CFD Modeling of the Multipurpose Hydrogen Test Bed (MHTB) Self-Pressurization and Spray Bar Mixing Experiments in Normal Gravity: Effect of Accommodation Coefficient on the Tank Pressure

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Overview

- Problem Description
- Computational Model Description
- Results
    - *Self-Pressurization of MHTB Tank*
    - *Cooling of MHTB Tank using Spray*
- Conclusions
- Future Work

Introduction

- Affordable and reliable cryogenic storage for use in propellant systems is essential to meeting NASA's future exploration goals.
- Cryogen mass loss occurs when heat leaks into the tank from the surroundings.
- Heat is carried to the interface by natural convection currents → evaporation → vapor compression→ rise in tank pressure.
- Pressure control is necessary to keep tank pressure within design limits (venting or active control)
- Predicting self-pressurization and depressurization rates is important for designing future tanks and pressure control systems.

Problem Description: MHTB Self-Pressurization and Spray Bar TVS Ground-Based Experiment

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Tank Internal volume 37.5 m3

Cylindrical midsection with:

height = 3.05 m

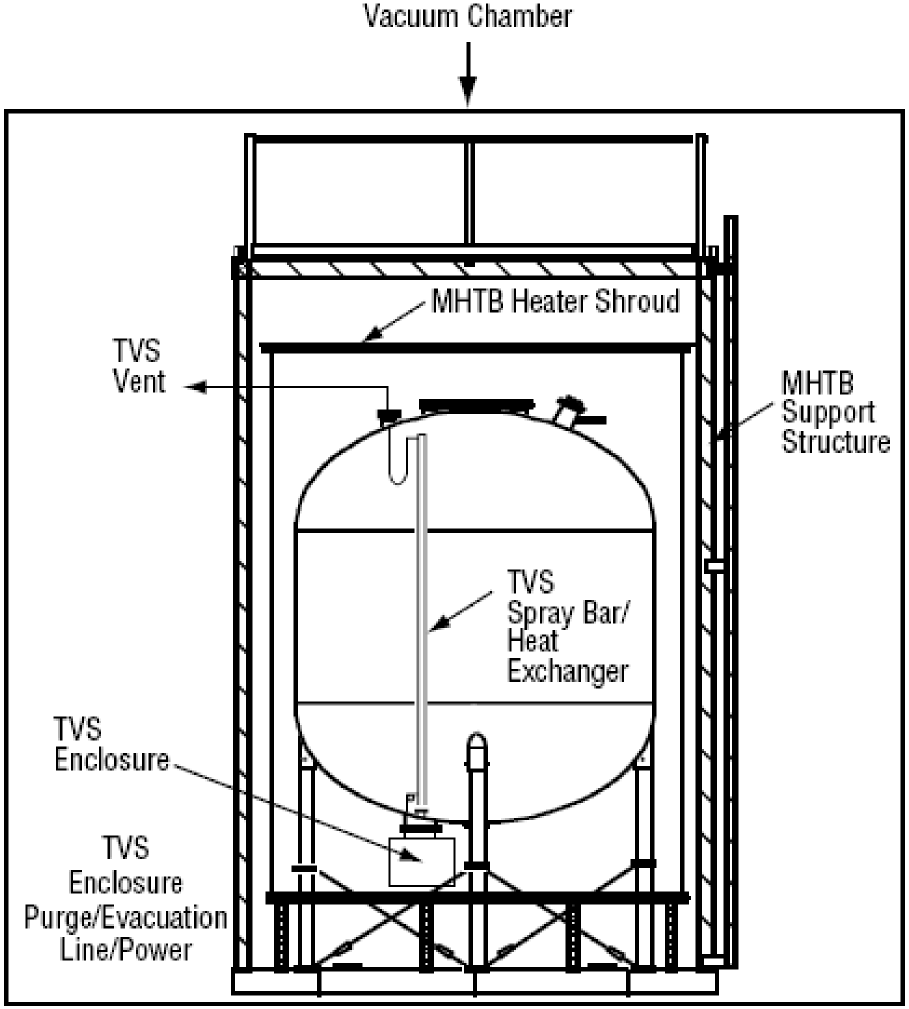
diameter = 3.05 m

2:1 elliptical end caps

Tank is enclosed in a vacuum shroud

4 spray bar tubes attached to center tube heat exchanger

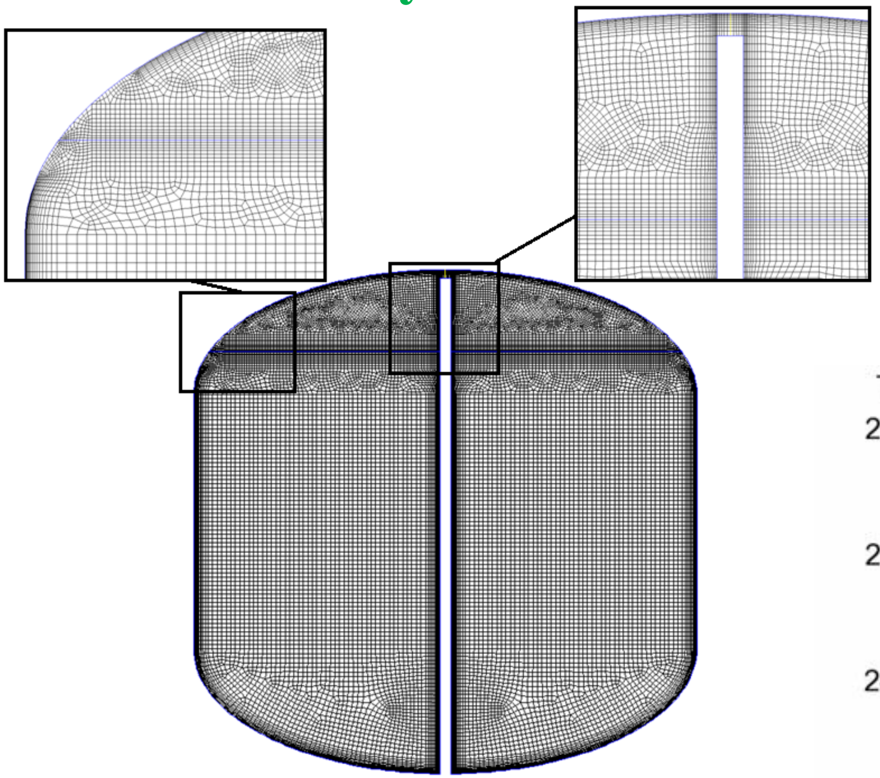
NASA TM-212926, 2003



Goal of this work is to simulate first self-pressurization and then cooling of the tank via spraying cold liquid in to the vapor using ANSYS Fluent Lagrangian Spray model combined with in-house developed UDFs

