Initiation of Richtmyer–Meshkov instability by a detonation wave

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Abstract. As part of the HyCFS-R numerical code development, a module for the simulation of multiphase chemically reacting flows based on the Euler–Euler approach was implemented. The code was verified on simple 0D and 1D problems, such as constant volume explosion and 1D shock tube problem. For more comprehensive testing the numerical simulation of the Richtmyer–Meshkov instability in reactive heterogeneous media was performed. The comparison against the reference solution revealed that numerical method implemented in the HyCFS-R either introduce too much dissipation and suppress the detonation wave front instabilities or lead to numerical artifacts in the Richtmyer–Meshkov instability flow pattern.

1. Introduction
HyCFS-R is a code currently being developed at Khristianovich Institute of Theoretical and Applied Mechanics to simulate a wide range of compressible flows. A number of numerical schemes were implemented for spatial and temporal approximation, as well as various models for calculating the rates of chemical reactions. As part of this work, a module for modeling multiphase chemically reacting flows was implemented. The code was mainly tested on the external flow, namely high-speed flows around bodies. When adding new physical models, verification is complicated by the need to check the effects of the interaction of various options and solvers with each other. It turned out that modeling a Richtmyer–Meshkov instability (RMI) in a reacting heterogeneous medium can serve as a fairly good comprehensive test.

2. HyCFS-R numerical code
The HyCFS-R [1, 2] code solves 3D unsteady Euler and Navier-Stokes equations in general curvilinear coordinates. The convective terms are approximated using the shock-capturing MUSCL TVD or the 5th order weighted essentially non-oscillatory (WENO) scheme. In the TVD scheme, the variables are reconstructed on the faces of the cells from the values in the cell centers with 2nd or 3rd order of accuracy. After that the limiter minmod is applied. Numerical fluxes are calculated using approximate solvers for the Riemann problem: HLLE (Harten–Lax–van Leer–Einfeldt) solver or hybrid AUSM–van Leer solver. The explicit time advancement schemes, the so-called Runge–Kutta TVD schemes of 2nd and 3rd orders of accuracy, are used.

The module for multiphase reacting flows [3] uses the description of the dispersed phase based on the Euler approach. The model for the oxygen laden with aluminum particles from the works of Fedorov and Khmel [5–9] is used at the current stage of the HyCFS-R
development. The basic verification of the implemented model was performed using simple 0D and 1D problems, including the constant volume explosion and 1D shock tube. As a part of more comprehensive code testing it was decided to simulate numerically the Richtmyer-Meshkov instability in a chemically reactive heterogeneous media. The HyCFS-R was verified by comparing the computation results against the reference solution obtained using the Fortran code developed in the cited above papers of Fedorov, Khmel and Kratova.

3. Richtmyer-Meshkov instability

Richtmyer-Meshkov instability occurs when a boundary between two fluids with different densities is impulsively accelerated by the shock wave (SW). In this case, small amplitude perturbations begin to increase. Such instability is found in hydrodynamics, astrophysics, nuclear engineering, etc. Therefore, RMI research is of both fundamental and practical interest [11,12]. Usually in the RMI numerical simulation the fluids interface is artificially disturbed in a shape of a sine wave with an amplitude smaller than the wavelength. A plane SW propagates through a lighter medium, interacts with the curved interface and leads to the increase in distance between the minimum and the maximum of the sine wave. In the detonation wave (DW), the cellular structure is formed, so the DW front is always curved. But will an RMI emerge if the curved DW front hits a plane interface?

To test this hypothesis, a numerical experiment was conducted. A plane 2D channel with a length of \( L = 1.4 \) m and a width of \( H = 0.06 \) m with specular walls (see figure 1) is filled with oxygen \((\rho = 1.28 \text{ kg/m}^3, T = 300 \text{ K, } P = 1 \text{ atm})\). A cloud of 1 \( \mu \)m aluminum particles \((\rho = 1.56 \text{ kg/m}^3)\) is placed in the middle section of the channel. The combustion of these particles ensures the formation of the DW cellular structure. The detonation is initiated by a Mach 5 SW, propagating through the oxygen layer in the left section of the channel. The interaction of the SW with a cloud of particles results in their heating, subsequent ignition and transition to detonation. To accelerate the formation of detonation cells, the boundary of the particle cloud has a sine curve shape (amplitude \( \sim 7\% \) of the wavelength). This interface disturbance also leads to the appearance of RMI on the left boundary. The DW can also be initiated by creating a small spot of gas with the temperature much higher than the ignition temperature of particles [10], but in this case the transition to detonation develops more slowly, and the computational domain needs to be much longer.

