INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
Int. J. Numer. Meth. Fluids (2007)
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/fld.1574

Closure models for multimaterial cells in arbitrary Lagrangian–Eulerian hydrocodes‡

M. Shashkov*, †

Los Alamos National Laboratory, T-7, MS B284, Los Alamos, NM 87545, U.S.A.

SUMMARY

High-speed multimaterial flows with strong shear deformations occur in many problems. Due to the nature of shock wave propagation in complex materials, the arbitrary Lagrangian–Eulerian (ALE) methods are currently the only proven technology to simulate such problems. In ALE methods, the mesh does not move with the fluid, so that it is unavoidable that mixed cells containing two or more materials will appear; such mixed cells require a special closure model to be well posed. In this paper, we will discuss some of the possible models. Published in 2007 by John Wiley & Sons, Ltd.

Received 22 March 2007; Revised 18 June 2007; Accepted 19 June 2007

KEY WORDS: multimaterial hydro; closure models; mixed cells; ALE; finite difference methods; compressible flow

1. INTRODUCTION

High-speed multimaterial flows with strong shear deformations occur in many problems of interest. Due to the nature of shock wave propagation in complex materials, the arbitrary Lagrangian–Eulerian (ALE) methods are currently the only proven technology that address such problems numerically. In ALE methods, the mesh does not move with the fluid, and so it is unavoidable that mixed cells containing two or more materials will appear.

Multimaterial cells are introduced in ALE methods to represent material interfaces that undergo large deformation. The main difficulties in this case are how to accurately determine the thermodynamic states of the individual material components and the nodal forces that such a zone generates, despite the lack of information about the velocity distribution within multimaterial cells.

*Correspondence to: M. Shashkov, Los Alamos National Laboratory, T-7, MS B284, Los Alamos, NM 87545, U.S.A.
†E-mail: shashkov@lanl.gov

Contract/grant sponsor: U.S. Department of Energy; contract/grant number: DE-AC52-06NA25396
Contract/grant sponsor: DOE Office of Science Advanced Scientific Computing Research (ASCR)

A separate set of material properties is normally maintained for each material in every multi-material cell along with the volume fractions that define the fraction of the cell's volume occupied by each material. The volume fractions can also be used to reconstruct material interfaces inside a mixed cell.

A subcell model (closure) is then required to define how the volume fractions and the states of the individual materials evolve during the Lagrangian step. This subcell model is required to close the governing equations, which are otherwise underdetermined.

One of the important classes of methods is based on the assumption of pressure equilibrium (PE), or on introducing some mechanism for pressure relaxation (PR) (see, e.g. [1–5]). The pressure at a material interface should be continuous; however, the pressure within a computational cell represents an average pressure integrated over the cell volume. This means that there is no physical requirement for absolute PE within a multimaterial cell. In fact, for the entire computational cell to come to PE, a shock wave would have to cross the cell many times, while the CFL stability condition prohibits a shock wave from crossing any cell in a single time step. However, pressure continuity at material interfaces does suggest that the pressure within a multimaterial cell should move toward PE, rather than to diverge from it. This can be achieved by introducing a relaxation mechanism like viscosity into the model (see, e.g. [2, 5]).

In addition to PE or PR, this class of method invokes conservation of volume and some form of conservation of total internal energy, which is still insufficient to close the model. There are several possibilities, e.g. methods like [2] assume that the flow is isentropic. Another model, in which the change in entropy of each material is assumed equal, is proposed in [4] and has the important property that it leads to a hyperbolic system of equations that satisfy an entropy inequality under CFL-like restrictions. Methods in this class also differ with respect to how the equations are approximated, ranging from fully implicit as in [4, 5], to fully explicit as in [2]. It is important to note that in this class of method, one assumes no knowledge of the actual configuration of materials in the cell.

