An adaptive 3–D CFD solver for explosion modeling on large scales

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Abstract

An adaptive 3–D CFD solver for modeling detonations on large scales is presented. As a detonation itself is a small scale event, adaptive mesh refinement and coarsening is used to resolve all relevant scales. Results are compared with experimental data.

Introduction

Studies of gas cloud explosions in industrial environments increasingly rely on numerical simulations of the accident sequence. This field of study puts enourmous requirements on the numerical simulation methods for the following reasons:

- The phenomena are inherently unsteady.
- The geometrical configuration is often both very large and very complex.
- The chemical source terms are highly nonlinear and require a very good spatial resolution.
- In a gas explosion, chemistry and fluid flow are coupled by nonlinear effects, therefore a detailed modeling is needed here.
- The total problem is a multi–scale problem in space and time, due to the fact that the geometrical scales vary from 10^{-3}m for the flame itself to 10^{+2}m for the size of the industrial environment.

To cover most of these needs, the adaptive CFD code REACFLOW was developed at JRC-Ispra. In this extended abstract we describe briefly the governing equations and the adaptive methods for our 3–D version of the code. As a quantitative example a 3–D transient simulation of a detonation on large scale will be presented.

Governing equations

The governing fluid dynamics equations are the equations for conservation of mass, chemical species, momentum and energy. Due to the very short time scales of a detonation, diffusive processes do not have to be taken into account and only the Euler equations are solved. In weak form they can be written in the following compact notation (in a cartesian coordinate system)

$$\frac{\partial}{\partial t}\left(\int_\Omega U dV\right) + \int_{\partial\Omega} n_i F_{i,\mathrm{conv}}(U) dS = \int_\Omega S dV \tag{1}$$

where $U = (\rho_\gamma, \rho u_i, \rho E)$ is the vector of conserved quantities which are the unknowns of the system. Here, ρ_γ, $(\gamma = 1, \Gamma)$ are the partial densities, ρu_i is the momentum vector and ρE is the total energy. $F_{i,\mathrm{conv}}$ is the convective flux. S is the source term including chemical reactions. The integration is performed for each control volume (CV) over the domain Ω with boundary $\partial\Omega$ and outward normal n_i.

In detonation modeling the chemical reaction rate can be described by a reduced chemical kinetics scheme. The progress reaction rate of the r'th reaction becomes

$$\omega_\gamma = k_{f,r}(T) \prod_{\gamma=1}^{\Gamma} C_\gamma^{\nu_{\gamma r,f}} - k_{b,r}(T) \prod_{\gamma=1}^{\Gamma} C_\gamma^{\nu_{\gamma r,b}} \tag{2}$$

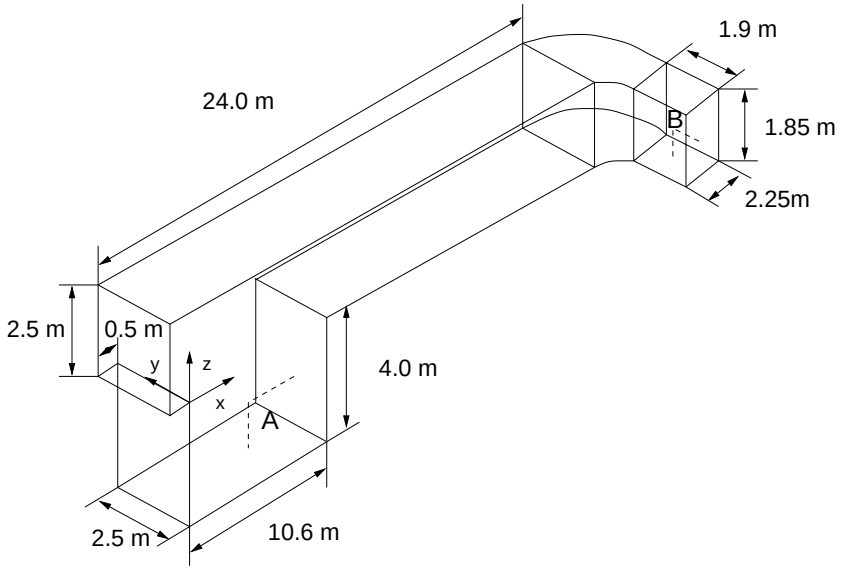

Figure 1: Outline of the RUT facility.

where $\nu_{\gamma r,f}$ is the stoichiometry of the γ'th component in the r'th forward reaction, and the forward and backward Arrhenius' rates for the r'th reaction, $k_{f,r}(T)$, $k_{b,r}(T)$, have the following form:

$$k_{f,r}(T) = A_{f,r} T^{b_{f,r}} e^{-E_{f,r}/RT} \tag{3}$$

Eq. 1 is solved by a finite volume approach. For details see [1].

