Internal Flashing Flow of Ammonia

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Abstract:
Ammonia is considered a carbon-free alternative fuel for energy systems. Its low boiling point makes liquid ammonia prone to flash boiling, especially under standard temperature and pressure. The phase change occurs on a timescale similar to the nozzle's flow-through time, requiring finite-rate modeling. This study presents a numerical simulation of internal flashing flow in superheated ammonia using a multidimensional thermal non-equilibrium model. The model was validated against experimental data, with simulations at two different back pressures showing a significant increase in vapor formation as back pressure decreased.

Keywords: Flashing, Ammonia, Convergent-Divergent Nozzle, Homogenous Relaxation Model.

Introduction:
Amid the growing demand for decarbonization, ammonia has garnered significant attention as a fuel due to its carbon-free nature, high energy density, and much higher volumetric and gravimetric hydrogen density as compared to conventional hydrocarbons [1]. Most research on utilizing ammonia as fuel has primarily focused on the external spray dynamics and flash boiling characteristics of liquid ammonia through numerical simulations and experimental techniques [2]. To achieve high-power output, liquid ammonia must be injected at high pressure and temperature, raising the fuel's enthalpy above the local or downstream saturation enthalpy, leading to flash boiling. The time scaleof rapid depressization inside the nozzl resulting in the phase change can be comparable to flow through time inside the nozzle. As per the author's knowledge, there is no previous study on the investigation of the internal flashing flow of ammonia. Therefore, this study conducts a preliminary numerical investigation into the internal flashing flow of liquid ammonia using a multi-dimensional finite rate non-equilibrium phase change model.

Numerical Methods And Approach:
The flash-boiling flow simulation presented here is based on fundamental conservation laws. Assuming no-slip conditions within a cell, the pseudo-fluid approach maintains the same core conservation principles as those for a single fluid. While the energy equation is included, all simulations are conducted under adiabatic conditions. Nevertheless, incorporating an energy or enthalpy equation is crucial for ensuring time accuracy. The k-ω turbulence model was employed to capture the complex flow dynamics associated with flash boiling, given its proven effectiveness. Details of the governing equations can be found in our previous manuscript on internal flashing flow in water [3] and are omitted here for brevity.

The non-equilibrium vaporization rate of superheated fuel is crucial for accurate modeling, significantly affecting fluid properties. This process is typically modeled as a first-order system using the Homogeneous Relaxation Model (HRM) [4], with a characteristic time derived from experimental data. The HRM accounts for internal bubble nucleation, growth, collapse, and motion. Initially developed for water, HRM has been adapted for liquid ammonia. The thermodynamic and transport properties of liquid NH3 are predicted using a surrogate model [5], though the values of the exponents in equation 1 remain unknown and await experimental validation. Thus, the same value of the exponents are used in the present study. Mathematically, HRM for upstream pressures up to 10 bar is

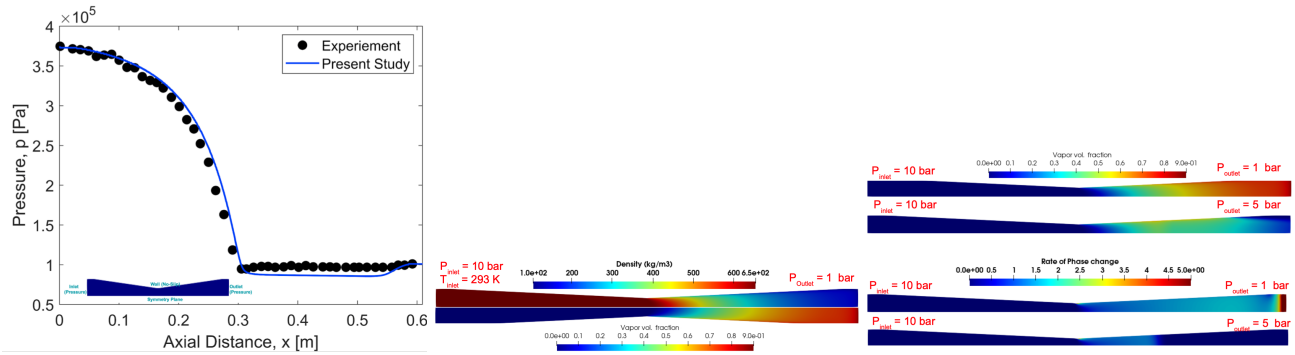
$$\frac{dx}{dt} = \frac{x_{eq} - x}{\Theta}; \quad \Theta = \Theta_o \epsilon^{\alpha} \phi^{\beta}; \quad \alpha = -0.257; \quad \beta = -2.24; \quad \Theta_o = 6.51 \times 10^{-4}; \tag{1}$$

Eqn.1,describes the exponential relaxation of the quality, x, to the equilibrium quality, $\bar{x}$, over a timescale, θ. The phase change process is connected to the conservation of mass and momentum through a chain rule approach, rather than relying on a traditional equation of state model. All variables, except for interpolated fluxes, were positioned at cell centers, located at the cell faces. Details about the numerical method and algorithm is

provided in our previous work [3].

Results and discusison:

The HRM model has been validated using experimental data from the study by Abuaf et al. on a converging–diverging (C-D) nozzle [6], with water as the working fluid. For detailed nozzle dimensions, please refer to [6]. Assuming axisymmetric behavior in the flashing flow, the numerical domain was simplified to a 2-D axisymmetric section with a wedge angle of 5° for analysis. A schematic of the numerical domain, boundary conditions, and code validation is presented in Fig. 1a. The calculated static pressure from this study aligns well with the experimental results from [6], as shown in Fig. 1a. The density contour for a pressure ratio of 10 (inlet to outlet) is shown in Fig. 1b, where flashing initiation is observed at the vena-contracta of the nozzle. The vapor volume fraction domain has been mirrored along the axis, allowing simultaneous visualization of both fields. Vapor formation in the divergent section accounts for only a small portion of the liquid due to the extreme density difference between liquid and vapor, supporting the choice not to include an additional momentum equation. A comparison for two different outlet pressures is shown in Fig. 1c. As back pressure decreases, the fluid experiences a greater pressure drop, leading to more vapor formation as the liquid reaches saturation. This increase in vapor generation at the nozzle exit occurs because the lower pressure allows more latent heat to be used for phase change, intensifying the flashing. Additionally, it was observed that the rate of phase change significantly increases with decreasing back pressure. **Conclusion**:



(a) (b) (c)

Figure 1: (a) Validation of the numerical model (b) Predicted density and vapour volume fraction (b) Comparison of flow field between two back pressure.

The HRM has been validated through multidimensional CFD simulations and applied to model the internal flashing behavior of subcooled liquid ammonia, utilizing the correlations proposed by Downar-Zapolski et al. The results demonstrate a reasonably high accuracy in predicting the pressure drop across the nozzle. As back pressure decreases, the increased pressure differential between the fluid and the surroundings accelerates the flashing process within the nozzle. This larger pressure drop causes the fluid to reach saturation pressure earlier, leading to a more rapid and intense phase change into vapor.

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