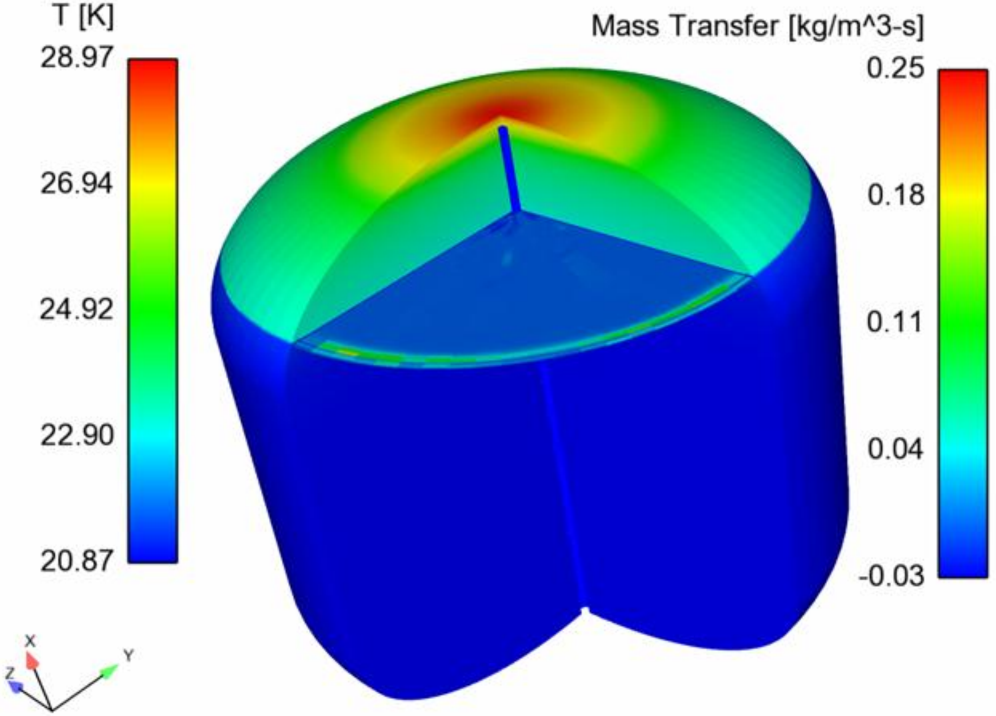
Problem Description: Modeling Approach

2D axisymmetric



Before starting spray run, 2D-axi results interpolated to 3D grid and self-pressurization continued for a short time to ensure no problems

3D 90° sector



Self-pressurization simulation performed on 2D-axisymmetric grid.
Spray Bar Mixing simulation will use 3D 90° sector grid.
Spray-Bar/Heat Exchanger assembly is approximated as lying along centerline

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Computational Model Description: Equations Solved

Continuity: $$\frac{\partial \rho}{\partial t} + \nabla(\rho \vec{v}) = 0$$

Momentum: $$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla(\rho \vec{v}\vec{v}) = -\nabla p + \nabla\left[\mu_{eff}\left(\nabla \vec{v} + \nabla v^T\right)\right] + \rho \vec{g} + \vec{F}_{vol}$$

Energy: $$\frac{\partial}{\partial t}(\rho E) + \nabla(\vec{v}(\rho E + p)) = \nabla\left(k_{eff} \nabla T\right) + S_h$$

Volume of Fluid (VOF) model:

Energy and Temperature are defined as mass average scalars: $$E = \frac{\sum_{q=1}^{2} \alpha_q \rho_q E_q}{\sum_{q=1}^{2} \alpha_q \rho_q}$$

Properties: $$\rho = \sum_{q=1}^{2} \alpha_q \rho_q, \quad \mu_{eff} = \sum_{q=1}^{2} \alpha_q \mu_{eff\ q}, \quad k_{eff} = \sum_{q=1}^{2} \alpha_q k_{eff\ q}$$

Continuity of Volume Fraction of the *q*-th phase: $$\frac{1}{\rho_q}\left[\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right) + \nabla \cdot \left(\alpha_q \rho_q \vec{v}_q\right) = S_{\alpha_q}\right]$$

Continuum Surface Force (Brackbill et al.): $$F_{vol} = \sum_{\text{pairs } ij,\ i<j} \sigma_{ij} \frac{\alpha_i \rho_i h_j \nabla \alpha_j + \alpha_j \rho_j h_i \nabla \alpha_i}{\frac{1}{2}\left(\rho_i + \rho_j\right)}$$

where $h_i = \nabla \cdot \hat{n}$

Interfacial mass transfer per unit volume: $$S_{\alpha_q} = \dot{\mathbf{m}}_i \cdot \mathbf{A}_{i,}\left[\frac{kg}{m^3 \cdot \sec}\right]$$

$\mathbf{A}_i = \left|\nabla \alpha\right|$, is an interfacial area density in 1/m, $\dot{\mathbf{m}}_i$ is a mass flux vector in kg/(m^2·sec).

where α is a volume fraction of the primary phase

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Computational Model Description: Equations Solved

Schrage's Relation :

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

where σ – accommodation coefficient

M – molar mass of hydrogen

R – universal gas constant (8.314472 $J/mol\,K$)

P_i and P_v – interfacial and vapor pressures, Pa

T_i and T_v – interfacial and vapor temperatures, K (assumed that $T_i = T_v \simeq T_{sat}$ at the interface)

