ENERGETIX: THE NEXT EVOLUTION IN HAZARD DIVISION 1.3 EVENT ANALYSIS

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INTRODUCTION

The prediction of explosive effects in confined spaces presents a complex and multifaceted problem in the domain of explosives safety, yet is a growing requirement given advancements in weapons technology, including the development, manufacturing, storage, and transportation of next-generation energetic materials. Another recent growth driver for this requirement is the Army's accelerated ammunition plant modernization program, where limited space within existing facilities necessitates the development of new sites and associated protective construction and safety testing. Hazard Division (HD) 1.3 events represent a particularly challenging explosive effects characterization problem for subsequent protective design. Explosive effects from an HD 1.3 event can vary greatly from a moderate burn to an explosive deflagration depending on factors such as loading density, degree of confinement, and overpressure venting capacity. An escalated HD 1.3 event can pose significant risks due to overpressure buildup, structural confinement effects, and potential transition to violent rupture[1], particularly in the absence of adequate venting.

However, the challenge of accurately predicting key physical phenomena relevant to HD 1.3 events, such as overpressure, venting dynamics, and fragment dispersion, has a continued reliance on empirical testing and simplified models for safety assessments. Existing modeling approaches rely on empirical correlations and simplified thermodynamic models, which, while useful, lack the granularity required to accurately simulate real-world scenarios involving structural containment.[2] Unlike detonation events, which can be modeled using well-established shock physics principles, deflagration in confined environments presents unique challenges due to; the dynamic interaction between gas expansion, structural response, and venting mechanisms[3]; the transition from slow burn to violent pressurization leading to structural breach[4]; and fragmentation dynamics, which depend on both the material properties of the containment and the thermodynamic state of the energetic material.

Co-developed by Synthetik Applied Technologies (Synthetik) and Protection Engineering Consultants, LLC (PEC), the EnergetiX modeling framework has been developed to provide a robust solution that balances many of the limitations surrounding existing approaches, improving predictive accuracy while maintaining computational feasibility. EnergetiX is a validated, adaptable computational framework developed for modeling HD 1.3 events in confined environments, optimizing venting strategies, and ensuring compliance with Department of Defense Explosives Safety Board (DDESB) standards.

Developed through extending the capabilities of the open source DoD-funded blastFoam[5] CFD solver, EnergetiX leverages new physics-based models for combustion, afterburn, and structural response, to better quantify explosive effects for confined HD 1.3 events and enables high-fidelity simulation in support of explosives safety siting and facility design assessments.

Validated through extensive testing, ensuring its effectiveness in predicting pressure rise, venting efficiency, and fragmentation behavior in HD 1.3 events, EnergetiX has been benchmarked against real-world test data, including Koenen tube experiments, thermal ignition scenarios, and reinforced structure containment tests. Validation included comparisons with existing benchmark tools showing improved accuracy in modeling HD 1.3 combustion behavior, enhancing explosives safety assessments for regulatory compliance as well as offering a viable simulation tool to support explosives safety projects.

DEVELOPMENT OF THE EnergetiX COMPUTATIONAL FRAMEWORK

EnergetiX was developed to model HD 1.3 events, specifically those occurring in confined environments. The development approach emphasized both physical fidelity and practical applicability, ensuring that the tool is

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[2] Brode, H. L. "Numerical solutions of spherical blast waves." Journal of Applied Physics, vol. 26, 1955, pp. 766-775.
[3] Han Sun, Guogang Yang, Zhonghua Sheng, Zhuangzhuang Xu, Xiaoxing Yang, Shengzheng Ji, Effects of vent position and numbers on hydrogen explosion dynamic characteristics, Clean Energy, Volume 9, Issue 1, February 2025, Pages 223–238
[4] Oran, E. S., & Gamezo, V. N. (2007). Origins of the deflagration-to-detonation transition in gas-phase combustion. Combustion and flame, 148(1-2), 4-47
[5] https://github.com/synthetik-technologies/blastfoam

capable of capturing complex multiphysics phenomena while remaining computationally tractable for use in operational safety assessment workflows.