Grid adaptation

Problems such as explosions in industrial environments are often characterized by very large and complex volumes where, at the other extreme, at any time the phenomena of interest are strongly localized, for instance at a blast wave or a flame front. These local areas of interest tend to move over time.

Under these circumstances it may be advantageous to let the computational grid adapt itself to the solution by inserting extra computational points (nodes) in the regions of interest, removing them once the flow features of interest decay or move away.

Two different criteria for the refinement/coarsening decisions have been implemented:

1. Simple difference between neighbours, based on the absolute difference in the selected variable between any two of the neighbours . The value of e_1 must be greater than the refinement criterion ξ.

$$e_1 = \Delta u = |u_i - u_j| \geq \xi \quad , \; i \neq j$$

2. Local evaluation of the interpolation error. Here we calculate an interpolated value, $\hat{u}_i$ for a given CV by a simple arithmetic mean of the neighbours. The adaptation criterion then becomes

$$e_2 = |u_i - \hat{u}_i| \geq \xi$$

This can be interpreted as making a comparison between the present grid and a fictitious coarser grid.

Large scale explosion simulation

As an example of the use of adaptive mesh refinement in large 3–D configurations we simulated the hydrogen detonation experiments performed in the Russian RUT Facility located near Moscow [2]. The facility has a total volume of about 263m^3. The volume has compartments of different size. There is a large volume, the so called canyon, followed by a 26m long channel. Some geometrical details are shown in Fig. 1.

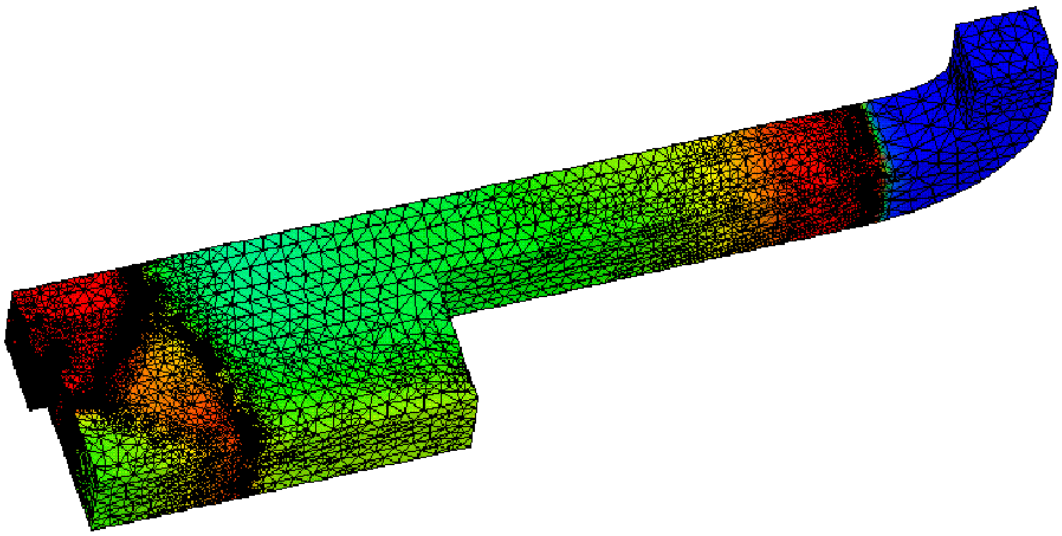

Figure 2: RUT detonation. Pressure isocolours at time $t = 10$ms after ignition shown with the grid on the surface.

For the simulation we chose test **hyd5** with a uniform hydrogen concentration of 20% Hydrogen (by volume) in air at ambient conditions. The detonation was initiated by 200g of high explosives at a low position inside the canyon. Experimental data were recorded by pressure transducers at various positions in the test facility.

The chemical source terms were calculated using the Finite-Rate scheme of Eq. 2. We used a scheme with 8 elementary chemical reactions [3]. To avoid the well-known problem of numerical detonation speeds, we added a cutoff temperature for the chemical source terms below which no reactions take place, as suggested by Klein [4]. The cutoff temperature was chosen as $T = 1200$K.

For the simulation with REACFLOW we used an initial grid with 3615 nodes and 15592 elements. The mesh distribution is nearly uniform. This corresponds to an initial resolution of $\Delta x \simeq 0.5$m. In the simulation the detonation was initiated by imposing a high temperature and pressure value for the nodes around the experimental ignition point. For the grid adaptation criterion the difference between pressure at neighbouring nodes were used (method 1 in Section). Nodes were added down to a minimum resolution of 1.5 cm. During the calculation nodes were added and removed up to a maximum of 235000 nodes which was the maximum set by the memory restrictions of 1 GB of the DEC–alpha workstation used for the calculation.

