Validation of a Computational Fluid Dynamics Model of Axial Jet Mixing for Cryogenic Propellant Tank Pressure Control

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The Fluid Dynamics Branch at the NASA Marshall Space Flight Center is preparing to support flight programs through analysis of a variety of cryogenic fluid management (CFM) applications. Many vehicles being considered for future manned missions to the moon and beyond use chemical or nuclear thermal propulsion systems that rely on cryogenic propellants. Storing cryogenic propellants for later use is a challenge, though. Many areas of active CFM research, testing, and design involve propellant conditioning to ensure propellant remains a usable liquid for propulsion. Multiple technologies may be used to achieve adequate conditioning including the subject of this paper, a jet-based mixer. Mixing serves to homogenize fluid temperatures and decrease ullage pressure. Development and validation of a modeling methodology for jet-based mixing was conducted to prepare for in-line design work.

I. Introduction

Cryogenic propulsion systems have long been used for launch vehicles due to their high thrust, throttle ability, and high specific impulse, compared to other chemical systems. For these reasons, the propulsion systems are also being implemented in landers and ascent vehicles for celestial bodies beyond Earth, among other spacecraft. However, thermal conditioning of cryogenic propellants is still a challenge for long duration missions. The low vapor pressure of cryogenic propellants results in evaporation or boiling even for small heat leaks to the liquid making cryogenic fluid management (CFM) difficult. Systems may be developed that are robust to temperature and pressure changes caused by heat leaks, e.g., propellant tanks with high maximum operating pressures, technologies yielding active thermal conditioning, and systems with ample pressurant for conditioning. Development of a predictive capability of an aspect of active thermal control is the topic of this work.

Active thermal control has traditionally been conceptualized as a group of technologies working in concert to homogenize and subcool a cryogenic propellant while reducing and rejecting heat leaks. Using multiple technologies, a maximum amount of propellant is expected to remain a usable liquid. One of the considered technologies is a mixer that is designed to recirculate liquid in a propellant tank. Mixing homogenizes liquid temperatures precluding disparate temperature growth along liquid interfaces with structure or the ullage gas. As a result, heat entering the system is evenly distributed avoiding local evaporation or boiling that could subsequently pressurize the tank necessitating venting. Any venting is a loss of commodities and may represent a direct loss of performance as well. As vehicles are optimized for increased payload capacity and reliance upon in-situ resource utilization for long duration missions, mixers are likely to be leveraged for both ground and space-based use.

Cryogenic mixer technologies have been tested before. The most common mixers recirculate liquid propellant by pulling it through a pump and injecting it back into the tank. Jet-induced mixing for cryogenic tanks has primarily consisted of jets aimed along the symmetry axis. Test data for these axial jet mixers at various flow rates, tank scales, and fluid types exist including some subscale microgravity test data. A particular set of ground test data for a 1 m radius liquid hydrogen propellant tank tested at the NASA Glenn Research Center K-Site facility [1] was used to validate a modeling capability of axial jet mixing.

Computational fluid dynamics (CFD) simulation was used to model the jet mixing process using the Loci/STREAM code with a recently implemented sharp interface method of distinctly representing both fluid phases to reduce computational expense versus other two-phase approaches. In particular, a boundary condition was used to

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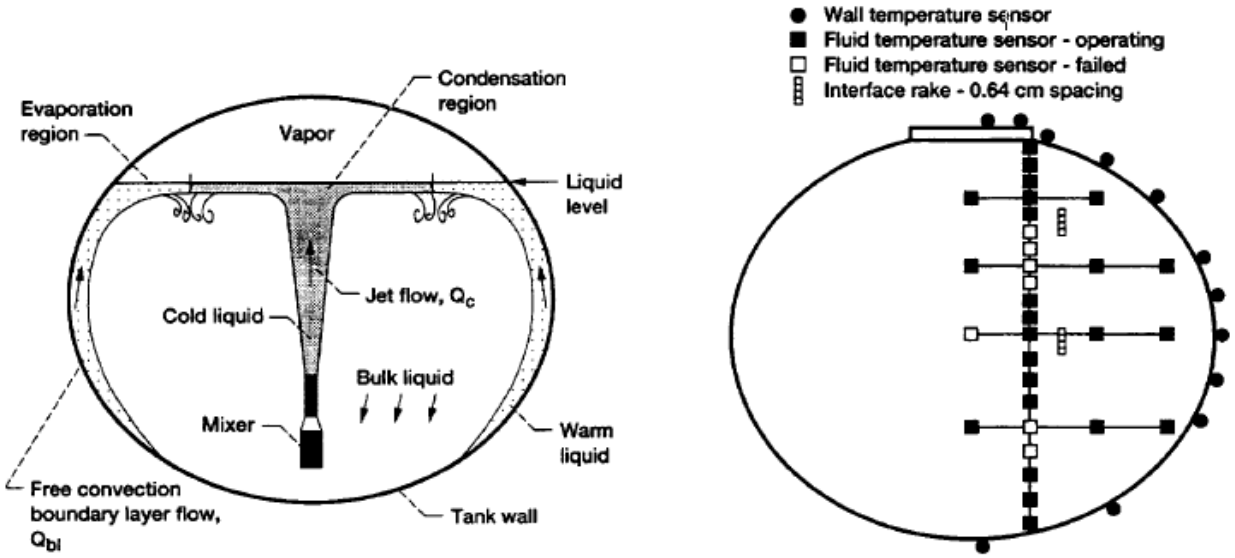
communicate between the gas and liquid phase domains along a static interface. Both heat and mass transfer occur across the interface while momentum for each phase is coupled to prevent interface normal velocity but allow parallel velocity, i.e., shear flow. This method of simulation is only necessarily applicable when the gas-liquid interface is unperturbed, but results can demonstrate model features needed in other more general simulation approaches like the volume of fluid approach.