Building on the DoD-funded *blastFoam* solver, a reactive compressible flow computational fluid dynamics (CFD) platform designed for defense-related blast analysis, EnergetiX incorporates a suite of enhancements tailored to the unique challenges posed by HD 1.3 deflagration events including:

- Physics-based solid propellant regression modeling, based on modified Saint-Robert's laws, which allows for accurate simulation of propellant burn behavior under confinement.
- Multi-species afterburn chemistry, accounting for reactions involving nitrogen-rich species and residual combustion products. These chemical mechanisms are modeled using Arrhenius-based rate laws, enabling time-resolved combustion source terms.
- Coupled fluid-structure interaction (FSI) modeling, facilitating the prediction of structural deformation, breach, and door/hatch response to internal overpressures, including the use of rigid body dynamics to simulate moving components.
- Three-dimensional resolution and spatial adaptability, which allows for refined local prediction of pressure gradients, flame front evolution, and fragmentation dynamics in complex geometries.

These capabilities were incorporated with the objective of better representing real-world explosive environments, where confinement, structural complexity, and non-ideal combustion behavior significantly influence hazard outcomes.

EnergetiX is implemented in C++ using the OpenFOAM framework and is compatible with both desktop and HPC environments. Pre- and post-processing are conducted using ParaView and standard OpenFOAM utilities. The solver is currently in use for safety assessments supporting DDESB reviews and is available for authorized government and contractor use.

GOVERNING EQUATIONS

The underlying physics implemented within EnergetiX are based on compressible Navier-Stokes equations for mass, momentum, and energy, with additional transport equations for species mass fractions and source terms for combustion and regression:

Continuity: $\partial\rho/\partial t + \nabla\cdot(\rho u) = S_m$

Momentum: $\partial(\rho u)/\partial t + \nabla\cdot(\rho u \otimes u) = -\nabla p + \nabla\cdot\tau + \rho g + S_u$

Energy: $\partial E/\partial t + \nabla\cdot((E + p)u) = \nabla\cdot(\kappa\nabla T) + Q\_comb + S\_E$

Where, S_m, S_u, and S_E represent source terms due to combustion, mass regression, and afterburn chemistry.

Unlike simplified control volume approaches, EnergetiX's governing equations resolve the evolution of mass, momentum, energy, and species concentration across transient, multiphase flows, making EnergetiX uniquely suited to simulate the gradual-to-violent pressure rise characteristic of HD 1.3 events, including those with mixed confinement and venting regimes.

The governing equations are as follows:

Mole conservation:	**Conservation of energy:**
$\frac{\partial n_i}{\partial t} = \dot{n}_{i,in} - \dot{n}_{i,out} + \dot{\omega}_i$ $\dot{n}_{i,in} = -f_i \frac{\partial m_s}{\partial t}$ $\frac{\partial m_s}{\partial t} = -k\left(\frac{p}{p_{ref}}\right)^{\alpha}$ $\dot{n}_{i,\,out} = v_{out} n_i$ $\dot{\omega} = K_f n_{CO} n_{O2}$ $K_f = A\exp\left(-\frac{T_r}{T}\right)$	$\frac{\partial nU}{\partial t} = \dot{n}_{in} H_{in} - \dot{n}_{out} H_{out} + q_{gen}$ $q_{gen} = \dot{\omega} H_C$ Where, n_i - Number of moles of specie I U – Interna energy H – Enthalpy m_s - Mass of solid propellant p – Pressure

The following equations describe how structural interactions such as door motion are incorporated.

Conversation of angular momentum:	Where,
$I\frac{\partial^2 \theta}{\partial t^2} = F \times \boldsymbol{R}$	θ – angle of door I – Moment of inertia $\boldsymbol{R}$ – Radius or rotation p - Pressure
Force acting on door:	$\boldsymbol{A}$ – Area of door (single)
$F = \left(p - p_{ref}\right)\boldsymbol{A} - \boldsymbol{g}\sin(\theta)\, m_{door}$	$\boldsymbol{g}$ – Gravitational acceleration m_door - Mass of door

Combustion and Regression Modeling: Solid propellant regression is modeled using pressure-dependent burn laws derived from modified Saint-Robert's equations. Afterburn chemistry incorporates nitrogen-rich species and residual oxidizer reactions through Arrhenius kinetics, enabling more accurate simulation of delayed energy release in partially confined geometries.

Structural Interaction: The solver includes a simplified fluid-structure interaction (FSI) capability for modeling door and hatch motion under internal pressure. Rigid body dynamics equations are used to predict movement and venting evolution over time.

Numerical Framework and Mesh Adaptability: EnergetiX employs finite volume methods on unstructured, three-dimensional meshes. Adaptive resolution in regions of steep pressure gradients and flame fronts allows for improved local accuracy without excessive computational cost.

Configurability and Workflow Integration: EnergetiX supports flexible user input for defining chamber geometry, vent size, propellant configuration, and boundary conditions. Pre-processing is conducted using OpenFOAM tools, while results are analyzed via ParaView and Python-based utilities. The model is deployable on both desktop and cluster environments.

