CNS RateStick Validation

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1 Introduction

1.1 Overview

The RateStick module simulates steady-state detonation in explosives under different types of confinement. It provides both the velocity of detonation (VOD), as well as the full flow field around the detonation wave front, enabling the extraction of additional characteristic quantities such as front curvature, confining material pressure and more.

The main features of the RateStick module are:

- High-performance simulations through the use of GP-GPUs for the computations allowing for rapid steady-state solutions, with convergence achieved within minutes.
- Simulation of any size of explosive charge and confinement thickness for two types of charge geometries: slab and cylinder.
- Two-phase reactive model with explicit representation of the reaction zone to enable capturing the confinement effect with a single set of explosive parameters.
- Large selection of confinement materials ranging from unconfined (air) to strong confining materials (e.g. steel)

While the current front-end application for RateStick provides a set of predefined material configurations with corresponding equation of state parameters, the underlying implementation of RateStick is modular and designed to support additional equations of state (symbolic or tabular) based on the scientific literature or experimental data. This modularity ensures flexibility for future expansions, which may include enhanced customisation options for user-defined materials. Additionally, a planned extension of this module is the direct integration with the chemical kinetics software, *CaThe*, which would enable the direct calculation of equation of state parameters for the products of any explosive, given its chemical composition.

1.2 Mathematical Model

The RateStick module solves the MiNi16 [2] multiphase formulation, which features two continuity equations that account for the explosive and inert materials, respectively. The explosive material is modelled using a two-phase formulation, with separate equations of state for the reactants and products. The system of equations is as follows:

$$
\begin{aligned}
\frac{\partial (z\rho_1)}{\partial t} + \nabla \cdot (z\rho_1 \mathbf{u}) &= 0,\\
\frac{\partial ((1-z)\rho_2)}{\partial t} + \nabla \cdot ((1-z)\rho_2 \mathbf{u}) &= 0,\\
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + pI) &= 0,\\
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot ((\rho E + p)\mathbf{u}) &= 0,\\
\frac{\partial z}{\partial t} + \mathbf{u} \cdot \nabla z &= 0,
\end{aligned}
$$

$$\frac{\partial (z\rho_1\lambda)}{\partial t} + \nabla \cdot (z\rho_1\lambda\mathbf{u}) = z\rho_1\mathcal{R}.$$

Here, ρ denotes the total density, $\mathbf{u}$ is the fluid velocity, p is the pressure, and E represents the total energy. The partial densities ρ_1 and ρ_2 correspond to the explosive and inert materials, respectively, while the volume fraction z determines the ratio of these two materials in each computational cell. The progress of the reaction in the explosive is tracked by the variable λ, and is governed by the reaction rate $\mathcal{R}$.

The formulation requires the definition of equations of state for each phase of the explosive, as well for the inert confining material. Additionally, a closure condition is needed for the system to be fully determined. The $p-V$ equilibrium conditions [3] are adopted in this implementation, enforcing pressure equilibrium between all materials and density equality between the two phases of the explosive. These closure conditions provide robustness and increased computational efficiency when compared to alternatives.

1.3 Numerical method

The mathematical formulation constitutes a non-linear hyperbolic system with source terms. Starting from the initial conditions, the numerical solution is advanced in time using the operator splitting method. This approach allows for separate treatment of the homogeneous part, which is solved with an appropriate hyperbolic solver, and the source terms, which are handled independently using an ordinary differential equation (ODE) solver.

The hyperbolic component is solved using the MUSCL-Hancock finite volume method [4], which is a high-resolution, shock capturing, Godunov-type reconstruction scheme that is second-order accurate in both time and space. To prevent spurious oscillations near steep gradients, which can arise in high-order schemes, the van Leer slope limiter is applied to the primitive variables. The scheme also requires a Riemann solver to compute fluxes at cell interfaces, and the HLLC solver is used for this purpose. The non-conservative equation governing the volume fraction is solved using the Godunov method for advection equations. The reaction rate source term, as well as the geometric source terms arising from the axisymmetric cylindrical coordinate setup, are solved using a fourth-order Runge-Kutta method.