Recently, a new class of closure models that attempts to emulate the behavior of separate Lagrangian subcells has been developed [6–8]. In this class of methods, one estimates the velocity normal to the interface between materials and then estimates the change in the volume for each material. In an ideal situation, the position and orientation of the material interface may be known (e.g. from interface reconstruction). Internal energy is updated separately for each material from its own $p\,\mathrm{d}V$ equation. A common pressure for a mixed cell, which is used in the momentum equation, is computed using the principle of conservation of total energy. One can also introduce an exchange of internal energy between the materials inside a mixed cell, which allows more freedom in the definition of the common pressure, [7, 8].

In this paper, we will describe two different closure models and present numerical comparisons for 1D compatible staggered discretizations of the Lagrangian equations with mixed cells.

2. STAGGERED COMPATIBLE DISCRETIZATION—PURE CELLS

In this section, we describe a standard staggered compatible discretization for Lagrangian gas dynamics (see, e.g. in [9, Chapter 5]) for the case that each cell (zone) of the computational mesh contains just one material; that is, all cells are pure cells. In a staggered discretization, the coordinates $\mathbf{x}_j$ and velocities $\mathbf{u}_j$ are located at the nodes j while the rest of the quantities: mass, $m_{j+1/2}$, density, $\rho_{j+1/2}$, internal energy, $\varepsilon_{j+1/2}$, volume, $V_{j+1/2}$, and pressure, $p_{j+1/2}$ are cell

Published in 2007 by John Wiley & Sons, Ltd. *Int. J. Numer. Meth. Fluids* (2007)
DOI: 10.1002/fld

centered. We will also need nodal mass M_j. We will adopt operator notation and spatial indices will be dropped almost everywhere.

Usually, the time integration of Lagrangian equations is implemented as a predictor–corrector scheme. In the predictor stage, one 'predicts' coordinates $\mathbf{x}^{n+1/2} = \mathbf{x}^n + (\delta t/2)\mathbf{u}^n$, and volumes $V^{n+1/2} = \mathscr{V}(\mathbf{x}^{n+1/2})$, as well as pressure under the assumption that the flow is isentropic

$$p^{n+1/2} = p^n - \rho^n (c^n)^2 \, \delta V^{n+1/2}/V^n, \quad \delta V^{n+1/2} = V^{n+1/2} - V^n \tag{1}$$

at the 'half' time step $n + 1/2$. In the corrector step, one updates velocity—$M(\mathbf{u}^{n+1} - \mathbf{u}^n)/\delta t = -\Delta(p^{n+1/2})$, coordinate $\mathbf{x}^{n+1} = \mathbf{x}^n + \delta t \, \mathbf{u}^{n+1/2}$, $\mathbf{u}^{n+1/2} = (\mathbf{u}^n + \mathbf{u}^{n+1})/2$, volume—$V^{n+1} = \mathscr{V}(\mathbf{x}^{n+1})$ density—$\rho^{n+1} = m/V^{n+1}$, internal energy—$m(\varepsilon^{n+1} - \varepsilon^n)/\delta t = -p^{n+1/2}\,\Delta^*(\mathbf{u}^{n+1/2})$, and finally pressure from the equation of state—$p^{n+1} = \mathscr{P}(\rho^{n+1}, \varepsilon^{n+1})$. In these formulas, we have used the operator notation $(\Delta\psi)_j = \psi_{j+1/2} - \psi_{j-1/2}$, $(\Delta^*\varphi)_{j+1/2} = \varphi_j - \varphi_{j-1}$ and for simplicity have omitted all terms related to artificial viscosity. The staggered compatible discretization is conservative [9]. For conservation, it is important that the same p is used in the momentum and internal energy equations; Δ and Δ^* are adjoint operators; and $\mathbf{u}^{n+1/2}$ is used in the internal energy equation.

3. MIXED CELL MODELS

In this paper, we consider two classes of closure models. The first class of models is based on the assumption of PE (PR) and the assumption that the flow is isentropic. The second class of models is based on modeling the dynamics of the pure subcells inside of a mixed cell. Let us mention several design principles for closure models. The first principle is *preservation of the contact*; that is, if initially all materials in a mixed cell have the same pressure, then that pressure does not change due to the closure model. The second principle is *pressure equilibration*; that is, after some transition time, all pressures in the mixed cell have to equilibrate. The third principle is *conservation of total energy*; that is, total energy has to be conserved exactly. For practicality, the closure models are implemented in the predictor stage.

