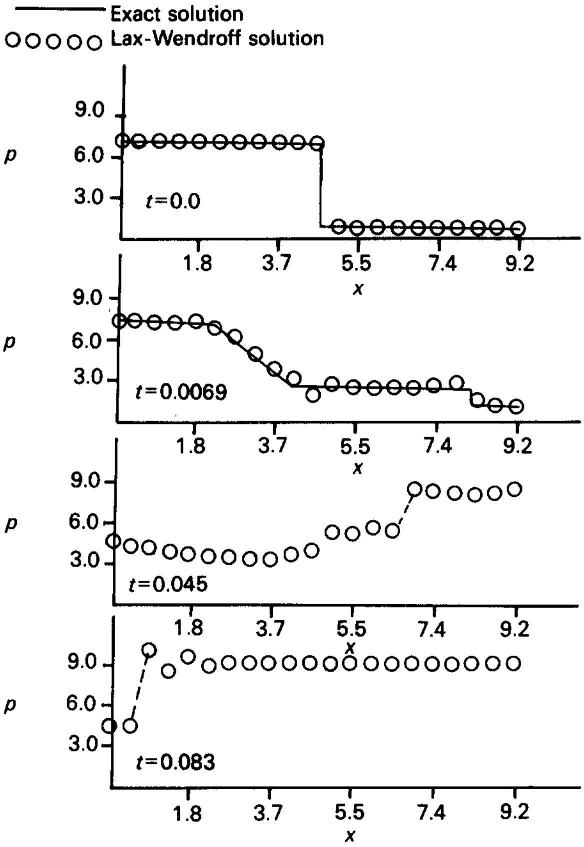


*Figure 3* Incident and reflected pressure wave

obtained, numerical values may be obtained for all the other unknowns.

Applying this method to the data obtained from Baltas gives the following solution to the problem:

| | | | |
|---|---|---|---|
| $\rho_1=1.222$ | $u_1=0.000$ | $p_1=0.1022.10^6$ | $a_1=342.2$ |
| $\rho_2=2.282$ | $u_2=238.8$ | $p_2=0.2523.10^6$ | $a_2=393.5$ |
| $\rho_3=4.074$ | $u_3=238.8$ | $p_3=0.2523.10^6$ | $a_3=294.4$ |
| $\rho_4=8.640$ | $u_4=0.000$ | $p_4=0.7227.10^6$ | $a_4=342.2$ |

in the notation of Figure 2. The shock travels with a speed $U=514.3$ m/s, and the analytical solution at $t=0.0069$ s, just before the shock impinges on the nozzle, is shown in Figure 3.

### Steady state solution

Once the transients have died away and the system is in a steady discharge state, a solution may be obtained from the following steady state equations:

*Reservoir to pipe*

$$\text{Energy:} \quad a^2+\frac{\gamma-1}{2}u^2=a_0^2 \tag{7}$$

$$\text{Entropy:} \quad p/\rho^\gamma=p_0/\rho_0^\gamma \tag{8}$$

where the subscript 0 represents a reservoir value.

*Pipe to nozzle*

$$\text{Continuity:} \quad \rho u=\psi\rho_e a_e \tag{9}$$

$$\text{Energy (sonic flow):} \quad a^2+\frac{\gamma-1}{2}u^2=\frac{\gamma+1}{2}a_e^2 \tag{10}$$

$$\text{Entropy:} \quad p_0/\rho_0^\gamma=p_e/\rho_e^\gamma \tag{11}$$

where the subscript $e$ represents a nozzle outlet value.