Fig. 2 shows pressure contour plots at $t = 10$ms after ignition. Here blue colour corresponds to low pressure of 1 bar and red to 10 bar and higher pressure. At this time the detonation has proceeded through the whole canyon and propagated 22m down the second part of the test facility. The reflected pressure waves at the end wall can be seen clearly, especially in the upper part of the canyon. The detonation front which is running down the second part of the canyon is now clearly planar. Fig. 2 shows the mesh at this time which has 146631 nodes and 756585 elements. Nodes are mainly added at positions of large pressure gradients. These are mainly found at the system of reflected shock waves and at the detonation front. Everywhere else the mesh is close to the initial mesh, as the nodes previously added have been removed.

Fig. 3 shows comparisons between experimental and simulated pressure time history plots at 2 different positions in the canyon. The detonation velocity is 1756 m/s in the experiment, whereas we find 1805 m/s in the simulation. The difference is about 3%. At the position at which the data in Fig. 3 (left) have been taken, the incoming shock wave propagates nearly perpendicular to the surface; therefore the peak pressure here is larger than in a case where the shock wave moves parallel to the surface (Fig. 3 right). This can be seen in the experiment as well as in the simulated results.

Summary

We have presented REACFLOW, a computer code for explosion modeling on large industrial scales. We have presented a grid adaptation system for this code which allows the grid to be adapted dynamically to changing flow conditions. In the example presented (RUT-detonation experiment), we have shown

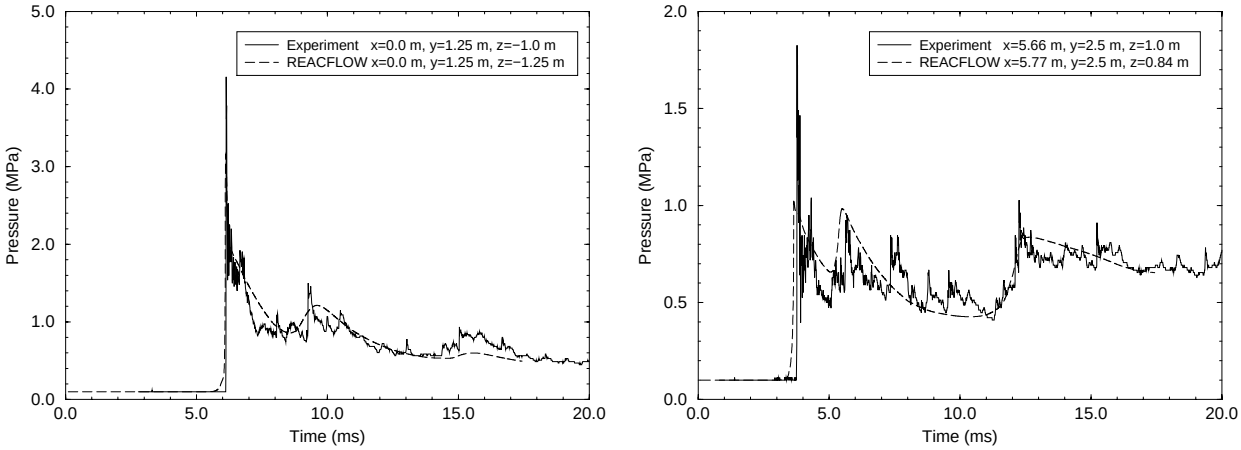

Figure 3: Hydrogen detonation in the RUT facility. Pressure versus time.

the use of adaptive mesh refinement in which used only about $2 \cdot 10^5$ nodes in our simulation where as a constant mesh would have required around $1 \cdot 10^7$ nodes if the maximum resolution was to be imposed everywhere in the domain. It is clear, therefore, clear, that saving two orders of magnitude of node points is worth the extra expenses for adaptive mesh refinement.

Acknowledgments

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References

[1] H. Wilkening and T. Huld. An adaptive 3–D CFD solver for modeling explosions on large industrial environmental scales. EUROTHERM: Preliminary Procedings of the Seminar 61, 's Hertogenbosch, Netherlands, Vol. II, Part 1, pp. G32-G58, October 1998.

[2] W. Breitung W., S. W. Dorofeev, A. A. Efimenko, A. S. Kochurko, R. Redlinger and V. P. Sidorov. Large Scale Experiments on Hydrogen-Air Detonation Loads and their Numerical Simulation. Proc. Int. Topical Meeting on Advanced Reactor Safety (ARS '94), Pittsburgh, USA April 94, Vol II, pp. 733-745, 1994.

[3] J. S. Evans and C. J. Jr. Schexnayder. Influence of Chemical Kinetics and Unmixedness on Burning in Supersonic Hydrogen Flames. *AIAA Journal*, 18:188-193, 1980.

[4] R. Klein, W. Breitung, W. Rehm, H. Olivier, L. He, P. Armand and M. Ang. Models and Criteria for Prediction of Deflagration–to–Detonation Transition (DDT) in Hydrogen-Air-Steam Systems under Severe Accident Conditions. Proc. FISA-97, Comm. Eur. Union, EUR 18258 EN, pp. 360-370, 1997.