The conducted CFD simulations demonstrate jet expansion and forced convection which reduces tank pressure through heat exchange and condensation at the interface. Both mixing characteristics and ullage pressure drop for different modeling methodologies were quantified through comparisons of transient temperatures and pressure within the tank. Demonstration of a predictive capability for such a mixer design enables rapid assessment and refinement of the technology for eventual infusion into future vehicles, supporting some of the most ambitious exploration and science missions humans have undertaken.

II. Test Description

Testing of the jet mixing process was conducted at the NASA Glenn Research Center K-Site facility [1]. The ground test was conducted within a vacuum chamber and thermal shroud to control the heat leak to the test article. The heat leak of 4.2 W/m^2 was quantified by measuring the steady boiloff rate using the procedure outline in references [2] and [3]. This heat leak was achieved by covering the tank in multilayer insulation (MLI).

The test article was a nearly ellipsoidal tank with a 1.2 major-to-minor axis ratio and a 2.2 m major diameter. The axial jet mixer from the Shuttle Centaur hydrogen tank was installed along the tank centerline in the test article. The inner diameter of the jet nozzle outlet was 0.0221 m and was located 0.51 m from the tank bottom. An illustration of the tank configuration and mixing process is shown in Fig. 1a. An array of temperature sensors and were installed as shown in Fig. 1b. A pressure sensor in direct communication with the ullage, and a capacitance probe used to measure the fill level were also installed.



(a) Mixing Dynamics Illustration [1] (b) Instrumentation Illustration [1]

Fig. 1 Test Article Configuration

Several operations preceded mixer testing to condition the liquid and vapor phases. The test article was initially filled with liquid hydrogen and continuously vented to a target pressure. This brought the hardware to a target liquid saturation temperature. Then, liquid was drained to just above a target fill level, and the vent was closed. This allowed the tank to pressurize due to heat leak into the system. During pressurization, the liquid becomes saturated with a warmer layer of liquid settling at the gas-liquid interface due to natural convection. The mixer was turned on once a target ullage pressure was reached, beginning the test. The cold jet expanded and mixed with the warmer layers near the interface dropping the pressure again. Testing ended once a steady ullage pressure was reached.

Two test cases with different jet mixer flow rates were used for validation purposes. Some of the characteristics of the tests are shown in Table 1. The initial measured temperatures in the liquid and ullage vapor near the interface as a function of axial location are shown in Fig. 2.

Table 1 Test Case Definitions

Test Case	Fill Level by Volume (% of Total)	Jet Flow Rate (m^3/hr)	Initial Ullage Pressure (MPa)
434	86.3%	3.47	0.1861
436	85.3%	1.82	0.1870

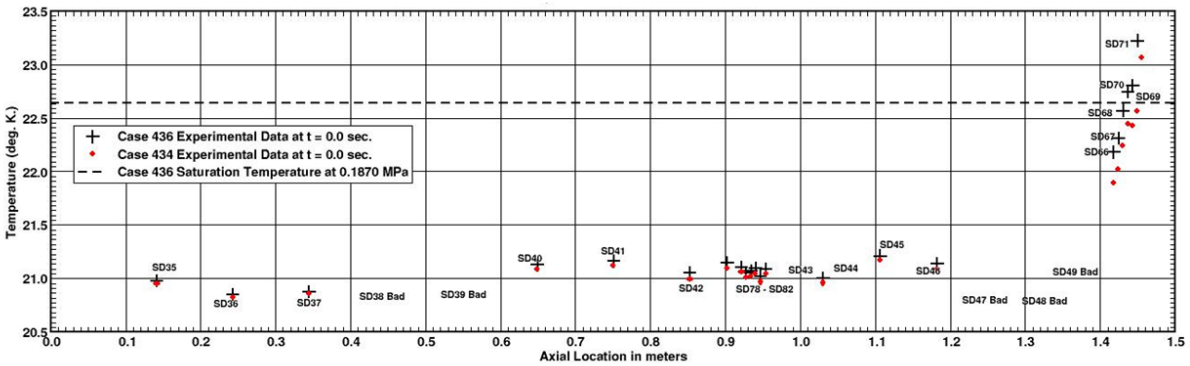


Fig. 2 Initial Experimental Temperature Distributions

III. CFD Methodology

A two-dimensional (2D) axisymmetric version of the tank test article and jet mixer were modeled. The full tank version of the model geometry is shown in Fig. 3. The simplified tank was bare except for the mixer, and the tank walls were used as boundary conditions to apply the estimated heat flux from the test. Conjugate heat transfer was not investigated but is expected to have a negligible effect on the mixing and depressurization process primarily due to the thermal conditioning operations performed prior to testing.