To ensure usability for explosives safety professionals and protective designers, EnergetiX has been developed with flexibility in mind. Input parameters and boundary conditions can be easily configured to represent a wide range of storage configurations, propellant types, and venting scenarios. Ongoing development includes efforts to expand automation and user accessibility, with the goal of producing a tool that not only meets high scientific standards but also integrates seamlessly into DDESB-aligned assessment workflows.

EnergetiX represents a deliberate effort to bridge the gap between fidelity and feasibility, a challenge that has historically limited the adoption of high-resolution models in routine safety evaluation. By building upon a validated, DoD-funded foundation and tailoring its architecture to the specific needs of HD 1.3 event modeling, EnergetiX provides a robust and credible alternative to existing tools.

CODE VALIDATION AND BENCHMARKING

A critical component of EnergetiX's development process was ensuring that the model could reliably reproduce key observables associated with confined HD 1.3 events. In line with standard practices for defense-related computational tools, EnergetiX underwent a staged validation campaign using both small-scale and full-scale test data. The goal of this process was to establish confidence in the model's predictions across a wide range of configurations and to demonstrate its suitability for regulatory-grade safety assessments.

Validation against experimental data focused on several core phenomena:

- Overpressure development in confined geometries
- Vent area effectiveness and pressure relief rates
- Flame propagation and transition from slow burn to violent pressurization
- Structural breach timing and dynamics
- Fragmentation onset and distribution

In particular, EnergetiX was benchmarked against:

- Koenen tube and strand burner tests to validate pressure-dependent burn rate models and ignition behavior.
- Thermal ignition trials performed at Sandia National Laboratories, which provided detailed temperature and pressure evolution data for HD 1.3 propellants under confinement.
- Large-scale structural breach tests involving the combustion of M1 propellant in reinforced concrete test cells, as documented in NAWCWD TM 8742.[6]

Simulation results showed consistent agreement with recorded data, including accurate prediction of ignition delays, pressure rise rates, and breach onset. Additionally, comparisons with control-volume approaches such as the Integrated Violence Model (IVM) highlight EnergetiX's improved resolution of local pressure gradients, secondary combustion phenomena, and geometric complexity.

The validation process followed technical standards consistent with DDESB, the US Army Technical Center for Explosives Safety (USATCES), Naval Ordnance Safety and Security Activity (NOSSA), and Air Force Safety Center (AFSEC). EnergetiX's predictive performance across combustion, gas dynamics, and structural response domains supports its use in regulatory-aligned safety modeling.

COMPARISON WITH OTHER CODES

EnergetiX was compared to the Integrated Violence Model[7] (IVM) using standard HD 1.3 benchmark scenarios, including evaluations in an ECM (150-barrel, 7500 kg) and ISO container (10-barrel, 500 kg) configuration. As shown below, EnergetiX produced closely matched or improved fidelity in transient pressure predictions and structural response timing.

[6] Aubrey Farmer. (2015). Combustion of Hazard Division 1.3 M1 Gun Propellant in a Reinforced Concrete Structure.
[7] https://ivm13.com/#/

