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Modeling of the quenching of blast products from energetic materials by expansion into vacuum

Sungjin Choi [a], D. Scott Stewart [a,*], Sunhee Yoo [b]

[a] Department of Mechanical Science and Engineering, University of Illinois at Urbana Champaign, IL 60801-2906, USA
[b] Jacobs Engineering, Munitions Directorate, Eglin AFB, FL, USA

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ABSTRACT

Condensed phase energetic materials include propellants and explosives. Their detonation or burning products generate dense, high pressure states that are often adjacent to regions that are at vacuum or near-vacuum conditions. An important chemical diagnostic experiment is the time of flight mass spectroscopy experiment that initiates an energetic material sample via an impact from a flyer plate, whose products expand into a vacuum. The rapid expansion quenches the reaction in the products so that the products can be differentiated by molecular weight detection as they stream past a detector. Analysis of this experiment requires a gas dynamic simulation of the products of a reacting multi-component gas that flows into a vacuum region. Extreme computational difficulties can arise if flow near the vacuum interface is not carefully and accurately computed. We modify an algorithm proposed by Munz [1], that computed the fluxes appropriate to a gas–vacuum interface for an inert ideal gas, and extend it to a multi-component mixture of reacting chemical components reactions with general, non-ideal equations of state. We illustrate how to incorporate that extension in the context of a complete set of algorithms for a general, cell-based flow solver. A key step is to use the local exact solution for an isentropic expansion fan, for the mixture that connects the computed flow states to the vacuum. Regularity conditions (i.e. the Liu–Smoller conditions) are necessary conditions that must be imposed on the equation of state of the multicomponent fluid in the limit of a vacuum state. We show that the Jones, Wilkins, Lee (JWL) equation of state meets these requirements.

1. Introduction

Condensed phase energetic materials include propellants and explosives. They are usually composed of a mixture of granular solids that include explosive or oxidizing crystallites, various metal powders like aluminum, sometimes carbon black, resins and plastics. The performance of the aggregate composite depends on the chemistry and the mechanisms of energy release, which occur in nearly all phases of materials, gas, liquid and solid. Propellant and explosives reactive decomposition produces huge volume expansion. The products start at near solid densities and at high pressures and expand to very low densities and lower pressures. In the case of explosives, the pressure drops from hundreds of kilo-bars to 1 atmosphere or less, which is 5 to 6 orders of magnitude across a reaction zone that is often no more than 1/10 of a

* Corresponding author.
E-mail addresses: dss@illinois.edu (D. Scott Stewart), syoo1@illinois.edu (S. Yoo).

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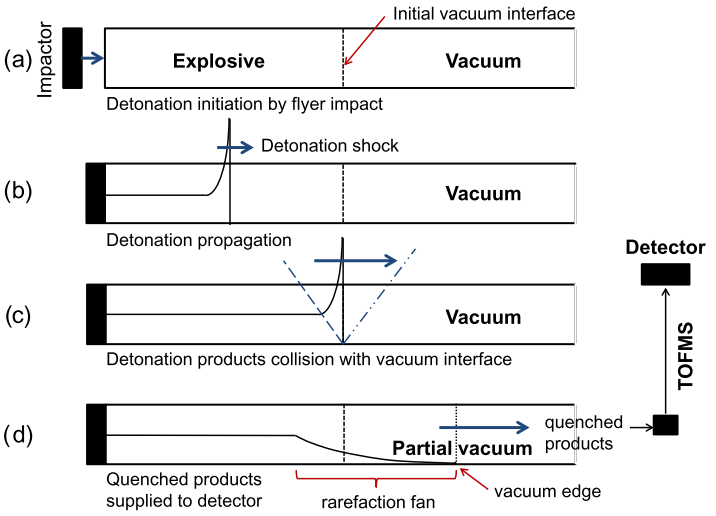

Fig. 1. The schematic diagram of numerical simulation of initiation, detonation and expansion for an explosive sample in the TOFMS experiment.

millimeter thick. This enormous pressure gradient provides the means to cut materials or drive surrounding materials to large velocities by virtue of this expansion power. Likewise, solid propellants in rocket motors vent gases with pressures that range from 1 to 200 atmospheres, down to vacuum conditions. Many orders of magnitudes of pressure change are realized and the pressure gradient in propellant exhaust stream provides the means to generate thrust. The problem of computing the transition of material states from very high pressure to vacuum or near vacuum states is a generic one for any multi-material simulation where two materials may collide and have individual or shared boundaries, for which one of the materials is adjacent to a region with very low pressure and density or a vacuum. Difficulties generally arise if the region of expansion between the high and low pressure regions is not accurately computed.

A time of flight mass spectrometry (TOFMS) experiment by Fossum et al. [2], initiated small samples of energetic materials by laser flyer plate impact. After impact, the products expanded into a vacuum region where spectroscopic analysis of the products was performed. A larger version of a similar experiment was carried out by Blais et al. [3] that used a large quantity of explosive to drive an ampule of nitromethane, which detonated upon being shocked. The premise of the TOFMS experiments is that the pressure drop caused by the expansion in a long vacuum region freezes/quenches the reaction amongst product species in a sequential manner, ordered by the events in the reaction zone in the material that was established prior to the expansion. In order to interpret TOFMS experiments, accurate model simulations of the gas dynamics of reacting multi-component mixtures are required. The range of thermodynamic states is extreme. The reactants start at standard room pressure and temperature conditions, are raised to high pressure, density detonation or highly shocked states in condensed materials, convert to (mostly) gas species products that expand to a vacuum or near-vacuum state. Such simulations are very challenging to carry out since non-ideal equations of state forms must be used for the reactants and products, and the location of the vacuum/materials boundary must be calculated in a precise manner.

Computational methods and techniques are not widely available for multi-component reactive flow, when the components are subjected such huge ranges in the thermodynamics states. Since we had an interest in finding an accurate and robust way to simulate the TOFMS experiments, we decided to make a modification to the basic vacuum interface tracking algorithm pioneered by Munz [1]. Our extension is used in combination with a (now) standard, higher order, cell-based, totally variation diminishing (TVD) Euler scheme, in a fairly general multicomponent framework. One should be able to use our method to compute the approach to the vacuum in the continuum limit, and combine it with simulations of the Boltzmann equation or with molecular dynamic simulations. The continuum simulations we describe would generate the near vacuum continuum flows as a far-field limit, or be used to establish averaged initial conditions for molecular based simulations. In this paper, we describe these algorithms and implementations in detail, and present worked examples that simulate the flow in the TOFMS experiment as a targeted application.

Fig. 1 shows a sketch of a typical sequence of events that occur in a simulation of the quenching of blast products that expand into a vacuum region on the right. a) The explosive sample and vacuum regions are initially separated, prior to impact by the flyer. b) If the sample detonates, a detonation shock and its supporting reaction zone propagate through the explosive. c) The detonation wave hits the vacuum interface. d) Then a rarefaction travels back into the detonation reaction zone structure. As the pressure and density drop, the reactions amongst product species slow as the products flow into the vacuum section, past the detector which monitors the mass concentration of the products at a fixed probe locations. Since the number density drops in the vacuum region, the species are thought not to undergo significant collisions and hence no further chemical changes occur.