3.1. Tipton's mixed zone pressure relaxation model

As an example of a PR model, we consider our interpretation of the so-called *Tipton's mixed zone pressure relaxation model* [2]. In this model, one assumes that $p_i^{n+1/2} + R_i^{n+1/2} = \hat{p}^{n+1/2}$, where i is the material index, $p_i^{n+1/2}$ is the pressure in the ith material and $R_i^{n+1/2}$ is the relaxation term. An expression for $p_i^{n+1/2}$ is derived under the assumption that the flow is isentropic, $\mathrm{d}S_i/\mathrm{d}t = 0$, and a particular time centering, that makes it linear in $\delta V_i^{n+1/2}$, and a relaxation term that resembles linear viscosity

$$p_i^{n+1/2} = p_i^n - \rho_i^n (c_i^n)^2 \delta V_i^{n+1/2}/V_i^n, \quad R_i^{n+1/2} = -\rho_i^n c_i^n (L^n/\delta t)(1/V_i^n)\delta V_i^{n+1}$$

Here, L^n is a characteristic length related to the mixed cell; c_i^n is the adiabatic speed of sound for the ith material, V_i^n is the volume occupied by the ith material at the previous time step, and $\delta V_i^{n+1/2}$ (which is unknown) is the change in volume for the corresponding material.

As was done for a single material in the predictor stage, one now computes the new volumes and the changes of volume for all cells including mixed cells. After this, one needs to solve a

system of linear equations (closure model) for $\hat{p}^{n+1/2}$ and $\delta V_i^{n+1/2}$

$$p_i^n - \tilde{B}_i^n(\delta V_i^{n+1/2}/V_i^n) = \hat{p}^{n+1/2}, \quad \sum_i \delta V_i^{n+1/2} = \delta V^{n+1/2}$$

where $\tilde{B}_i^n = \rho_i^n (c_i^n)^2[1 + L^n/(c_i^n\,\delta t)]$ and $\delta V^{n+1/2}$ is known change of the volume of the entire mixed cell. This system has a very simple structure whose explicit solution is

$$\hat{p}^{n+1/2} = \overline{p}^n - \overline{B}^n \frac{\delta V^{n+1/2}}{V^n}, \quad \delta V_i^{n+1/2} = \frac{V_i^n}{\tilde{B}_i^n}\left[(p_i^n - \overline{p}^n) + \overline{B}^n \frac{\delta V^{n+1/2}}{V^n}\right] \tag{2}$$

where

$$\overline{p}^n = \sum_i \left(\frac{f_i^n}{\tilde{B}_i^n} p_i^n\right) \Big/ \sum_i \left(\frac{f_i^n}{\tilde{B}_i^n}\right), \quad \overline{B}^n = 1 \Big/ \sum_i \frac{f_i^n}{\tilde{B}_i^n} = \sum_i f_i^n \Big/ \sum_i \frac{f_i^n}{\tilde{B}_i^n}$$

and $f_i = V_i/V$ is the volume fraction. The equation for $\delta V_i^{n+1/2}$ indicates that the change in volume in the ith material is due to the difference of pressure in this material with respect to the 'averaged' pressure and also due to the change of the volume of entire mixed cell. Because $V_i = f_i V$, the equation for $\delta V_i^{n+1/2}$ implies the following equation for $\delta f_i^{n+1/2}$:

$$\delta f_i^{n+1/2} = f_i^n(p_i^n - \overline{p}^n)/\tilde{B}_i^n + f_i^n(\overline{B}^n/\tilde{B}_i^n - 1)\delta V^{n+1/2}/V^n$$

In the corrector stage of Tipton's method, the pressure $\hat{p}^{n+1/2}$ is used in the momentum equation and $\delta f_i^{n+1} = 2\,\delta f_i^{n+1/2}$ is used to distribute the change in volume of the entire mixed cell among the individual materials. The pressure $\hat{p}^{n+1/2}$ and δV_i^{n+1} is then used in the internal energy equations

$$m_i(\varepsilon_i^{n+1} - \varepsilon_i^n) = -\hat{p}^{n+1/2}(V_i^{n+1} - V_i^n) \tag{3}$$

Finally, a new pressure for each material is determined from its own equation of state. Conservation of total energy directly follows from Equation (3).

