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Code-to-Code Validation of SCORPION Against TEXAS-V for KROTOS K37 with a UO2-ZrO2 Oxidic Corium Melt

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1. Introduction

Steam explosions induced by fuel coolant interaction during severe accidents can generate short duration but intense pressure loads that challenge containment integrity [1]. Reliable prediction of peak pressure and impulse is essential for evaluating structural margins and for supporting integrated severe accident management strategies. Because the explosion phase evolves over very short time scales and involves strong thermal hydraulic coupling, a computational tool must remain both physically consistent and numerically robust. To address this, the SAFARI project has been initiated to provide a framework for efficient and systematic severe accident analysis, including dedicated modules for key energetic phenomena such as steam explosions.

Within the SAFARI framework, the steam explosion module SCORPION is being developed to predict pressure transients during the explosion phase in a computationally efficient manner. SCORPION is formulated as a lumped parameter model that advances coupled mass and energy inventories while representing rapid melt fragmentation and vapor generation. The module is designed to be integrated with other severe accident components in SAFARI, enabling consistent initialization from premixing conditions and fast evaluation of multiple scenarios. Through this development, SCORPION aims to provide a practical tool for repeated analyses and code validation studies while preserving the dominant physics governing pressure load generation [2].

2. Methodology

2.1 SCORPION model overview

The steam explosion module SCORPION is formulated as a non-equilibrium lumped parameter model designed to capture the mass and energy conservation mechanisms that govern pressure load generation during the short explosion transient. The formulation follows the one dimensional lumped modeling philosophy developed in the UWFCI [3], while avoiding the explicit resolution of detailed multiphase momentum fields. The system is represented by a small number of control volumes, where molten fuel, fine fragments, coolant, vapor, and the overlying slug are tracked through their evolving masses and energies. The coolant region is divided into a mixing zone, in which rapid fragmentation, enhanced interfacial heat transfer, and vapor generation occur, and a slug zone that represents the upper water column accelerated by the pressure rise as shown in Fig 1.

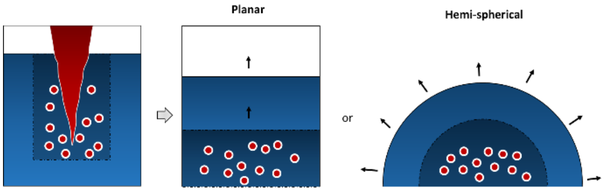

Fig. 1. Geometry constraint options

The coupled ordinary differential equations are integrated in time using the LSODA algorithm, and vapor pressure and temperature are evaluated from the conserved vapor mass, energy, and volume without direct solution of full momentum equations. Through this compact structure, SCORPION aims to reproduce the key energetics that control peak pressure and impulse while maintaining computational efficiency suitable for repeated analyses and code validation studies.

2.2 Governing Equations

The governing equations of SCORPION are formulated based on coupled mass and energy conservation for each control volume and material component. The model tracks the time evolution of molten fuel, fine fragments, coolant, vapor, and the slug. The mass conservation equations describe the transfer of melt into fine fragments through the fragmentation rate, the generation of vapor from coolant due to heat transfer, and the redistribution of coolant between the mixing zone and the slug region. In this formulation, fragmentation reduces the mass of intact melt while increasing the mass of fine fragments, and vapor generation increases the vapor inventory while decreasing the corresponding coolant mass. These balances ensure that all mass exchanges between phases are consistently accounted for within the lumped parameter framework.

The energy conservation equations account for interfacial heat transfer, vapor generation, phase change, and pressure work associated with volume variation. Heat transfer terms between fuel, fragments, coolant, and vapor determine the redistribution of internal energy, while vaporization contributes to the growth of vapor mass and enthalpy. The pressure work terms represent compressible expansion effects that are directly linked to pressure rise and slug acceleration. Pressure and temperature are then evaluated from the conserved vapor mass, energy, and volume, closing the thermodynamic state of the system. Through this set of coupled ordinary differential equations, the model captures the dominant energetic pathways that control pressure and impulse during the short explosion transient in a compact and computationally efficient manner. [4]

Mass Conservation

$$\frac{dm_f}{dt} = -\dot{m}_{fr} \tag{1}$$

$$\frac{dm_{fr}}{dt} = \dot{m}_{fr} \tag{2}$$

$$\frac{dm_c}{dt} = -\dot{m}_g + \dot{m}_s \tag{3}$$

$$\frac{dm_g}{dt} = \dot{m}_g \tag{4}$$

$$\frac{dm_s}{dt} = -\dot{m}_s \tag{5}$$

Energy Conservation

$$\frac{dE_f}{dt} = -\dot{Q}_{fg} + \dot{m}_{fr} V_f P - \dot{m}_{fr} h_{fn} \tag{6}$$

$$\frac{dE_{fr}}{dt} = -\dot{Q}_{frg} - \dot{m}_{fr} V_f P + \dot{m}_{fr} h_{fn} \tag{7}$$

