Applied Numerical Mathematics 76 (2014) 145–165

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

A Riemann problem solution methodology for a class of evolutionary mixture equations with an arbitrary number of components

M.W. Crochet [1], K.A. Gonthier [*,2]

Department of Mechanical and Industrial Engineering, Louisiana State University, Baton Rouge, LA 70803, USA

ARTICLE INFO

Article history:
Received 29 April 2013
Received in revised form 28 August 2013
Accepted 13 September 2013
Available online 19 September 2013

Keywords:
Multiphase flows
Granular mixtures
Riemann solver
Hyperbolic systems
Nonlinear algebraic equations
Nonconservative sources

ABSTRACT

The solution of the two-phase Riemann problem is a critical component of upwind finite-volume numerical schemes used to solve systems of evolutionary equations, which are routinely used to model compaction and combustion phenomena in gas–granular explosive mixtures. Extensions of a common two-phase model are currently being used to analyze the thermomechanics and combustion of explosive mixtures consisting of N components. Although a solution to the two-phase Riemann problem has been formulated, there is currently no available analogue for the N-phase system in the literature, due to the inherent difficulty of determining the correct wave ordering within the Riemann solver. The development of a solution for these systems is therefore an important step in the formulation of numerical schemes applied to N-phase mixtures. Here, an extension of the exact two-phase solution methodology is proposed for the N-phase case, which may be utilized in the construction of finite-volume schemes for multiphase systems, and can be used with general, convex equations of state. Finally, example problems for three-phase mixtures are considered to illustrate the accuracy of the solution compared to the results of a centered numerical scheme. These solutions also demonstrate the complexity of the possible wave configurations that arise when multiple solid phases are present, as well as the algorithmic challenges which must be addressed to provide a robust implementation.

1. Introduction

Systems of hyperbolic partial differential equations are frequently used to analyze wave phenomena in two-phase flows [3,2,23,24,12]. In particular, the two-phase Baer–Nunziato (BN) model [4] was formulated to study deflagration-to-detonation transition (DDT) in granular energetic materials, where a mixture of reactant granular solid and product gas simultaneously exist. The system of equations consists of mass, momentum, and energy balance equations for each phase, as well as a volume fraction evolution equation required for closure. Volumetric source terms in these equations account for mass, momentum, and energy interactions between phases due to combustion, drag, heat transfer, and compaction. In this study we ignore phase interaction processes and focus on terms that account for nonlinear wave formation and propagation, which can be computationally challenging to resolve. The effects of volumetric source terms can be computationally examined separately based on standard operator splitting techniques [27].

* Corresponding author. Tel.: +1 225 578 5915.
E-mail addresses: mcroch2@tigers.lsu.edu (M.W. Crochet), gonthier@me.lsu.edu (K.A. Gonthier).
[1] Graduate Research Assistant.
[2] Associate Professor. Tel.: +1 225 578 5915.

0168-9274/$36.00
http://dx.doi.org/10.1016/j.apnum.2013.09.004

The one-dimensional form of the two-phase equations that accounts for nonlinear convection is given by:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{q})}{\partial x} = \mathbf{g}(\mathbf{q}) \frac{\partial \phi_s}{\partial x}, \tag{1}$$

where

$$\mathbf{q} = [\phi_s \rho_s, \phi_g \rho_g, \phi_s \rho_s u_s, \phi_g \rho_g u_g, \phi_s \rho_s E_s, \phi_g \rho_g E_g, \phi_s]^\top, \tag{2}$$

$$\mathbf{f}(\mathbf{q}) = \left[\phi_s \rho_s u_s, \phi_g \rho_g u_g, \phi_s \rho_s u_s^2 + \phi_s P_s, \phi_g \rho_g u_g^2 + \phi_g P_g, \phi_s \rho_s u_s (E_s + P_s/\rho_s), \phi_g \rho_g u_g (E_g + P_g/\rho_g), 0\right]^\top, \tag{3}$$

$$\mathbf{g}(\mathbf{q}) = [0, 0, P_g, -P_g, P_g u_s, -P_g u_s, -u_s]^\top. \tag{4}$$

Here, t is time and x is spatial position. For $i = s, g$, ϕ_i is volume fraction; ρ_i is density; u_i is velocity; $E_i = e_i + u_i^2/2$ is the total specific energy, where e_i is the specific internal energy, and P_i is pressure. The subscripts s and g denote the solid and gas phases, respectively. This system is closed by equations of state (EOS's) $e_i = e_i(\rho_i, P_i)$ for both the gas and solid phases, and the saturation constraint $\phi_s + \phi_g = 1$. The compaction equation convects ϕ_s at the local velocity u_s. Some multiphase models convect ϕ_s at a different velocity U [24,18], such as the mass-weighted velocity of the phases. The Riemann solver presented here is generally not applicable in such cases. The sources $\mathbf{g}(\mathbf{q})\partial\phi_s/\partial x$ are referred to as nonconservative products in the literature, and are required to satisfy the strong form of the entropy inequality for the mixture. Formulating accurate discretizations of these products within finite-volume schemes has proven to be particularly challenging [17,6], and their proper mathematical treatment remains an active area of research [16,11,9,22,20,21].