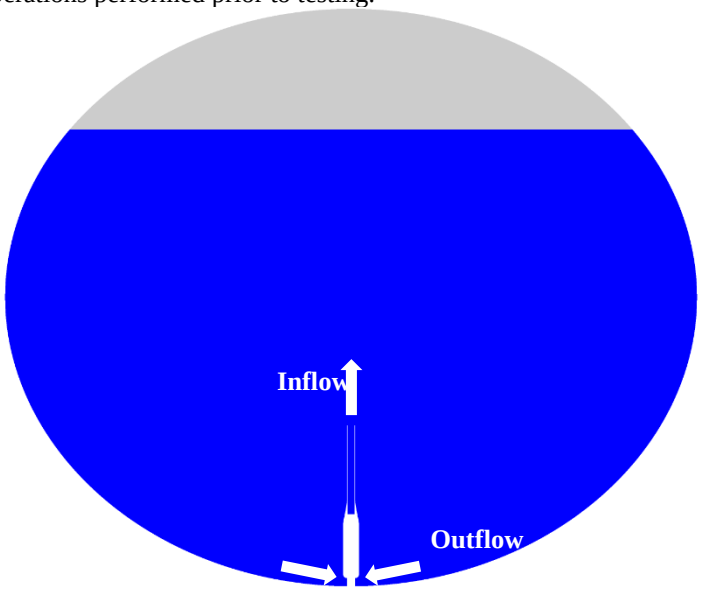


Fig. 3 Model Geometry with the Target Liquid Fill Level (blue)

The precise mixer geometry was not known except for the location and inner diameter of the jet exit. Other features of the mixer were chosen to reflect available information about the mixer including photos. Most of the mixer features are expected to have a negligible effect on results due to a lack of interaction with the flow field and thermal pre-

conditioning. One mixer feature that was unknown that may have an impact on jet spreading was the jet exit contour. A rounded lip was modeled but the true contour was not documented. The impact of this feature is expected to be small affecting the initial jet expansion rate coming into the tank. Sensitivity to this geometric feature was not investigated.

Multiple sensitivity studies were conducted to find the best method of simulating jet mixing. These sensitivities included the jet flow rate, jet average temperature, turbulence model, phase change model, spatial resolution, and temporal resolution. Results of each sensitivity study are shared in Section IV.

A. Computational Tools

Loci/STREAM, a pressure-based solver, was used in the preparation of these results. Loci/STREAM [4][5] is an all-speed CFD code for generalized grids in the rule-based programming framework called Loci [6]. The Loci framework allows the solver to integrate new multidisciplinary physics using a modular manner and automatic handling of massively parallel computing. The Loci/STREAM code has been applied and validated over a wide range of problems, including incompressible laminar flows to compressible turbulent flows with heat transfer. Loci/STREAM has been shown to also scale very well on significant problems [4][5]. Loci/STREAM is a pressure-based solver with SIMPLE, SIMPLEC, and PISO algorithms available for pressure-momentum coupling. Also available are various turbulence models that can be executed in Reynolds-Averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) mode. It has support for reacting flows and flamelet models for turbulent combustion. Loci/STREAM supports first and second-order discretization for inviscid fluxes as well as first and second-order temporal discretization. The code has been in use at NASA MSFC for large-scale simulations of low-speed flows, turbulent combustion, cavitation, and other problems.

The code employs multiple methodologies to represent distinct fluid phases and their shared interface. The volume of fluid (VoF) method distinctly represents a liquid and gaseous phase in the same simulation by tracking the volume of a particular fluid and the geometric liquid interface in each cell of the discretized computational domain. This simulation technique can capture gas-liquid interface deformation and breakup and has been applied extensively to propellant tank dynamics and cryogenic fluid management applications.

Recently, a method of distinctly representing two fluid phases with a common static interface was recently developed for Loci/STREAM that is referred to as a sharp interface model and is described below. By eliminating interface movement with the corresponding calculations and temporal resolution requirements for stability and accuracy, the sharp interface method is expected to reduce computational expense by more than an order of magnitude as compared to a VoF method for practical problems.

Sharp Interface Model

The Loci/STREAM implementation of a sharp interface method to model CFM applications is similar to previous studies [7],[8]. The model comprises a specialized interface boundary condition between the liquid and the gas phases that does not allow momentum transfer normal to the interface. The sharp interface boundary separates two regions of the mesh, each containing a pure gas or a pure liquid phase. The sharp interface model augments the existing VoF module to allow the use of the same liquid equation of state and liquid model files and minimize changes to the Loci/STREAM input file.

The momentum boundary conditions were derived by setting the tangential velocity and tangential components of the interfacial stress on the gas and liquid sides to be the same ($v_l\hat{t} = v_g\hat{t}, \tau_l\hat{t} = \tau_g\hat{t}$). The normal velocity at the interface is set to zero for both gas and liquid, and the interfacial phase change mass source term is applied at the gas side cell center of the interface.

The interface boundary is used to compute the mass and heat transfer between the two phases by obtaining the conditions across the interface to compute the correct evaporation or condensation rates and the corresponding heat-transfer augmentation on either side of the interface boundary. Two different methods for calculating the mass transfer are available:

Balance Method

This method is implemented as outlined in Kassemi *et al.* [8]. The temperature at the gas-side interface (T_i) is computed from the pressure ($P_{i,sat}$) in the gas cell using the Clausius-Clapeyron method in Equation 1 or using the Antoine equation in Equation 2:

$$\frac{P_{i,sat}}{P_{ref}} = e^{\left[\frac{L}{R}\left(\frac{1}{T_{ref}}-\frac{1}{T_i}\right)\right]} \tag{1}$$

where P_{ref} and T_{ref} are reference pressure and temperature, and L is the latent heat of phase change.

$$\log_{10} P_{i,sat} = A - \frac{B}{(C+T_i)} \quad (2)$$

Here, P is the pressure, T is temperature, and A, B, and C are component-specific constants.