3.2. Sub-cell dynamics approach to closure models

In the subcell dynamical closure models, each material has its own pressure, density and internal energy. One of the main difficulties in such models is how to estimate the velocity of interface between two materials. If we have an estimate for this velocity, we can also estimate how the volume and density of each material will change. The next question is how to define the one pressure of the mixed cell that will be used in the momentum equation? And finally, how does one conserve total energy?

To estimate the interface velocity u_1 between two materials in 1D, one can use the acoustic Riemann solver $u_1 = [(\rho_1 c_1)u_1 + (\rho_2 c_2)u_2 + (p_1 - p_2)]/(\rho_1 c_1 + \rho_2 c_2)$, where the indices 1 and 2 denote states on different sides of interface. Clearly, different choices for u_1, u_2 are possible, as well as other estimates for the interfacial velocity.

In subcell closure models, each material has its own '$p\,\mathrm{d}V$' equation $m_i\,\mathrm{d}\varepsilon_i/\mathrm{d}t = -p_i\,\mathrm{d}V_i/\mathrm{d}t$. The conservation of total energy argument can be used derive one pressure for the mixed cell:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum m_i\,\varepsilon_i\right) = m\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = -\sum p_i\,\frac{\mathrm{d}V_i}{\mathrm{d}t} = -p\,\frac{\mathrm{d}V}{\mathrm{d}t} \to p = \sum p_i\,\frac{\mathrm{d}V_i}{\mathrm{d}V}$$

Published in 2007 by John Wiley & Sons, Ltd.

DOI: 10.1002/fld

The are several questions related to the formula $p = \sum p_i\,(\mathrm{d}V_i/\mathrm{d}V)$. What to do if $\mathrm{d}V = 0$? What to do if some of $\mathrm{d}V_i/\mathrm{d}V$ have different signs? In such a case, the averaged pressure can be negative even if all p_i are positive.

3.2.1. Barlow's method. As a specific example of a subcell dynamical closure model, we consider our interpretation of Barlow's method [6] for the case of two materials. The design principle for Barlow's method is to choose $\beta_i \sim \mathrm{d}V_i/\mathrm{d}V$, such that $1 \geqslant \beta_i \geqslant 0$ and $\sum \beta_i = 1$. Having β_i, we can define $\mathrm{d}V_i = \beta_i\,\mathrm{d}V$ and $p = \sum \beta_i\, p_i$.

In Barlow's method, the interfacial velocity is defined from an acoustic Riemann solver under the assumption that $u_1 = u_2$, and is obtained by linear interpolation of velocities $u_\mathrm{L}, u_\mathrm{R}$ at the end points of the mixed cell using volume fractions $u_\mathrm{I}^n = f_2^n\, u_\mathrm{L}^n + f_1^n\, u_\mathrm{R}^n + (p_1^n - p_2^n)/(\rho_1^n\, c_1^n + \rho_2^n\, c_2^n)$. In the predictor stage, this velocity is used to compute the changes in volumes of each material. Then if $\delta V^{n+1/2} = 0$ then $\beta_i^{n+1/2} = f_i^n$; if all $\delta V_i^{n+1/2}/\delta V^{n+1/2}$ have the same sign then

$$\beta_i^{n+1/2} = \delta V_i^{n+1/2}/\delta V^{n+1/2} \tag{4}$$

otherwise, $\delta V_i^{n+1/2}$ are corrected as follows: if $\delta V_1^{n+1/2} \cdot \delta V^{n+1/2} < 0$ then $\delta V_1^{n+1/2} = 0$, $\delta V_2^{n+1/2} = \delta V^{n+1/2}$; If $\delta V_2^{n+1/2} \cdot \delta V^{n+1/2} < 0$ then $\delta V_1^{n+1/2} = \delta V^{n+1/2}$, $\delta V_2^{n+1/2} = 0$, and formula (4) is used.