Particle Energy Equation:

$$m_p c_{p_p} \frac{dT_p}{dt} = h \cdot A_p\left(T_\infty - T_p\right) - L\dot{m}_p$$

UDFs used:

VOF (DEFINE_MASS_TRANSFER)

- Calculate mass transfer using Schrage relation and supply it to Fluent for phase interaction at the interface

Lagrangian spray (DEFINE_DPM_SCALAR_UPDATE, DEFINE_SOURCE)

- Perform particle tracking in the vapor, remove particles from the vapor domain when they reach the interface and add their contributions to the liquid through source terms.
- Define sources for the spray bar liquid jets.
- Model heat and mass transfer between particles (droplets) and vapor

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Computational Model Description: Numerical Methods

NASA

- Simulations performed using ANSYS Fluent version 16
- **2D-Axisymmetric** formulation for self-pressurization; **3D 90° sector** for Spray cooling study
- Compressible ideal gas
- Laminar or k-ω SST turbulence model of Menter et. al
- Temperature dependent properties for vapor and liquid viscosity and thermal conductivity; vapor specific heat
- Interfacial mass transfer and mass transfer between droplets and continuous phase (vapor) is modeled based on Schrage's relation via user's subroutine
- Surface tension effects via Continuum Surface Force method of Brackbill et al.
- Contact angle for hydrogen 0°

- Second Order Upwind scheme was used for discretization of the Turbulence, Energy and Momentum equations (cell values)
- PISO scheme was used for the Pressure-Velocity coupling (cell values)
- Least Squares Cell Based scheme was used for the gradient calculations (face values)
- Body Force Weighted scheme was used for the Pressure interpolation (face values)
- Point Implicit (Gauss-Seidel) linear equation solver with Algebraic Multi-Grid (AMG) method was used for solving linearized systems of equations
- Bounded Second Order Implicit temporal discretization was used with implicit VOF model; First Order Implicit scheme was used with explicit VOF model

Computational Model Description: Grid

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3D 90° sector (184400 hex cells)

First row: 0.0094 m
Growth Factor: 1.05
Number of Rows: 17

Number of Intervals
on the Vapor Side: 136
Average Interval size: 0.02 m

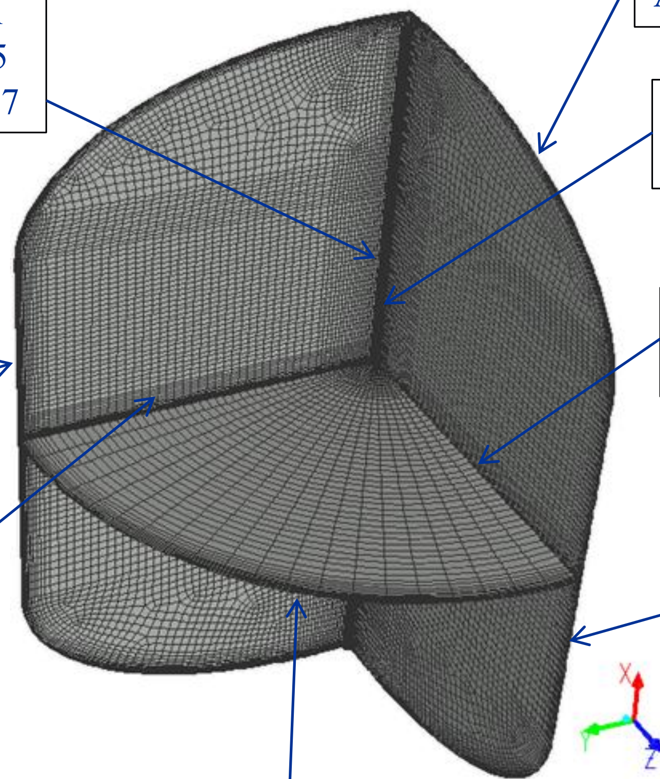
Number of Intervals: 151
Average Interval size: 0.025 m

