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Direct Numerical Simulations of Shock Propagation in a Heterogeneous Mixture of Two Gases

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Introduction

Numerical simulations of heterogeneous mixtures represent a relevant problem, and numerical methods should be able to model it, above all, as applied to shock propagation.

- **1. First approach** is based on averaged description of thermodynamic parameters, such as density and energy, with a single EOS for mixture.
- 2. Second approach (more general) is based on complete thermodynamic distinction of mixture components each having its own EOS. This case requires closure models for gas dynamics equations in mixed cells.

In any case, some data are needed for verification of the common EOS or closure models. Three options are available:

- Experimental data, but these are scarce and limited
- Theoretical studies, but these involve certain assumptions and simplifications
- Direct numerical simulations, which represent matter in the form of some structures

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Problem of Shock Propagation in a Heterogeneous Gas Mixture

The problem has been proposed in [6], and the analytical solution obtained in [7]. In [8], 1D Lagrangian simulations have been performed, in which matter is represented as a layered periodical structure.

In this work, numerical investigations of the problem have been extended from the assumption of layered structure to other more realistic structures. Simulations have been done for both 1D (for comparison with [8]), and 2D and 3D approximations (depending on the structure involved) using the code EGAK [9] on a fixed Eulerian mesh.

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Problem Statement



The domain is occupied by a heterogeneous mixture of two gases with EOS $P = (\gamma - 1)\rho e$ Initial gas parameters (t=0)

Gas #	ρ	e ₀	u ₀	P ₀	γ	β ₀
1	1	0	0	0	3.0	0.5
2	1	0	0	0	1.2	0.5

Analytical solution has been obtained assuming that the components experience single shock loading and have equal pressure.

$$\rho_{i} = \frac{\gamma_{i} + 1}{\gamma_{i} - 1} \rho_{i0}, \quad D = \frac{\rho}{\rho - \rho_{0}} u, \qquad u^{2} = P\left(\frac{1}{\rho_{0}} - \frac{1}{\rho}\right), \quad e = \frac{1}{2} P\left(\frac{1}{\rho_{0}} - \frac{1}{\rho}\right)$$
$$P_{i} = P, \qquad e_{i} = \frac{P}{(\gamma_{i} - 1)\rho_{i}}$$

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Setup and Processing of Eulerian Simulations

Simulations were run on N, 2N, and 4N meshes, where N in all the setups means a mesh with a linear cell size of h=0.002. Boundary condition is inflow of gas 1 with parameters behind the shock front from the analytical solution (ρ =2, e=1.419, u=2).

As a major output we present shock front velocities, $D_{fr}(t)$, calculated at time t_k as

$$D_{\phi p}(t_{k}) = \frac{dX_{\phi p}}{dt} \approx \frac{X_{\phi p}(t_{k}) - X_{\phi p}(t_{k-1})}{t_{k} - t_{k-1}}$$

In the multidimensional case, data are obtained by pre-averaging the quantities in the cross section.

1D Simulation Setup Image: Constraint of the setup

Mixture components are represented by 300 alternating layers of equal thickness, $L_1=L_2=0.05$, along the shock path.

1D Simulation Results



Density and velocity profiles

2D Simulation Setup (Plane Geometry)



2D Simulation Results



Flow patterns at t=5





Density and velocity profiles at t=5

3D Simulation Setup



3D Simulation Results





Density and velocity profiles at t=1



Density and velocity profiles at t=5



Gas density profiles at t=5

t	3D_3		3D_4		
	N	2N	N	2N	
1.0	2.812	2.798	2.796	2.810	
1.5	2.792	2.786	2.836	2.788	
2.0	2.792	2.788	2.800	2.810	
3.0	2.788	2.781	2.804	2.797	
4.0	2.788	2.780	2.808	2.785	
5.0	2.785	2.785	2.806	2.784	

Shock velocity



Shock front velocity as a function of mesh size

	1D	2D_1	2D_2	3D_1	3D_2
N	2.879	2.872	2.876	2.847	2.845
2N	2.892	2.869	2.875	2.839	2.840

Conclusions

Direct numerical simulations of strong shock propagation in a mixture of two perfect gases have been performed. The problem has an analytical solution obtained assuming that the mixture components are subject to single compression and that their pressures are equal.

The simulations have been done in 1D, 2D and 3D setups, of which the 3D setup is most realistic. The simulations have demonstrated that this particular setup gives shock front velocities closest to the analytical solution. This proves that the assumptions made in obtaining the analytical solution are credible.

Thank you for attention!

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