The interface temperature is then used to calculate the mass flux based on the following equation,

$$\dot{m}L = Q_L - Q_G \quad (3)$$

where $\dot{m}$ is the mass flux, Q_L and Q_G are the heat fluxes from the liquid and gas side to the interface, respectively.

Kinetics - Balance Iterative Method

This method is also implemented as outlined in Kassemi *et al.* [8]. The interface mass transfer rate is first estimated based on a kinetics formulation developed by Schrage [9], widely used in phase change problems, as shown in the following equation:

$$\dot{m} = \alpha\left(\frac{M}{2\pi R}\right)^{1/2}\left(\frac{P_i}{T_i^{1/2}} - \frac{P_v}{T_v^{1/2}}\right) \quad (4)$$

where α is the accommodation coefficient, M is the molar mass, and R is the universal gas constant. P_i is the interfacial pressure, assumed to be the saturation pressure, and P_v is the vapor pressure in the cell closest to the interface. Equations 1 (or 2), 3, and 4 are solved for temperature and interfacial mass transfer rate, as shown in Equation 5 using a secant method. The temperature of the interface is allowed to deviate from the saturation temperature.

$$f(Ti) = \alpha\left(\frac{M}{2\pi R}\right)^{1/2}\left(\frac{P_r}{T_i^{1/2}} e^{\left[\frac{L}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T_i}\right)\right]} - \frac{P_v}{T_v^{1/2}}\right) - \frac{1}{L}\left[\frac{k_g T_v}{\Delta_g} + \frac{k_l T_l}{\Delta_l} - T_i\left(\frac{k_g}{\Delta_g} + \frac{k_l}{\Delta_l}\right)\right] \quad (5)$$

An alternate form of Equation 5 is used in this study, where the interface mass transfer rate of Schrage is simplified to the Hertz Knudsen form which assumes the interface and vapor temperature are equal:

$$\dot{m} = \alpha\left(\frac{M}{2\pi RT}\right)^{1/2}(P_i - P_v) \quad (6)$$

Equation 6 is substituted into Equation 5 with other all solution details remaining the same.

The treatment of turbulence at the liquid-gas interface is an area of ongoing research, with multiple investigators [10], [11] suggesting that damping of the turbulence on the interface is necessary, although questions remain on how to apply that damping and what level of damping is appropriate. For the sharp interface method, a simpler approach has been taken where the interface on the gas and liquid side can be treated as wall-like (e.g., infinite damping) or as a zero gradient (no damping). In this study, it was found that applying a wall treatment at the interface produced the best results, and all presented analysis uses this approach. It remains future work to determine the appropriate treatment for other CFM problems, or to develop a higher fidelity model of interface turbulence.

B. Computational Domain and Mesh

Multiple views of the nominal resolution computational mesh are presented in Fig. 4. A 2D surface mesh of mixed cell type was extruded through a 1° wedge forming a single layer of volume cells. The mesh consisted of about 62,000 volume cells. The boundary fitted mesh included refined normal wall spacing and stretching to the mesh interior. The gas and liquid domains were made separately. Each domain connected to the gas-liquid interface which was node matched on either side. The domains were combined into a single file, but volume cells remained linked to the gas-liquid interface boundary. This allowed boundary condition specification on the interface. The interface was refined in the same manner as the solid walls to capture velocity and temperature gradients there.

The meshes simulated to investigate spatial resolution sensitivity are shown in Fig. 5. Normal spacing from walls and the gas-liquid interface was 0.01 mm for every mesh to yield a y+ of less than 1 throughout the domain. Peak velocity was within the mixer, so spacing could be increased elsewhere in the domain. Stretch rates were maintained for each mesh. The maximum edge length was 50 mm, 10 mm, and 5 mm for the coarse, nominal, and fine meshes, respectively. Similarly, the total volume cell count was 36,500, 62,500, and 119,700.