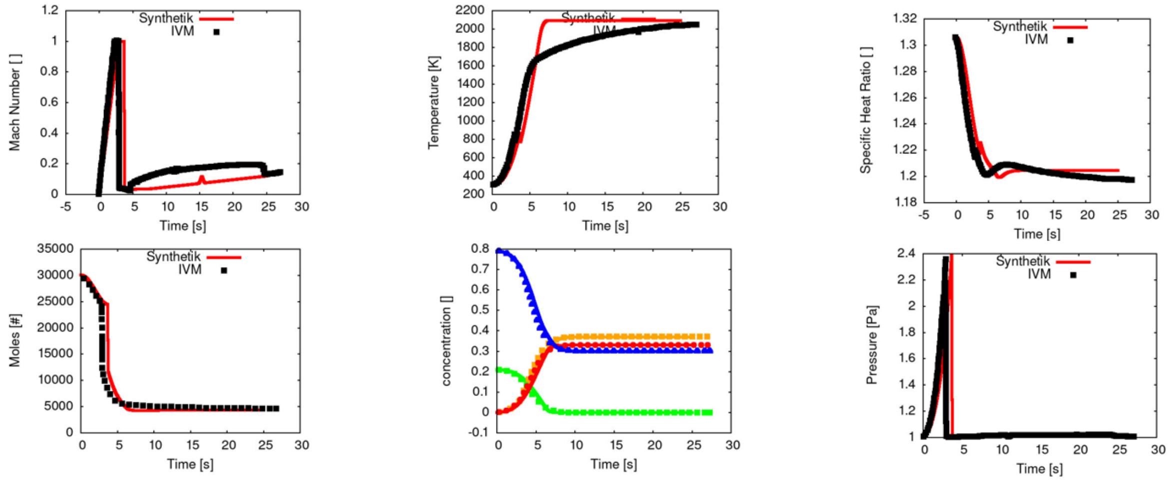

Figure 1: Comparison between EnergetiX and IVM predictions for ECM configuration with 7500kg (150 barrels) of propellant.

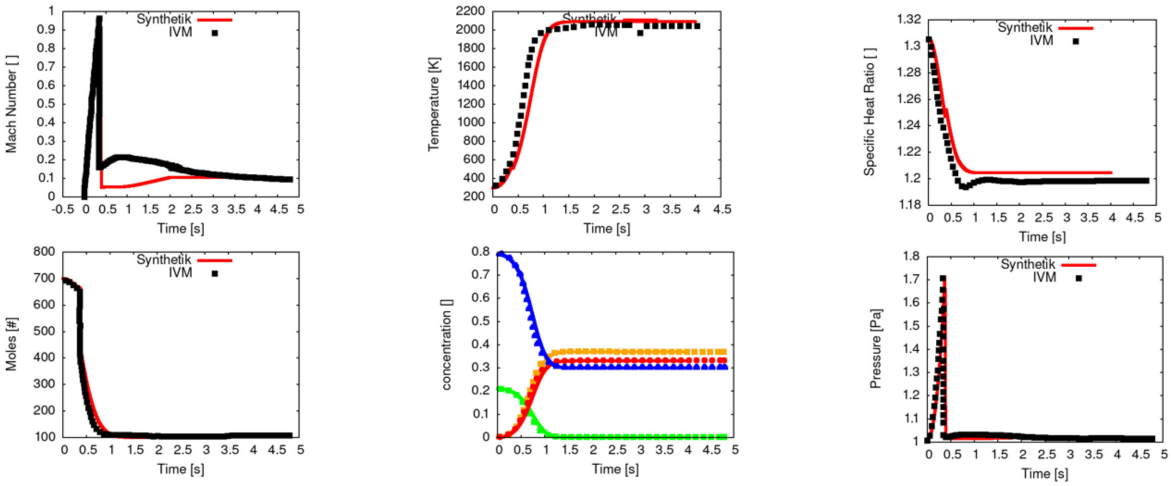

Figure 2: Comparison between EnergetiX and IVM predictions for ISO Container configuration with 500kg (10 barrels) of propellant.

Key comparative observations include:

- Improved prediction of localized overpressure gradients and structural loading patterns in non-symmetric vent configurations.
- Accurate resolution of flame acceleration and secondary combustion (afterburn) effects, which existing tools typically simplify or neglect.
- Flexible handling of geometry and confinement complexity, enabling simulations of real-world storage or handling configurations without reducing the problem to a series of idealized compartments.

EnergetiX's increased fidelity is especially apparent in scenarios involving partial confinement, vent obstruction, or transitioning flame regimes—situations that often fall outside the validated use envelope of empirical or semi-empirical models.

The validation process adhered to guidelines consistent with those employed by key U.S. Department of Defense stakeholders, including DDESB, USATCES, NOSSA, and AFSEC. Confidence in the application of EnergetiX is supported by its demonstrated consistency in reproducing outcomes observed in independent experimental studies. The model has shown reliable performance across multiple interconnected physical domains, including combustion, structural response, and gas dynamics. Furthermore, its development is grounded in peer-reviewed methodological rigor, with governing equations and numerical implementations based on established principles in reactive flow and structural mechanics

This validation record supports the use of EnergetiX as a defensible analytical tool for HD 1.3 event modeling, suitable for informing explosive safety siting, facility design, and compliance reviews. While no model can eliminate uncertainty entirely, EnergetiX represents a valid competitor, as well as an advancement in the resolution and scope of predictive capabilities currently available for deflagration hazard assessment.

APPLICATION FOR EXPLOSIVES SAFETY ASSESSMENTS

EnergetiX was developed to support defense stakeholders in conducting accurate, physics-informed hazard analyses for HD 1.3 events, particularly in cases where traditional empirical models and control-volume-based tools may not capture the full complexity of real-world configurations. With increasing demand for defensible modeling in explosives safety submissions to DDESB, there is a growing need for simulation tools that can offer transparent, validated, and physically grounded predictions of overpressure, venting efficiency, and fragmentation in confined or semi-confined environments.