$$\begin{aligned} \frac{dE_c}{dt} = \dot{Q}_{fc} + \dot{Q}_{frc} - \dot{m}_g c_{pc}\left(T_c - T_{ref}\right) \\ + P\dot{V}_c - \dot{m}_s c_{pc}(T_s - T_{ref}) \end{aligned} \tag{8}$$

$$\begin{aligned} \frac{dE_g}{dt} = \dot{Q}_{fg} + \dot{Q}_{frg} - \dot{Q}_{fgc} - \dot{Q}_{frgc} \\ + \dot{m}_g\left(h_{fg} + c_{pc}\left(T_c - T_{ref}\right)\right) - P\dot{V}_g \end{aligned} \tag{9}$$

$$\frac{dE_s}{dt} = -\dot{m}_s c_{pc}\left(T_c - T_{ref}\right) + P\dot{V}_s \tag{10}$$

2.3 Fine Fragmentation Model

Fine fragmentation plays a central role in steam explosion energetics because it directly controls the interfacial area available for heat transfer between melt and coolant. As molten fuel undergoes rapid breakup, the characteristic fragment size decreases and the total surface area increases significantly. This enhanced surface area intensifies heat transfer, accelerates vapor generation, and promotes rapid pressure rise within the mixing zone. Therefore, an appropriate representation of fine fragmentation is essential for capturing the causal chain that links melt breakup to pressure load generation.

In SCORPION, fine fragmentation is modeled through a semi mechanistic approach that relates the evolution of fragment mass and characteristic size to local thermodynamic and kinematic conditions. The model introduces a time dependent fragmentation rate that transfers molten fuel mass into fine fragments. This rate is formulated to reflect the influence of pressure growth, vapor expansion, and effective hydrodynamic constraints within the mixing zone. As fragmentation progresses, the interfacial heat transfer term in the energy conservation equations is updated based on the evolving fragment surface area. In this way, fragmentation is not treated as an instantaneous event but as a dynamic process that interacts with vapor production and pressure evolution.

$$\frac{dm_{fr}}{dt} = -6C_{fr} m_f \sqrt{\frac{\Delta P_{fr}}{\rho_c {R_f}^2}} f(\alpha) g(\tau_{fr}) \tag{11}$$

The fragmentation model is designed to remain compact while preserving the dominant physical trends observed in fuel coolant interaction experiments [5]. Instead of resolving detailed interface instabilities or multiphase flow structures, the formulation embeds their net energetic effect into source terms that are consistent with the lumped parameter framework. This approach enables efficient computation and stable coupling with the pressure evolution model, while retaining sensitivity to key parameters that influence peak pressure and impulse.

2.4 ResNet-Based Model for Thermodynamic Property Prediction Near the Critical Point

Accurate evaluation of thermodynamic properties is crucial in steam explosion simulations because pressure and temperature are determined from the conserved vapor mass, internal energy, and volume. In conventional steam table calculations, pressure and temperature are often obtained by inverting relationships between specific volume and internal energy. However, near the thermodynamic critical point, property gradients become steep and the Jacobian matrix involved in the inversion process can become ill-conditioned. This may lead to numerical instability, oscillatory pressure predictions, or convergence failure during time integration.

To address this issue, a ResNet-based surrogate model has been developed to directly map vapor specific volume and specific internal energy to pressure and temperature. The neural network is trained using high fidelity thermodynamic data covering a wide range of states, including regions close to the critical point. By learning the nonlinear relationship between state variables and target properties, the surrogate avoids explicit iterative inversion of steam tables. This significantly improves numerical robustness when the vapor state approaches near critical conditions during rapid pressure rise.

In SCORPION, the ResNet model is integrated within a hybrid property evaluation scheme. For regular thermodynamic regions, conventional formulations can be used, while the surrogate is employed when the state approaches conditions where inversion instability is likely. This strategy stabilizes pressure prediction and reduces computational time compared with repeated nonlinear iterations. As a result, the module can maintain both physical consistency and numerical efficiency, which are essential for repeated analyses and for systematic code-to-code validation.

3. Results

3.1 Initial Condition of KROTOS K37 Experiment

Table I: Initial and boundary condition of KROTOS K37 experiment

Experiment	**KROTOS K37**
Melt Composition	80 $wt\% \, UO_2$ $+ \, 20 \, wt\% \, ZrO_2$
Released Mass [kg]	3.22
Release Diameter [m]	0.03
Melt Temperature [K]	3018
Free Fall in Gas [m]	0.44
Water Depth [m]	1.105
Pool Diameter [m]	0.20
Water Temperature [K]	296
Water Subcooling [K]	77
Pressure [MPa]	0.1
External Trigger	Yes

Table I lists the initial and boundary conditions adopted for the simulations of KROTOS K37. The calculations were defined to be consistent with the reported melt composition, released mass, coolant temperature, subcooling, system pressure, and facility geometry of the experiment. The melt consisted of a prototypic corium composition of UO2 and ZrO2, and the test was conducted under subcooled water conditions with an external trigger. These conditions were used to define the initial thermodynamic state and the representative participating melt inventory for the explosion phase [6].