The two-phase BN model has been extended to include mixtures containing an arbitrary number of condensed phases to examine the thermomechanics and combustion of multi-component energetic solids [14,28,5]. Here, the solid subscript s is replaced by the index i, for $i = 1, 2, \ldots, M$, where M is the total number of solid phases. The gas–solid mixture consists of $N = M + 1$ components, and the one-dimensional system of equations is given by:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{q})}{\partial x} = \sum_{i=1}^{M} \mathbf{g}_i(\mathbf{q}) \frac{\partial \phi_i}{\partial x}, \tag{5}$$

where

$$\mathbf{q} = \left[\{\phi_i \rho_i\}_{i=1}^M, \phi_g \rho_g, \{\phi_i \rho_i u_i\}_{i=1}^M, \phi_g \rho_g u_g, \{\phi_i \rho_i E_i\}_{i=1}^M, \phi_g \rho_g E_g, \{\phi_i\}_{i=1}^M\right]^\top, \tag{6}$$

$$\mathbf{f}(\mathbf{q}) = \left[\{\phi_i \rho_i u_i\}_{i=1}^M, \phi_g \rho_g u_g, \left\{\phi_i \rho_i u_i^2 + \phi_i P_i\right\}_{i=1}^M, \phi_g \rho_g u_g^2 + \phi_g P_g, \left\{\phi_i \rho_i u_i (E_i + P_i/\rho_i)\right\}_{i=1}^M, \phi_g \rho_g u_g (E_g + P_g/\rho_g), \{0\}_{i=1}^M\right]^\top, \tag{7}$$

$$\mathbf{g}_i(\mathbf{q}) = \left[\{0\}_{i=1}^M, 0, P_g \mathbf{a}_i, -P_g, P_g u_i \mathbf{a}_i, -P_g u_i, -u_i \mathbf{a}_i\right]^\top. \tag{8}$$

The notation $\{\cdot\}_{i=1}^M$ indicates a sequence of elements for $i = 1, 2, \ldots, M$, and the $\mathbf{a}_i$ are vectors of length M such that the j-th component a_{ij} is given by:

$$a_{ij} = \begin{cases} 0 & \text{if } j \neq i, \\ 1 & \text{if } j = i. \end{cases} \tag{9}$$

Finite-volume numerical methods are commonly used to solve systems of hyperbolic partial differential equations such as those given by Eqs. (1) and (5). Many of these methods are based on upwind Godunov methods, which approximate the solution as piecewise-continuous polynomials within each computational cell. Discontinuities at cell interfaces constitute initial states for Riemann problems that are locally solved to obtain interface fluxes needed to evolve the solutions in space and time. Embid and Baer first analyzed the eigenstructure of the BN equations [10], and the solution of the associated two-phase Riemann problem has been investigated by Andrianov and Warnecke [1] and Deledicque and Papalexandris [8], with Schwendeman et al. [25] providing the first direct solution for ideal and stiffened equations of state. This solution is also utilized in [25] to evaluate the nonconservative products analytically. However, there is currently no available solution to the Riemann problem for Eq. (5) for $M > 1$, primarily due to the complexity of possible wave configurations and difficulties that arise in determining their spatial order during the solution procedure. An analysis of this solution is a critical component in the construction of upwind finite-volume numerical schemes needed to predict flows governed by Eq. (5).

In this paper, a direct solution methodology for the Riemann problem for an arbitrary number of solid phases is formulated that can be used with any convex EOS. This solution can be used in the verification of numerical schemes applied to multiphase flow problems and may provide a framework for the implementation of exact or approximate Riemann solvers for Eq. (5) within existing upwind numerical schemes. The solution approach is based on the methodology used in [25], and utilizes an inner Newton method to solve for the phase shock speeds and an outer Newton iteration to obtain the specific volumes. All other flow properties may be calculated from these quantities. While it is possible to eliminate the shock speeds and solve the system of nonlinear equations with a single Newton iteration for the phase pressures, the resulting relations include square-root terms which can make the system discontinuous in large sub-domains of $\mathbb{R}^W$, where W is