First row: 0.002 m
Growth Factor: 1.2
Number of Rows: 14

Number of Intervals: 64
Interval size: 0.02 m

First row: 0.002 m
Growth Factor: 1.2
Number of Rows: 10

Number of Intervals
on the Liquid Side: 97
Average Interval size: 0.03 m

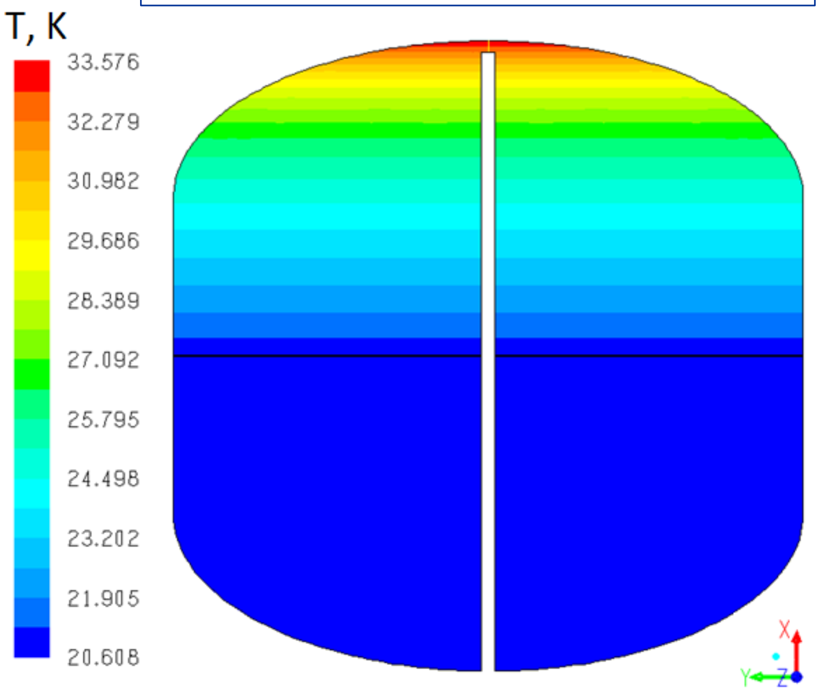


Number of Intervals: 20
Interval size: 0.12 m

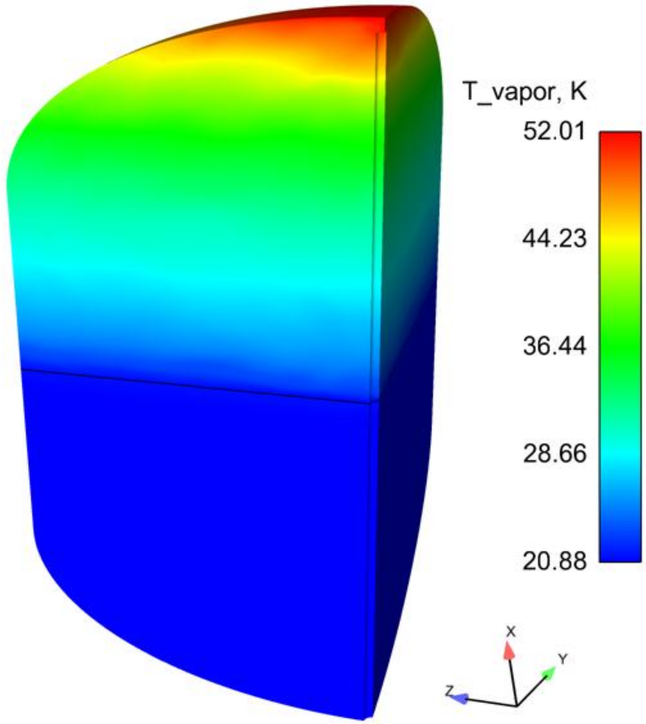
On all tank walls $y^+ < 5$

Computational Model Description: Initial Conditions

Beginning of Self-Pressurization



Beginning of Spray



Self-Pressurization

- T field from experimental data
- Velocity = 0.0 m/s
- Turbulent Kinetic Energy (in a turbulent run) = 1.0e-06 m^2/s^2
- Specific Dissipation Rate = 100 1/s
- Interface initialized at 50% or 90% liquid fill level
- 2D axisymmetric