For the reservoir values $p_0=0.7227.10^6$ and $a_0=342.2$, the following steady state solutions were obtained:

| | | | |
|---|---|---|---|
| $u_0=0.000$ | $p_0=0.7227.10^6$ | $\rho_0=8.640$ | $a_0=342.2$ |
| $u=91.21$ | $p=0.6874.10^6$ | $\rho=8.336$ | $a=339.8$ |
| $u_e=312.4$ | $p_e=0.3818.10^6$ | $\rho_e=5.477$ | $a_e=312.4$ |

## Numerical method of solution

### Lax-Wendroff method

The autoclave system is subdivided by the nodal points $j=0,1,2,\ldots,J$, as shown in Figure 1. The Lax-Wendroff method, in its two-step form[8]

$$V_{j+1/2}^{n+1/2}=\frac{1}{2}(V_{j+1}^n+V_j^n)-\frac{1}{2}\frac{\Delta t}{\Delta x}(G_{j+1}^n-G_j^n)+\frac{\Delta t}{4}(B_{j+1}^n+B_j^n) \tag{12}$$

$$V_j^{n+1}=V_j^n-\frac{\Delta t}{\Delta x}(G_{j+1/2}^{n+1/2}-G_{j-1/2}^{n+1/2})+\frac{\Delta t}{2}(B_{j+1/2}^{n+1/2}+B_{j-1/2}^{n+1/2}) \tag{13}$$

was used to calculate values at the nodes $j=1,2,\ldots,J-2$ of Figure 1.

### Numerical approximation at the boundary

The calculation of the values at the 0, $J-1$, and $J$ nodes of Figure 1 requires a numerical method that can be used in conjunction with the quasi-steady assumptions at the pipe-nozzle and pipe-reservoir boundaries.

At the pipe-nozzle boundary, a hybrid method of approximation was used. This method, along with its accuracy in the calculation of a reflected shock, has been fully discussed elsewhere.[9]

At the reservoir-pipe boundary, a characteristic approximation was used in conjunction with the quasi-steady state assumption. For subsonic flow from the reservoir to the pipe, two quasi-steady state assumptions are required. These, in the notation of Figure 1, take the form

$$\text{Energy:} \quad \frac{\gamma-1}{2}u_R^2+a_R^2=a_0^2 \tag{14}$$

$$\text{Entropy:} \quad (a_a)_R=(a_a)_0 \tag{15}$$

where the 0 subscript refers to the reservoir values.

Applying the method of Courant *et al.*[10] to the $C^{(2)}$ characteristic in Equation 4 leads to

$$x_R-x_Q=(u_A-a_A)K \tag{16}$$

and the characteristic relation

$$a_R-\frac{\gamma-1}{2}u_R=\frac{\gamma-1}{2}Q \tag{17}$$

where

$$Q=\frac{2}{\gamma-1}a_Q-u_Q+\frac{2}{\gamma-1}\frac{a_A}{(a_a)_A}((a_a)_R-(a_a)_Q)+\alpha_A K$$

Following Rudinger,[11] it is now possible to solve Equations 14 and 17 for the sound speed, $a_R$, giving

$$a_R=\frac{\gamma-1}{\gamma+1}\left[Q+\left(\frac{\gamma+1}{\gamma-1}a_0^2-\frac{\gamma-1}{2}Q^2\right)^{1/2}\right] \tag{18}$$

where it has been assumed that the flow is positive, $u_R>0$. Once a value for the sound speed, $a_R$, has been found, values for the pressure, $p_R$, and density, $\rho_R$, may be obtained from the isentropic relationships.

## Numerical computations

The Lax-Wendroff method with the hybrid and characteristic methods of approximation at the pipe boundaries was applied