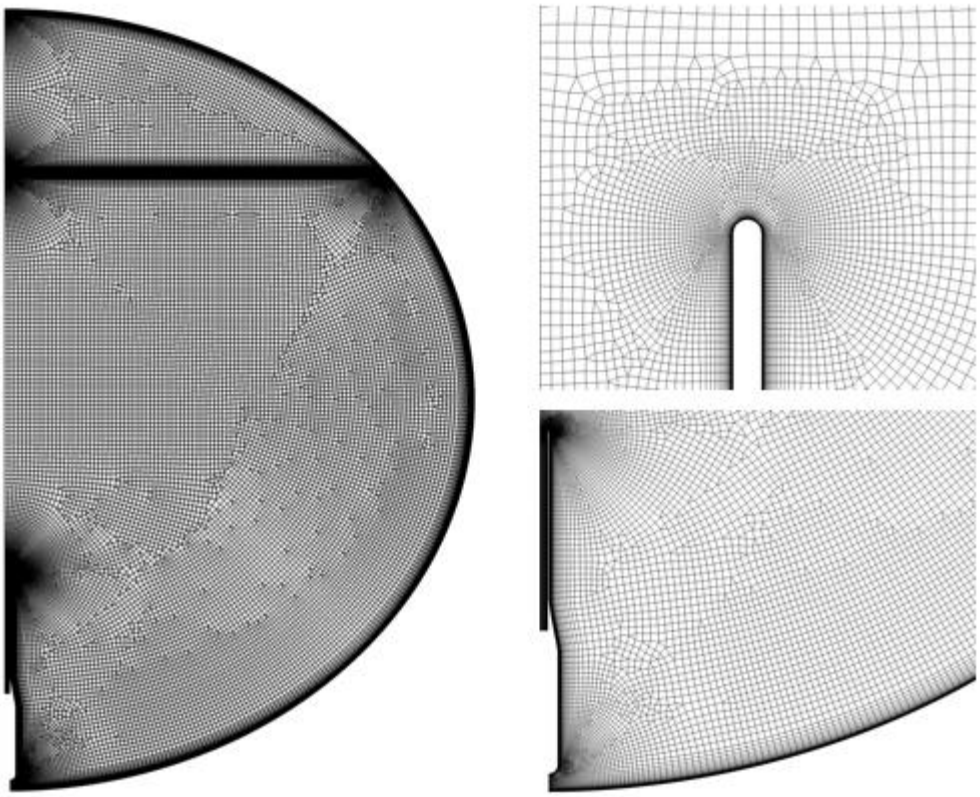
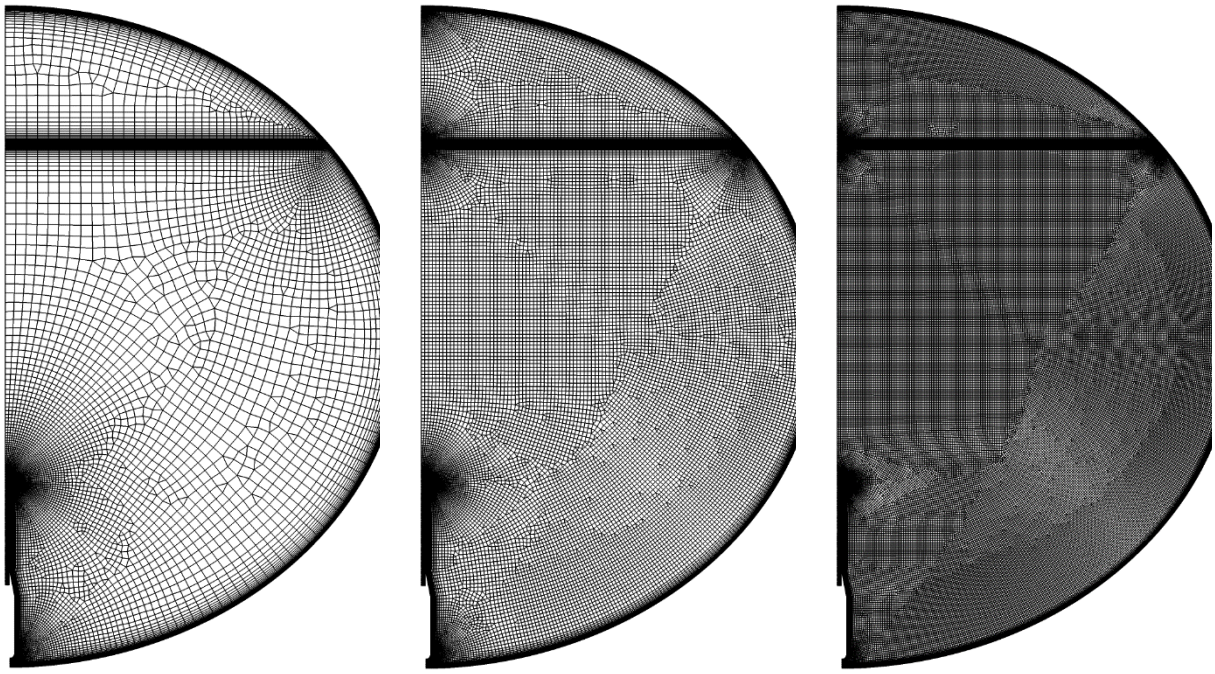


Fig. 4 Computational Mesh with Detailed Mixer Views



(a) Coarse Resolution Mesh (a) Nominal Resolution Mesh (a) Fine Resolution Mesh

Fig. 5 Comparison of the Analyzed Computational Meshes

C. Simulation Inputs

Equations were solved with a 2nd order accuracy scheme in space and a 1st order accuracy scheme in time. A time step of 0.1 s was used for nominal simulations. Liquid hydrogen (LH2) and gaseous hydrogen (GH2) were modeled in their respective domains. Table 2 contains the fixed fluid properties used for LH2 at the temperature and pressure shown [12]. The Boussinesq approximation was used to model buoyancy in the liquid phase only. The compressible gas phase was modeled as an ideal gas with a transport model calibrated to data [12]. The initial temperature field and ullage pressure measured for each test, shown in Fig. 2 and Table 1 respectively, were imposed as initial conditions onto a quiescent flow field.

The kinetics-based method of calculating local phase change across the gas-liquid interface described above was used throughout. The phase change model includes a coefficient which can act as a phase change limiter if set too low. The dimensionless coefficient that can vary from 0 to 1 was nominally set to 0.001, but a sensitivity study was also conducted. The Antoine equation with coefficients taken from data [12] was used to calculate the saturation conditions throughout the simulation.

The improved 2003 Shear Stress Transport model (SST) [13] was nominally used for the mixing simulations. Laminar equations and various other turbulence models were investigated, but those results are only briefly discussed in this paper. Initial turbulence quantities for k and μ_t in the computational domain were set low but non-zero values, at 1e-8 m^2/s^2 and 1e-10 Pa-s, respectively.