KROTOS K37 was selected because it represents a corium based, externally triggered experiment under relatively simple geometric and low pressure conditions. Compared with highly energetic cases, K37 is generally characterized by weak pressure development, providing a stringent test of whether a model can avoid overprediction of explosion strength. This feature makes the case suitable for code-to-code validation, as it allows a focused comparison of how SCORPION and TEXAS-V treat fragmentation driven vapor generation and pressure evolution under non-energetic or small energetic conditions.

3.2 SCORPION-TEXAS code-to-code Validation Results

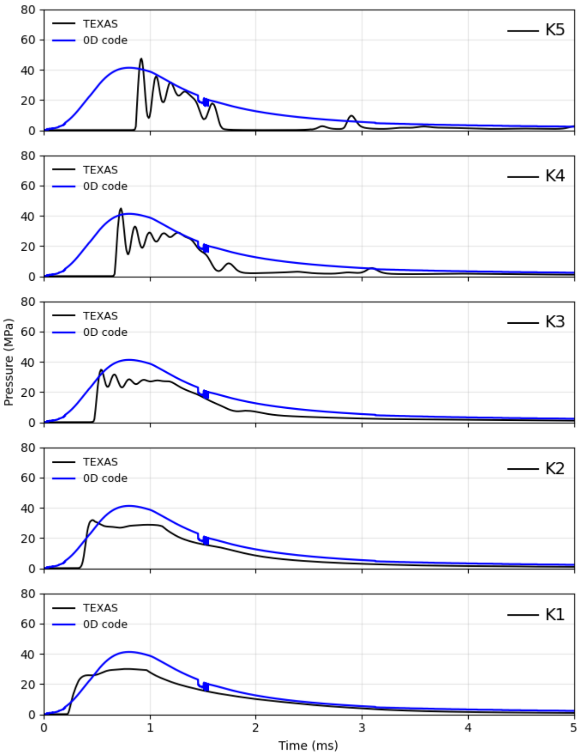

Fig. 2. TEXAS and SCORPION KROTOS K37 results

Figure 2 compares the pressure histories predicted by SCORPION and TEXAS at the five axial gauge locations for the KROTOS K37. Overall, SCORPION reproduces the main pressure pulse and the subsequent decay trend at all gauges, while TEXAS shows a sharper oscillatory structure after the initial rise. The agreement is relatively good in terms of the global pressure evolution, especially for the ordering of signal magnitudes and the progressive attenuation of the pressure wave along the measurement locations. In particular, both calculations indicate that the strongest response appears in the upper gauges, whereas the lower gauges exhibit a smoother and weaker transient.

SCORPION results are smoother and broader than the TEXAS results, with less pronounced short time oscillations and a slightly delayed decay in some gauges. This tendency is attributable to the lumped parameter formulation of SCORPION, which is intended to capture the dominant explosion induced pressure loading rather than the detailed local wave reflections resolved in a multi cell calculation. Despite these differences, the comparison suggests that SCORPION provides a reasonable representation of the overall pressure load characteristics for KROTOS K37, particularly with respect to the main peak level and the long tail behavior of the transient. This result supports the applicability of SCORPION to efficient code to code assessment for steam explosion load prediction.

4. Conclusions

In this study, the SCORPION steam explosion module within the SAFARI framework was validated against TEXAS-V through a code-to-code comparison for the KROTOS K37 experiment using a UO2-ZrO2 oxidic corium melt. K37 was selected as a relatively weak, externally triggered case conducted under low pressure conditions, providing a benchmark for avoiding overprediction of explosion strength.

SCORPION, formulated as a non-equilibrium lumped parameter model with a semi-mechanistic fine fragmentation treatment, reproduced the overall pressure development trends predicted by TEXAS-V under the same initial and boundary conditions. The comparison focused on the treatment of fragmentation driven vapor generation and its coupling to pressure evolution during the short explosion transient. The results indicate that the compact formulation of SCORPION can capture the energetic mechanisms governing pressure rise while maintaining computational efficiency.

The integration of the ResNet-based thermodynamic surrogate further improved numerical robustness near critical conditions, enabling stable evaluation of vapor pressure and temperature without iterative inversion instability. Overall, this study demonstrates that SCORPION provides a physically consistent and numerically efficient tool suitable for repeated analyses and systematic code-to-code validation within integrated severe accident assessment frameworks.

Nomenclature

P : Pressure
T : Temperature
V : Volume
α : Void fraction
R_f : Radius of fuel
ρ_c : Density of coolant
v : Specific volume
u : Specific internal energy

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