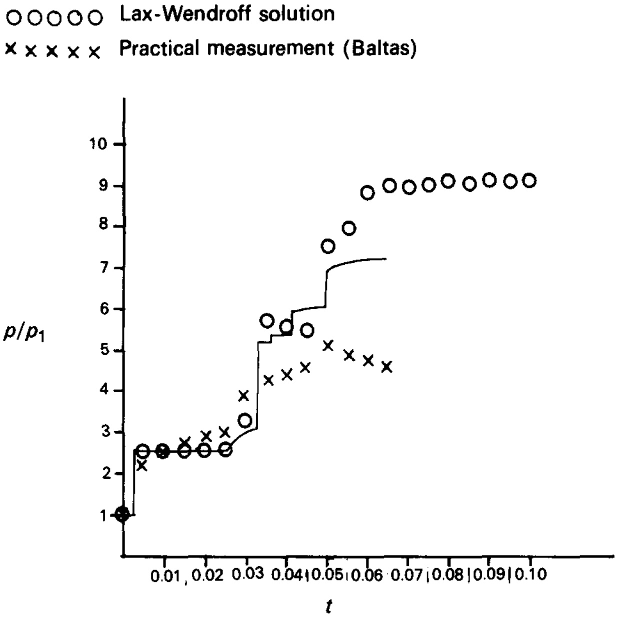


*Figure 4* Pressure ratio ($p/p_1$) against time

to the data obtained from Baltas. The computations were performed with 42 nodes, giving a mesh length $\Delta x = 9.212/40 = 0.2303$ m. The increment, $\Delta t$, was obtained from $\max(|u| + a)\,\Delta t/\Delta x = 0.9$ to satisfy the Courant-Friedrichs-Lewy stability criterion.[8]

The computed values at various times are shown in Figure 3. The results at time $t = 0.0069$ s demonstrate the accuracy of the Lax-Wendroff method, when compared with the exact solution, for the incident wave. The computations show that the incident shock wave impinges on the nozzle at an approximate time $t = 0.009$ s and produces a reflected shock wave of approximate magnitude 9.0 bar. As time increases, a steady discharge state is eventually reached through the interplay of waves between reservoir and nozzle ends. For $t \geqslant 0.8$, the Lax-Wendroff method gave steady state pipe values of

$$u = 91.2 \qquad p = 0.687.10^6 \qquad \rho = 8.34 \qquad a = 339.8$$

and steady-state nozzle values of

$$u_e = 312.4 \qquad p_e = 0.3818.10^6 \qquad \rho_e = 5.478 \qquad a_e = 312.4$$

showing agreement to three significant figures with the analytical steady state values previously obtained.

## Theoretical and practical comparisons

This section compares the solution to the autoclave problem given by the Lax-Wendroff method with the one obtained by Baltas from practical measurement.

In the practical measurements, a transient pressure measuring transducer was placed between the diaphragm and the outlet nozzle at a distance of 1.317 m from the diaphragm. The pressure ratio, $p/p_1$, where $p_1$ is the atmospheric pressure, against time measurements at this point are shown in Figure 4, along with the results obtained by the Lax-Wendroff method.

The results show good agreement in the time interval $0 \leqslant t \leqslant 0.01$, during which time the incident shock wave passes the transducer. The results are also in reasonable agreement in the time interval $0.01 \leqslant t \leqslant 0.05$, the increase in pressure arising here from the reflection of the shock and interface waves. For $t > 0.05$, the solutions show some differences, and some explanation is required. In the practical measurement, the pressure ratio reaches a maximum of 5.0 and then decreases. This may be explained by the fall in pressure at the reservoir, which cannot be maintained at the initial high pressure value for very long in a practical experiment. The Lax-Wendroff method for $t > 0.05$ shows a rise in the pressure ratio to a maximum of 9.2, followed by a gradual tailing off to the steady state pressure ratio of 6.7 for $t \geqslant 0.8$.

In summary, though these results show good agreement initially, significant differences do appear in the solutions at later times. These differences arise from the assumption of constant pressure at the reservoir used in the mathematical model. An improved model allowing for the decrease in pressure at the reservoir should produce better agreement, and work is continuing along these lines.

## Conclusion

This paper has obtained a solution to the autoclave problem through the application of the Lax-Wendroff method of solution. The numerical solution obtained from the Lax-Wendroff method has been compared with exact analytical solutions, for the initial and final steady state values, and good agreement has been obtained between the two methods. The solutions given by the Lax-Wendroff method have also shown reasonable agreement with those obtained from practical measurement.

## Acknowledgement

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