All solid walls were modeled with a no-slip boundary condition. A 4.2 W/m^2 heat flux was applied to tank walls while all others were assumed adiabatic. A fixed velocity was held on the inlet boundary forming the mixer jet, with low turbulence intensity specified. The initial temperature at the outlet at the bottom of the tank was nominally used as the inlet temperature. Inlet velocity was set for each simulation to yield the tested volumetric flow rate while the same volumetric flow rate was explicitly specified at the outlet. The gas-liquid interface was modeled as previously described with the interface turbulence nominally using the wall treatment in both fluid domains. All other boundaries were modeled with a symmetry boundary condition.

Table 2 Modeled Liquid Properties

Fluid Property	LOX
Temperature (K)	20.94
Static Pressure (MPa)	0.184674
Density (kg/m^3)	70.2803
Dynamic Viscosity (Pa*s)	1.29456e-05
Thermal Conductivity (W/m*K)	0.103933
Latent Heat (J/kg)	434699
Cp (J/kg*K)	10065.1
Cv (J/kg*K)	5698.50

IV. Axial Jet Mixing Validation

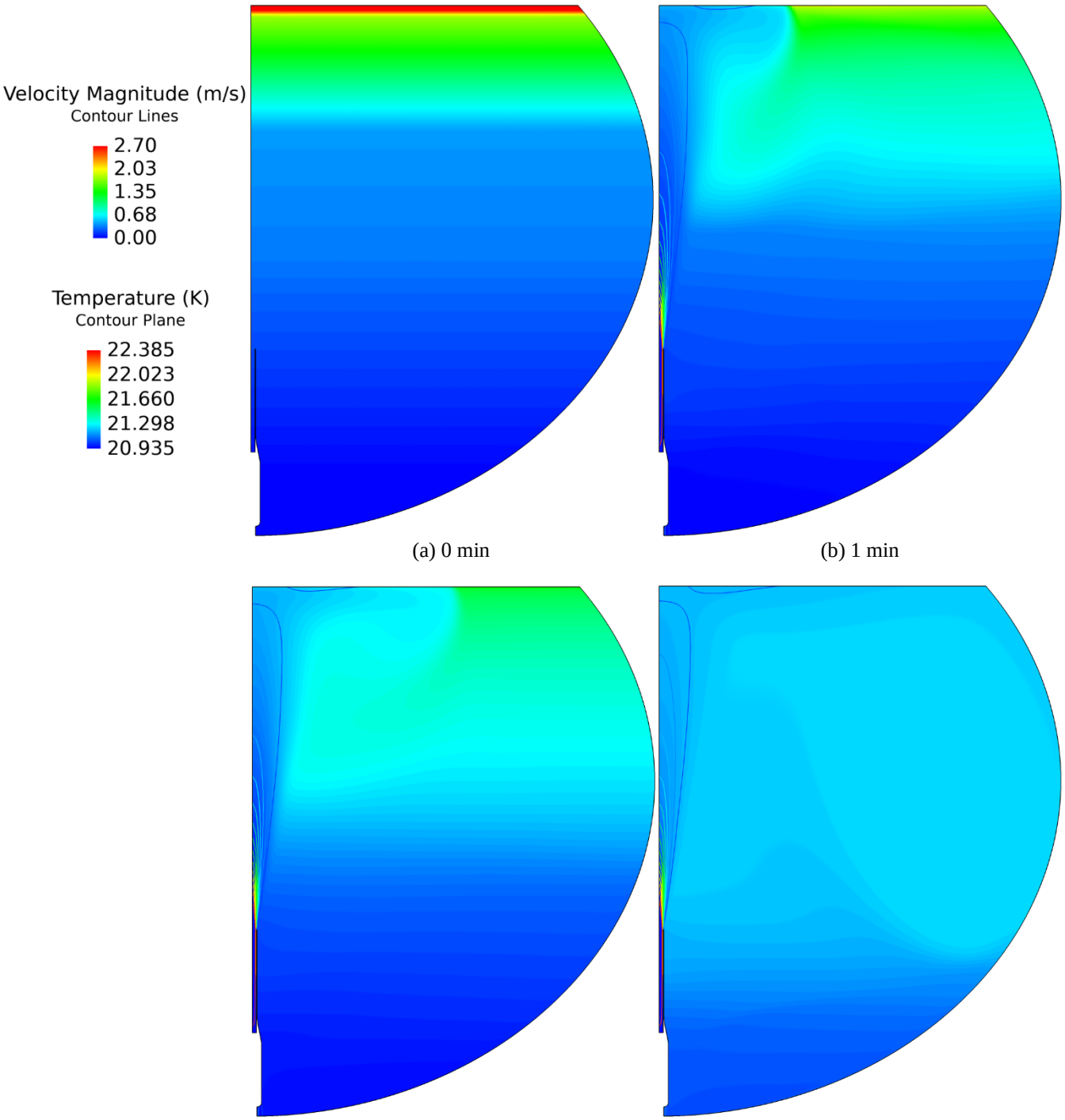
Results of jet mixing simulations are compared to corresponding test data in this section. Several sensitivity studies were conducted to ensure model convergence and identify modeling requirements for any future related in-line work.

The analysis results shown were generated from an initially quiescent flow field. Self-pressurization prior to mixing was also simulated but found to have negligible effect on the pressure drop rate as forced convection overwhelmed natural convection. It is expected that properly representing natural convection during the mixing process is needed when simulating sufficiently low mixing rates such that either a jet does not penetrate to the liquid surface or there is comparable energy in the forced and natural convection flow fields.

