

Gas Explosion Simulations with Flux Limiter Centred Method

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Introduction

A 2D and 3D numerical code for gas explosion simulations is proposed based on the 2. order total variation diminishing (TVD) flux limiter centred scheme (FLIC). The equations solved are the Euler equations with an energy source term, these equations are LES filtered. The combustion model used is a reactive Riemann solver for infinitely thin flames. A turbulence model for the turbulent kinetic energy is used to model the subgrid turbulence. The flame propagation is handled by the G-equations for turbulent flames. The FLIC scheme is chosen for its simplicity and its computational speed compared to upwind TVD schemes. To illustrate the performance of the code, results from numerical experiments have been compared with results from physical experiments.

Numerical Scheme

The 2. order flux limiter centred scheme combines the 1. order FORCE scheme and the 2. order Richtmyer version of the Lax-Wendroff scheme. The FORCE flux is a deterministic version of the Random Choice Method, where the stochastic steps of RCM is replaced by integral averages of the Riemann problem solutions. One outcome of this is that the FORCE flux is the arithmetic mean of the Richtmyer flux and the Lax-Friedrich flux.

$$\begin{aligned} \mathbf{F}_{i+\frac{1}{2}}^{\text{LF}} &= \frac{1}{2}[\mathbf{F}(\mathbf{U}_L) + \mathbf{F}(\mathbf{U}_R)] + \frac{1}{2} \frac{\Delta x}{\Delta t} [\mathbf{U}_L - \mathbf{U}_R] \\ \mathbf{U}_{i+\frac{1}{2}}^{\text{RI}} &= \frac{1}{2}[\mathbf{U}_L + \mathbf{U}_R] + \frac{1}{2} \frac{\Delta t}{\Delta x} [\mathbf{F}(\mathbf{U}_L) - \mathbf{F}(\mathbf{U}_R)] \\ \mathbf{F}_{i+\frac{1}{2}}^{\text{RI}} &= \mathbf{F}(\mathbf{U}_{i+\frac{1}{2}}^{\text{RI}}) \\ \mathbf{F}_{i+\frac{1}{2}}^{\text{FORCE}} &= \frac{1}{2}[\mathbf{F}_{i+\frac{1}{2}}^{\text{LF}} + \mathbf{F}_{i+\frac{1}{2}}^{\text{RI}}] \\ \mathbf{F}_{i+\frac{1}{2}}^{\text{FLIC}} &= \mathbf{F}_{i+\frac{1}{2}}^{\text{FORCE}} + \phi_{i+\frac{1}{2}}[\mathbf{F}_{i+\frac{1}{2}}^{\text{RI}} - \mathbf{F}_{i+\frac{1}{2}}^{\text{FORCE}}] \end{aligned}$$

The superscripts LF and RI stand for Lax-Friedrich and Richtmyer, respectively and ϕ is the flux limiter. Flux limiters eliminate spurious oscillations near high gradients by making the scheme 1. order accurate.

Turbulence Model

The turbulence model presented by Menon et. al. (2003) is applied to model the turbulent burning velocity. This model is a transport equation of the turbulent kinetic energy, k , where the source and sink terms, P and D describe production and destruction of turbulence.

$$\begin{aligned}(\bar{\rho}k)_t + \text{div}(\bar{\rho}uk) &= P^{\text{sgs}} - D^{\text{sgs}} + \text{div}\left(\frac{\nu_t}{\sigma} \text{grad}(k)\right) \\ P^{\text{sgs}} &= -\tau_{ij}^{\text{sgs}} \frac{\partial \tilde{u}_i}{\partial x_j}, \quad D^{\text{sgs}} = C_\varepsilon \bar{\rho} k^{\frac{3}{2}} / \bar{\Delta} \\ \tau_{ij}^{\text{sgs}} &= -2\bar{\rho}\nu_t(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{ij}\delta_{ij}) + \frac{2}{3}\bar{\rho}k\delta_{ij} \\ \nu_t &= C_\nu k^{\frac{1}{2}} \bar{\Delta}\end{aligned}$$

Sgs stand for subgrid scale. C_ε and C_ν are model constants set to 0.916 and 0.17. Δ is the filter size.

Combustion Model

The combustion model used to solve the energy source term is based on the Riemann solver as presented by Teng et. al.(1982). Our model is applicable for different heat capacity ratios, γ , for the burned and unburned states. This model is also previously used by Bjerketvedt et. al. (2004) in the 1D RCMLab code. In the article by Teng et. al. it is stated that the Riemann solver could produce several solutions or no solutions if applied to turbulent combustion. Our investigations conclude that it is not possible with more than one solution. This will be discussed in a separate paper. The model for determining the turbulent burning velocity presently used is a model proposed by Peters (2000), eq 2.200 in Peters.

Results and Discussion

A numerical experiment has been performed and compared with results from physical experiments. In both test cases a 3 m long cylindrical tube of inner diameter of 100 mm was filled with stoichiometric hydrogen-air at 1 atm. The tube was closed in both ends. The mixture was ignited at the end of the tube with a spark plug. Pressure transducers (Kistler 7001 and 603B) were placed at 0.5 m intervals along the tube wall. The numerical experiments were performed in 2D cylindrical coordinates, this is a rough assumption considering the Euler equations was filtered for LES.