![Figure 1. Computational domain geometry and the initial conditions set-up.](image)

Figure 2 shows the density flowfields of carrier and dispersed phases at different time moments. At time \( t = 0 \) the shock wave approaches a cloud of particles. The particles combustion process starting at \( t = 0.1 \) ms leads to the formation of detonation cells seen at \( t = 0.2 \) ms. By the time DW exits the particle laden section, the pronounced cellular structure of DW is observed. At the same time, the combustion products at the left boundary demonstrate the classical pattern of the RMI development.
Figure 2. Formation of cellular structure of DW.

The DW, exiting from a cloud of particles, generates an SW in the carrier phase (see Fig. 3). It can be seen that an RMI also emerges at the interface, slowly growing in time, and the number of disturbances coincides with the number of detonation cells.

It should be noted that RMI emerges during the transition of SW from a lighter gas to a denser one. In this case, the density of the combustion products compressed by DW, is more than 4 times higher than the density of the gas phase. But the speed of DW is about 6 times higher than the speed of sound. It indicates that the emergence of RMI in this case depends not only on the densities of the media, but also on the speed of sound and speeds of DW and SW in these media. The emergence of RMI during the transition of DW into an inert medium was observed earlier. So in [13,14], RMI-specific structures are observed when DW enters a cloud of neutral particles.

The data were extracted from the lines \( Y = \text{const} \) to measure the positions of the peak and the bubble RMI. The difference in these positions illustrates the rate of RMI development. Figure 4 shows the RMI development for both left and right boundary cases. For the left RMI, the distance at first corresponds to initial disturbance amplitude (0.004 m), and after the shock-interface interaction increases non-linearly, tends to a constant value. Because the right RMI is initiated by detonation cells, peaks and bubbles positions oscillate on DW front. As a result, the size of the RMI varies within the size of the detonation cell. After emergence of RMI, a non-linear increase in size is also observed, which tends to a constant value. Oscillations in the profiles are caused by acoustic waves.

The numerical simulation were repeated using the HyCFS-R code. Comparison with the results discussed above showed that the correct reproduction of RMI development pattern strongly depends on the choice of the Riemann problem solver and MUSCL reconstruction. In the calculations presented above, the 2nd order TVD scheme with the Roe solver was used. It is a well-known fact, that the Roe solver introduces rather small numerical dissipation to the flow. As a result, it is less robust than other solvers but does not suppress the development of various disturbances as much. On the other hand, HLLE and AUSM–van Leer solvers
Figure 3. Carrier density flowfields at different time moments.

Figure 4. Distance between the bubble and the spike as function of time.

introduce more artificial viscosity to the flow which makes them more suitable for external aerodynamics problems, containing strong shocks and large flow gradients. However, the RMI problem indicated that the combination of approximation methods and solvers in the HyCFS-R code could not correctly resolve the entire flow. In figure 5 the temperature field of the carrier phase obtained in calculations with the 2nd order MUSCL reconstruction just before the end of the particle combustion process. It can be seen that the left RMI is resolved quite correctly, at the same time, the structure of the detonation cells is rather smeared by the numerical dissipation.
In figure 6 the same flowfields are obtained with the 3rd order MUSCL reconstruction. The structure of detonation cells was well resolved, but the certain numerical artifacts distorting the shape of the left RMI can be seen. Obviously, numerical viscosity has major impact on this flow on this flow. To solve such a problem, the solver and the numerical scheme need to treat different scales of flow inhomogeneities with equal accuracy. In the present case a more detailed study of both the flow and the HyCFS-R solvers is required. The latter ones need to be compared with other numerical schemes to locate the source of numerical artifacts.
4. Conclusion
As part of the HyCFS-R numerical code development, a module for the simulation of multiphase chemically reacting flows based on the Euler-Euler approach was implemented. The code was verified on simple 0D and 1D problems, such as constant volume explosion and 1D shock tube problem. For more comprehensive testing the numerical simulation of the Richtmyer–Meshkov instability in reactive heterogeneous media was performed. The comparison against the reference solution revealed that numerical method implemented in the HyCFS-R either introduce too much dissipation and suppress DW front instabilities or lead to numerical artifacts in the RMI flow pattern. Thus, it can be concluded that further improvement of the numerical techniques is required. Future work will include implementation of TVD schemes of 4th and 5th order by Yamamoto and Daiguji, employment of other schemes for the dispersed phase advection, and 3D calculations.

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