A two equation $k-\omega$ SST turbulence model was used to generate all the analysis results shown. Laminar model equations were used separate from the results shown here that demonstrated negligible jet spreading and mixing. The pressure transient and final pressure consequently compared poorly with the data. Similar results, but with more mixing, were observed when running a Detached Eddy Simulation (DES). Turbulence production was predominately at the mixer exit where jet expansion begins. The lack of turbulent production further downstream halted jet expansion and mixing. Turbulence treatment on the gas-liquid interface was also investigated. Rather than a wall treatment where turbulent kinetic energy was driven to 0 for the nominal simulations, turbulence was extrapolated to the gas-liquid interface with zero gradient. The result was significant turbulent mixing at the interface that destroyed the thermally stratified liquid layer there. Corresponding comparisons with pressure drop measurements were poor. Higher fidelity

methodologies will be explored in the future, but consistent treatment at gas-liquid interfaces must be used for a wide parameter space if reliable predictions are to be made for flight programs.

A transient of the liquid temperature field for the nominal simulation of the high flow rate test, Case 434, is shown in Fig. 6. The imposed initial temperature stratification is disrupted by the axial jet impinging on the liquid surface. Mixing at the surface continues eventually leading to a nearly isothermal liquid by the end of the simulation. These results are typical of every simulation conducted for this analysis.



(a) 0 min (b) 1 min

(c) 2 min (d) 8 min

Fig. 6 Nominal Liquid Temperature Field Transient of High Jet Flow Rate Simulation

A. Jet Flow Rate Sensitivity

Pressure transients for both considered tests are shown in Fig. 7 along with nominal simulation results. Mixing at a lower flow rate consequently reduced the pressure drop rate, as expected. The analysis results match the pressure drop trend, magnitude, and timing well but with notable deviation. Of particular note, the final pressure for the low flow rate case, 436, differs between experimental measurement and analysis result. The analysis predicted a final gas-liquid interface temperature below that of the experiment resulting in the lower pressure, although the temperature difference is less the 0.1 K.

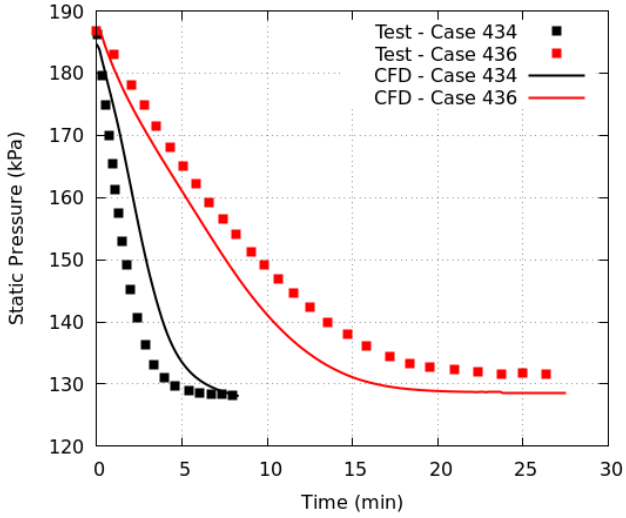


Fig. 7 Pressure Transient Comparison - Jet Flow Rate Sensitivity

B. Jet Temperature Dependence

Jet temperature was fixed for nominal simulations to the initial temperature near the mixer intake. A subsequent simulation was conducted where jet temperature was updated throughout the simulation to the mixer intake temperature. Effects of this change were minor as can be observed in Fig. 8. It is apparent that mixing did not significantly alter the liquid temperature at the bottom of the tank for the simulated conditions. It is possible that proper modeling of jet temperature is more impactful for different conditions, like higher mixing rates or longer duration mixing at lower flow rates, so the capability will be used in future support of this application.

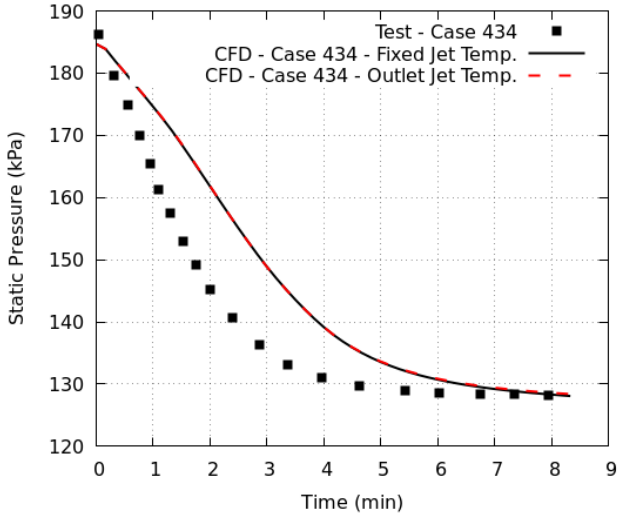


Fig. 8: Pressure Transient Comparison - Jet Temperature Sensitivity

C. Phase Change Model Sensitivity

The phase change model contains a coefficient which acts as a limiter on mass transferred in a time step. A value of 0 would inhibit mass transfer while a value of 1 would allow for a maximum amount of mass transfer. Numerical stability issues can arise from using too high of a phase change coefficient, so values between 0 and 1 are commonly used. Fig. 9 shows convergence of the phase change coefficient (alpha, α, from Eq. 6) by at least the nominal phase change coefficient value, 0.001, given the nominal mesh resolution and time step. Future simulations of jet mixing will target relaxing spatial resolution of boundaries necessitating additional phase change coefficient sensitivity studies.