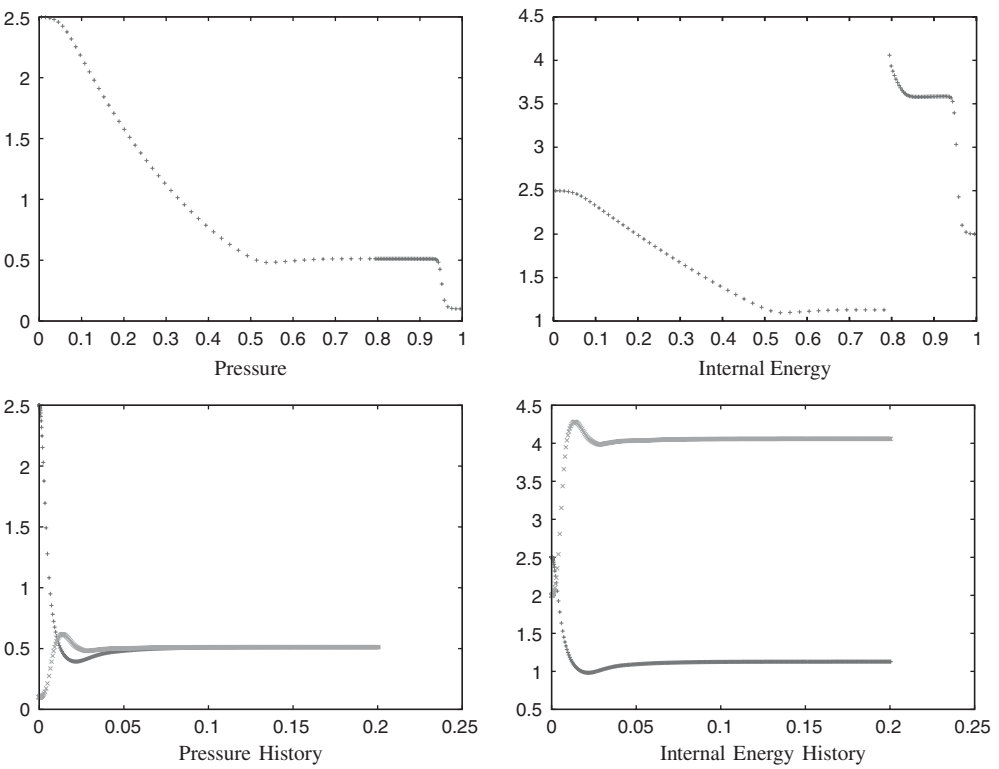

Figure 1. Results of the Lagrangian computation of two-material Sod problem—pure cells.

Updated values of $\delta V_i^{n+1/2}$ are used to compute the pressure in each material $p_i^{n+1/2} = p_i^n - \rho_i^n (c_i^n)^2 \delta V_i^{n+1/2} / V_i^n$. Finally, one pressure for the mixed cell is computed as follows $p^{n+1/2} = \sum \beta_i^{n+1/2} p_i^{n+1/2}$.

In the corrector stage, $p^{n+1/2}$ is used in the momentum equation, $\beta_i^{n+1/2}$ are used to distribute change in volume of entire mixed cell $\delta V_i^{n+1} = \beta_i^{n+1/2} \delta V^{n+1}$, and finally δV_i^{n+1} and $p_i^{n+1/2}$ are used to update internal energy for each material $m_i (\varepsilon_i^{n+1} - \varepsilon_i^n) = -p_i^{n+1/2} \delta V_i^{n+1}$.