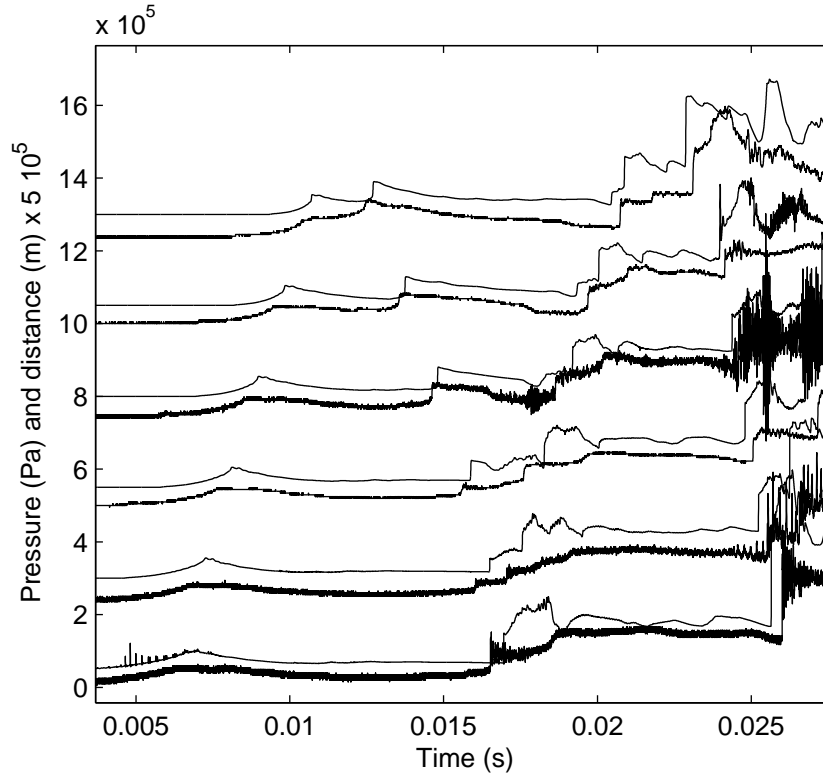


Figure 1. Pressure records for numerical and physical experiments with H_2 -air, $\phi=1$, $L=3$ m, $d=0.1$ m.

Figure 1 show the pressure records for the numerical and physical experiments at all transducer. The numerical results are elevated 50 kPa to discern them from the physical experiments. The initial numerical results are general in good agreement with the physical experiments. The first pressure peak that rises from the initial expanding flame, is simulated accurately as shown in Figure 1. This indicates that the code handles the large scale flame deformation well. When the first reflected pressure wave interacts with the flame, as shown in figure 2 at $x \approx 0.8$ m and $t \approx 0.016$ s, the total burning rate is increased as in the experiments, but pressure records show some discrepancies.

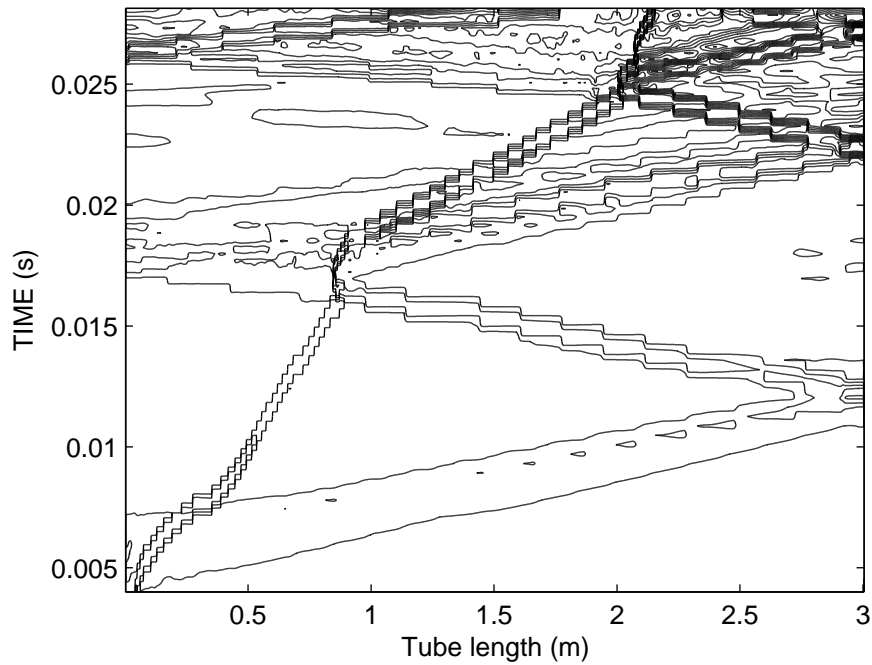


Figure 2. Wave pattern along the central line of the tube.

Conclusion

A code for simulation of gas explosions has been developed and the initial tests show promising results. The code performs relatively fast and it is numerically stable. Some of the future work will include an evaluation of the constants in the turbulence model and to validate the code in full 3D.

References

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