1.4 Implementation

The numerical methods are implemented using CUDA, with computations performed on high-performance GPUs. The implementation divides and distributes the computational load across GPU threads, while ensuring optimal memory usage for enhanced performance.

Computational efficiency is further improved by employing a moving frame of reference. This approach is motivated by the fact that the detonation steady state is reached after the detonation wave has propagated a certain distance through the explosive charge, known as the *run-to-detonation* length. Rather than simulating the entire run-to-detonation length, a smaller, dynamically moving domain is used to track the detonation wave at all times. This method does not influence the detonation propagation but provides significant computational gains in addition to allowing the domain size selection to be independent of the run-to-detonation length of the explosive.

2 Case Study

This section presents a case study that demonstrates the RateStick module's ability to match experimental results. This study explores the diameter effect observed in explosives, where the steady-state VOD increases with charge diameter. The confinement material plays a crucial role in this phenomenon, and multiple materials are examined to highlight the predictive capabilities of the RateStick module in capturing the effect of confinement.

Users can replicate the results presented in this report by entering the specified settings and material configurations into a new simulation within the CNS platform. This case study can also serve as a starting point for users to conduct their own simulations.

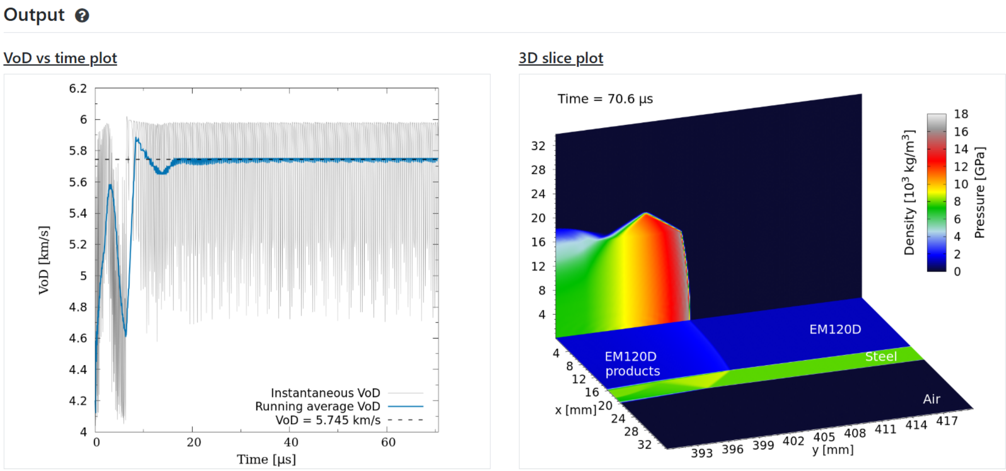

Figure 1: Indicative results from the platform showing a simulation of a cylindrical EM120D charge of 15 mm radius, with 4 mm thick steel confinement.

2.1 EM120D VOD

In this example, the RateStick module is employed to study the change of velocity of detonation (VOD) with radius of a cylindrical charge for the explosive EM120D under different confining materials.

The EM120D is an ANFO-based emulsion widely used in the mining industry. It is an example of a highly non-ideal explosive, characterised by long reaction zones and a strong dependence of the VOD on the radius of the explosive. The equation of state for both the reactants and products, as well as the reaction rate parameters, are derived from Wilkinson et al. [5]. However, due to differences in equilibrium conditions between the aforementioned study and the $p - V$ conditions used in this module, the reaction rate parameters were re-calibrated to match the unconfined VOD curve of the explosive. With this single calibration, the RateStick module can accurately reproduce the VOD curves under different confinement conditions, as will be demonstrated below.