4. NUMERICAL EXPERIMENTS

In this section, we compare numerical results for the two-material Sod problem. The computational domain is [0 : 1], the initial discontinuity is at 0.5. Materials on the left and right side are both ideal gases: left—$\gamma = 2$, $\rho = 1$, $p = 2$, $u = 0$, right—$\gamma = 1.4$, $\rho = 0.125$, $p = 0.1$, $u = 0$. First, the Sod problem is computed on a mesh of 100 cells, where the interface coincides with the discontinuity, that is, there are no mixed cells. Results are presented in Figure 1. In the two pictures at the top, we present a snapshot of pressure and internal energy at $t = 0.2$. In the two pictures at the bottom, we present the history of pressure and internal energy in the Lagrangian

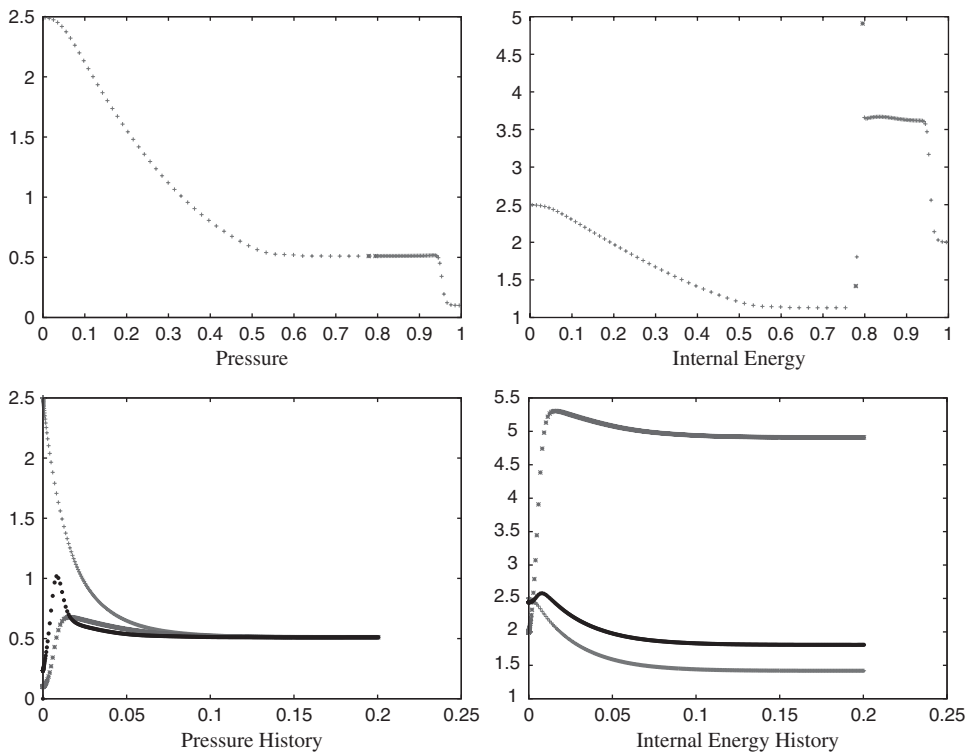

Figure 2. Two-material Sod problem—one mixed cell—Tipton's closure model.