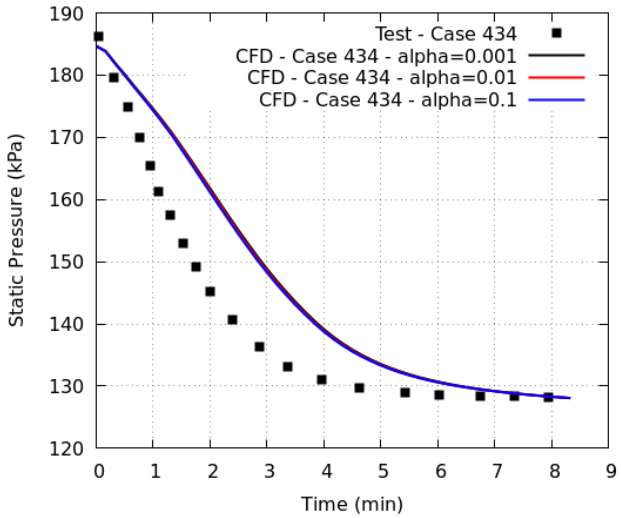


Fig. 9 Pressure Transient Comparison - Phase Change Coefficient Sensitivity

D. Spatial Resolution Sensitivity

Sensitivity of the pressure transient to nominal cell edge length is shown in Fig. 10. Only a minor difference exists between the coarse mesh and more refined meshes which is likely due to capture of jet expansion or turning at the gas-liquid interface, as the normal spacing at the interface is constant among these meshes. Convergence was clearly reached for nominal cell edge lengths. Additional assessment of other mesh features like boundary layer spacing will be studied in the future since it is driving mesh size and will have a profound impact on support of any related in-line work.

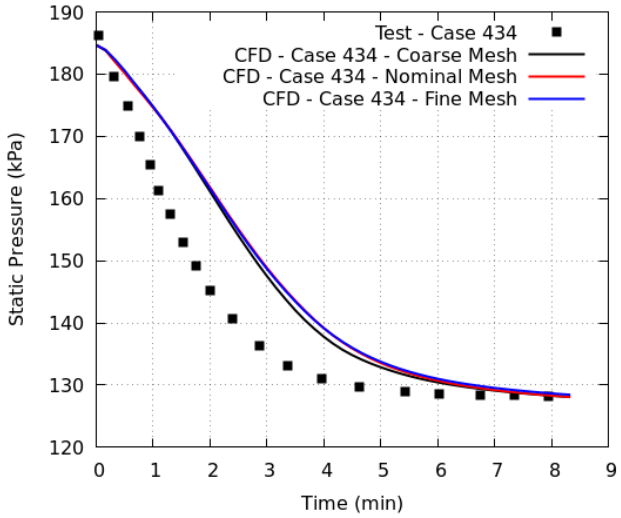


Fig. 10 Pressure Transient Comparison – Mesh Resolution Sensitivity

E. Temporal Resolution Sensitivity

Results of the time step sensitivity study are shown in Fig. 11. Little variation was observed up to the nominal time step of 0.1 s. This result is unsurprising since RANS models smooth spatial and temporal fluctuations relaxing resolution requirements compared to other methods that more explicitly resolve turbulence. Additionally, the phase change model was already shown to be converged at the nominal time step. The time step achievable in this study is enabling of future in-line work, where long duration simulations can be computationally prohibitive for practical applications and offers room for additional model complexity that is sure to be added with flight-like designs of tanks and mixers.

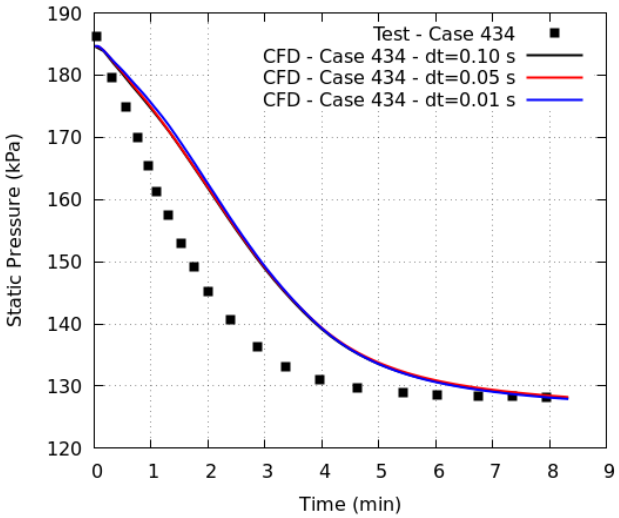


Fig. 11 Pressure Transient Comparison - Time Step Sensitivity

V. Conclusion

CFD simulations of axial jet mixing were conducted to develop and validate a modeling methodology in preparation for similar in-line design work. The nominal modeling methodology resulted in reasonable representation of the pressure drop trend, magnitude, and timing. There was little variation in the RANS model solutions for axial jet mixing across the multiple sensitivity parameters and spaces investigated. As such, a capability exists, at least within the analyzed parameter space, to make predictions of mixing flow rate and duration demands that inform a concept of operations and power budget.

Future study will include expanded sensitivity ranges to identify the limits of each modeling parameter. Turbulence modeling features like imposed damping on the gas-liquid interface will be implemented. Finally, features of the sharp interface method used within this study will be incorporated into the Loci/STREAM VoF method and validated. Having a capable VoF method for prediction of jet-based mixing will enable simulation of axial jet flow rates that significantly perturb the liquid interface, a scenario that may be preferential or unavoidable if in-space or reduced gravity.

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