Designed for seamless integration into safety assessment workflows, EnergetiX offers both the fidelity necessary for high-consequence evaluations, and the configurability to represent a range of practical storage, transport, and operational scenarios. It supports explosive material hazard classification, explosives safety quantity-distance (ESQD) siting, and protective design by enabling analysts to assess the impact of vent sizes, barrier placement, confinement levels, and energetic material inventories on resulting pressure loads and structural response.

As regulatory expectations evolve and the complexity of energetic systems increases, EnergetiX provides a scalable solution capable of producing insights that extend beyond the capabilities of legacy tools. The model is currently undergoing implementation in support of multiple assessment activities, including design studies, risk reviews, and facility compliance evaluations.

Protection Engineering Consultants, LLC (PEC) has collaborated closely with Synthetik Applied Technologies to apply the EnergetiX framework to live explosives safety projects requiring detailed deflagration hazard analysis. PEC's role has focused on interpreting regulatory guidance, defining realistic modeling inputs, and applying EnergetiX to analyze confined HD 1.3 events in scenarios representative of operational facilities and test environments for use in subsequent protective design applications. Through its application in real-world assessment scenarios, EnergetiX has supported the development of defensible technical arguments aligned with DDESB guidance, providing a credible basis for mitigation design, facility planning, and operational risk review.

As a code developer, Synthetik Applied Technologies is reliant on PEC's expertise in the application of EnergetiX for safety assessments. PEC continues to support the evolution of EnergetiX through real-world application and feedback, contributing domain-specific insights to improve usability and ensure the model's alignment with safety evaluation best practices. A near-term focus for Synthetik Applied Technologies and PEC is to identify the process by which EnergetiX can become properly verified and validated by the DDESB as an approved load characterization methodology to support explosives safety site plan and protective construction design submittals. The vision is for EnergetiX to eventually become the ConBLAST tools suite counterpart for evaluating load effects from an HD 1.3 event.

FUTURE DEVELOPMENT

Planned enhancements to EnergetiX aim to improve physical fidelity, broaden usability, and streamline regulatory adoption driven by both user feedback from applied assessments and emerging requirements from DDESB, USATCES, and NOSSA.

One area of focus is the extension of EnergetiX's capability to represent more complex structural interactions, including fracture mechanics for brittle materials and coupling with nonlinear finite element solvers for detailed structural stress and damage predictions. These enhancements will allow EnergetiX to more accurately resolve failure modes such as spalling, scabbing, and fragmentation beyond the current rigid-body representation.

Also under consideration, in order to streamline the user experience and lower the barrier to adoption within the safety engineering community, is the integration of a graphical user interface (GUI) to simplify geometry setup and parameter input, as well as automated post-processing features for safety criteria evaluation and reporting. These features will be especially beneficial in supporting consistent, traceable documentation for DDESB submissions.

Additional validation using extended test datasets remains a priority, particularly for edge cases involving marginal venting or high energy densities. These efforts will ensure continued alignment with empirical observations and extend the applicability of the model to a broader range of scenarios.

CONCLUDING REMARKS

EnergetiX is a computational modeling framework designed to resolve the complex multiphysics phenomena associated with deflagration events in confined environments containing HD 1.3 energetic materials. Developed by Synthetik Applied Technologies in collaboration with Protection Engineering Consultants, LLC (PEC), the model incorporates reactive flow physics, combustion kinetics, structural interaction, and transient venting behavior within a validated CFD platform.

As safety assessments become increasingly dependent on predictive modeling to inform decision-making and regulatory compliance, EnergetiX stands as a robust and credible alternative to existing tools. Based on the DoD-funded blastFoam platform and enhanced through the incorporation of multiphase reactive flow, solid regression, and afterburn modeling, EnergetiX is tailored to meet the specific demands of HD 1.3 deflagration analysis. Through extensive benchmarking against experimental datasets and comparative evaluation with existing tools, EnergetiX has demonstrated its capability to provide accurate, granular insights into explosive event dynamics while maintaining computational efficiency suitable for regulatory applications. It addresses the limitations of simplified methods by capturing essential physical details that influence outcome severity and safety zone definition.

With proven application in live safety projects and alignment with DDESB requirements, EnergetiX offers a credible scientific foundation for hazard evaluations and serves to strengthen confidence in the mitigation of HD 1.3 explosive risks.

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