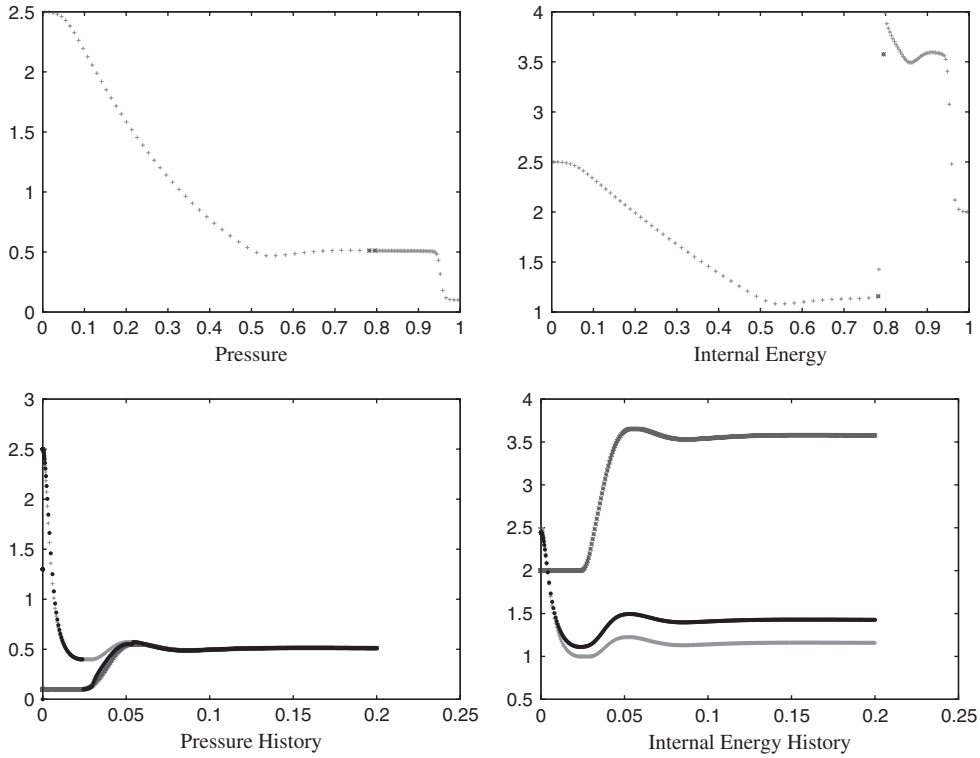

Figure 3. Two-material Sod problem—one mixed cell—Barlow's closure model.

cells left (marked by symbol '+' (red)) and right (marked by symbol '×' (green)) of the initial discontinuity. In Figures 2 and 3, we present the numerical results for Tipton's and Barlow's methods for the calculations where initially two cells adjacent to interface were combined in one mixed cell, where the interface was in the middle and initial parameters are discontinuous inside the mixed cell. In the graphs of pressure and internal energy values in pure cells are marked by symbol '+' (red), and values in different materials of the mixed cell are marked by symbol '∗' (blue). On the history plots, in addition to the values in each material (right (marked by symbol '∗' (blue)) and left (marked by symbol '+' (red))), the common pressure in mixed cells is marked by solid dots (black).

ACKNOWLEDGEMENTS

This work is result of numerous fruitful discussions with A. Abgrall, D. Bailey, A. Barlow, Yu. Bondarenko, D. Burton, B. Despres, J. Grove, A. Harrison, B. Kashiwa, M. Kucharik, R. Liska, R. Loubere, R. Lowrie, P.-H. Maire, L. Margolin, R. Schmitt, P. Vachal, B. Wendroff, and Yu. Yanilkin. This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396 and the DOE Office of Science Advanced Scientific Computing Research (ASCR) Program in Applied Mathematics Research.

REFERENCES

1. Stewart H, Wendroff B. Two-phase flow: models and methods. *Journal of Computational Physics* 1984; **56**:363–409.
2. Tipton RE. CALE mixed zone pressure relaxation model. Private communication, 1989.
3. Murrone A, Guillard H. A five equation reduced model for compressible two phase flow problems. *Journal of Computational Physics* 2005; **202**:664–698.
4. Despres B, Lagoutiere F. Numerical resolution of a two-component compressible fluid model with interfaces and mixing zones. *Preprint R04008 of the Laboratoire Jacques–Louis Lions*.
5. Bondarenko Yu, Yanilkin Yu. Computation of the thermodynamic parameters in the mixed cells in gas dynamics. *Mathematical Modeling* 2002; **14**:63–81.
6. Barlow A. A new Lagrangian scheme for multimaterial cells. *Proceedings of European Congress on Computational Methods in Applied Sciences and Engineering*. *ECCOMAS Computational Fluid Dynamics Conference 2001*, Swansea, Wales, U.K., 4–7 September 2001.
7. Delov VI, Sadchikov VV. Comparison of several models for computation of thermodynamical parameters for heterogeneous Lagrangian cells. *VANT*, *Mathematical Modeling of Physical Processes* 2005; **1**:57–70.
8. Goncharov EA, Yanilkin YV. New method for computations of thermodynamical states of the materials in the mixed cells. *VANT*, *Mathematical Modeling of Physical Processes* 2004; **3**:16–30.
9. Shashkov M. *Conservative Finite-difference Methods on General Grids*. CRC Press: Boca Raton, FL, 1996.

Published in 2007 by John Wiley & Sons, Ltd.

Int. J. Numer. Meth. Fluids (2007)
DOI: 10.1002/fld