2.1.1 Results

A series of simulations were performed for rate-sticks of various radii and confining materials. The radii ranged from 12-45 mm for the weak confiners (unconfined and concrete) and from 10-40 mm for steel, which is a strong confiner and allows for steady detonations to form at smaller radii. Figure 1 illustrates the results for a representative case with a 15 mm charge radius and steel confinement.

The numerical results are compared against experimental data from experiments conducted by Orica Mining Services [1] in Figure 2. Solid points with error bars indicate experimental data, while line segments represent numerical results from RateStick.

There is strong agreement between the experimental and numerical results. Even though the reaction rate was calibrated using the experimental data for a 20 mm unconfined rate-stick, the model can accurately capture VODs for the whole range of the unconfined curve. The diameter curves for steel and concrete confinement also show good agreement across a wide range of radii.

This case study demonstrates the predicting capabilities of the RateStick module in determining the effect of both weak and strong confinement on the VoD, despite using only unconfined rate-stick data during the calibration process.

3 Conclusion

The RateStick module provides an efficient and accurate tool for predicting detonation velocities in both confined and unconfined explosive configurations. It effectively captures diameter effects and confinement influences, demonstrating strong agreement with experimental results.

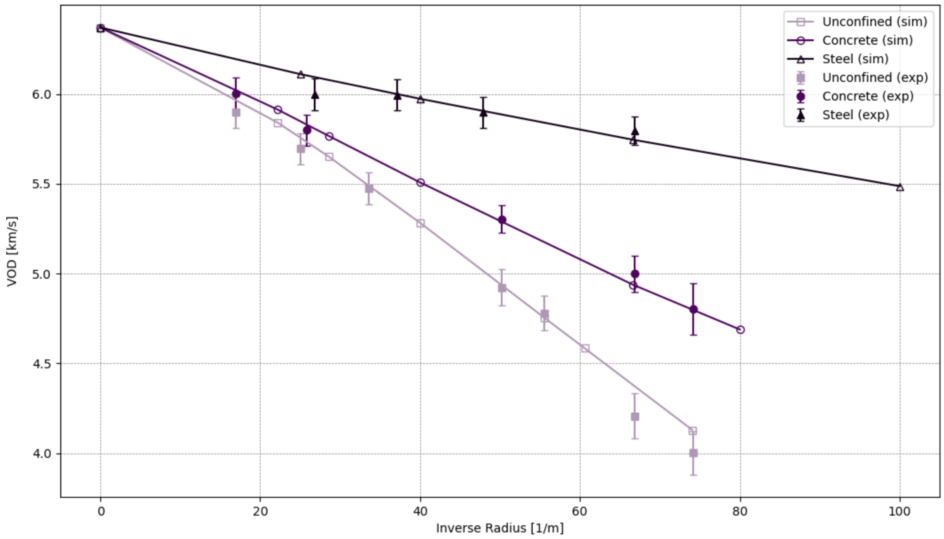

Figure 2: Radial dependence of the VoD for EM120D rate sticks under different confinement types. Numerical results (open symbols) are compared with experimental data [1](solid symbols), with error bars indicating experimental uncertainty.

By leveraging high-performance GPU computing and advanced numerical methods, RateStick enables reliable and efficient detonation modelling, making it a valuable tool for explosive research and development.

References

[1] A. N. Dremin. *Results from Detonic Research Contract II*. Tech. rep. Orica Canada, 1999.

[2] L. Michael and N. Nikiforakis. "A hybrid formulation for the numerical simulation of condensed phase explosives". In: *Journal of Computational Physics* 316 (July 2016), pp. 193–217.

[3] D. S. Stewart, S. Yoo, and W. C. Davis. "Equation of state for modeling the detonation reaction zone". In: *12th Symp.(Intl) on Detonation*. 2002, pp. 1–11.

[4] E. F. Toro. *Riemann solvers and numerical methods for fluid dynamics*. 3rd. Springer, 2009.

[5] S. D. Wilkinson et al. "A complete equation of state for non-ideal condensed phase explosives". In: *Journal of Applied Physics* 122.22 (2017), p. 225112.