Spray

- T, V, vof fields from the end of self-press simulation interpolated on to 3D 90 degree sector mesh

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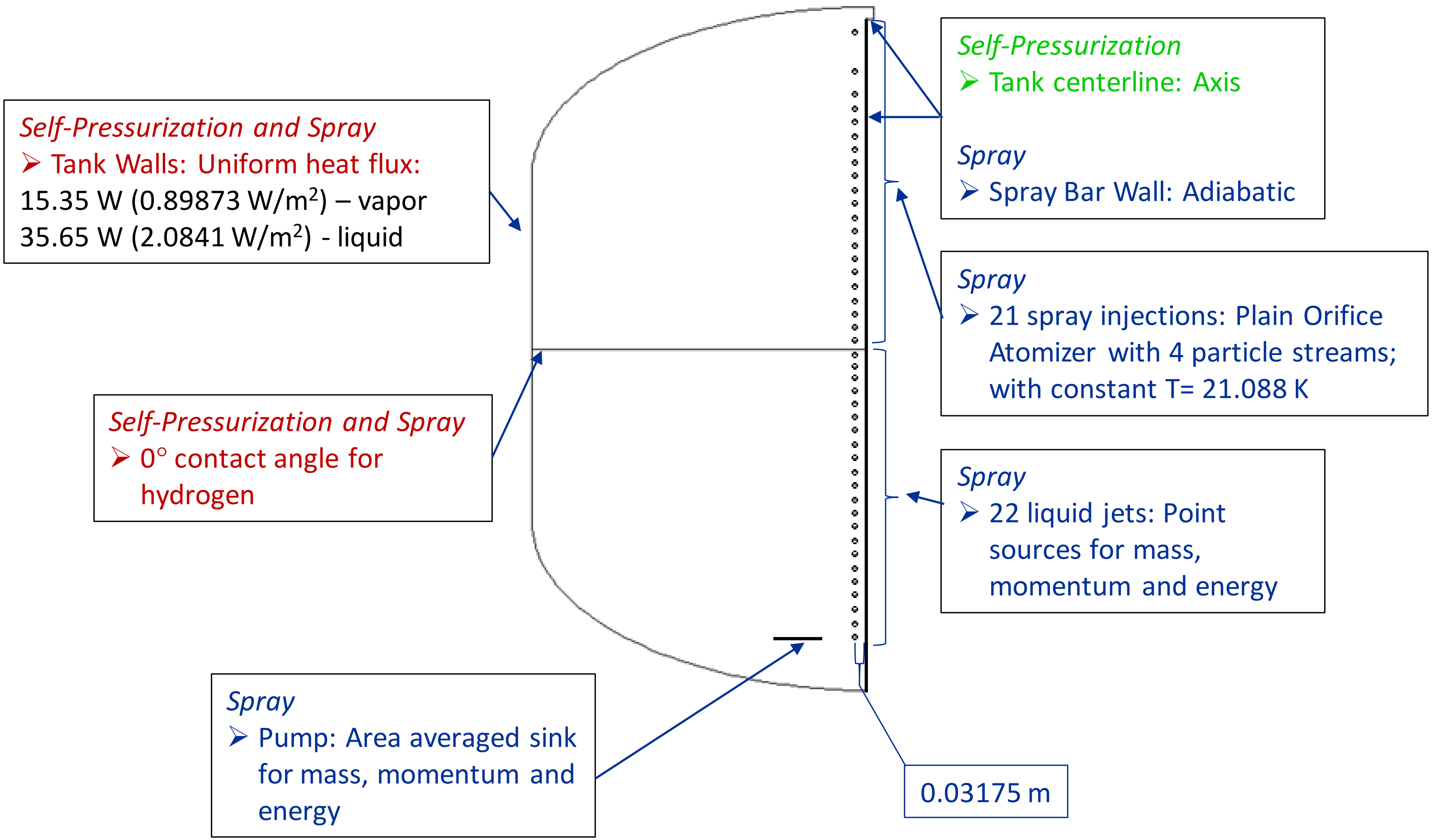
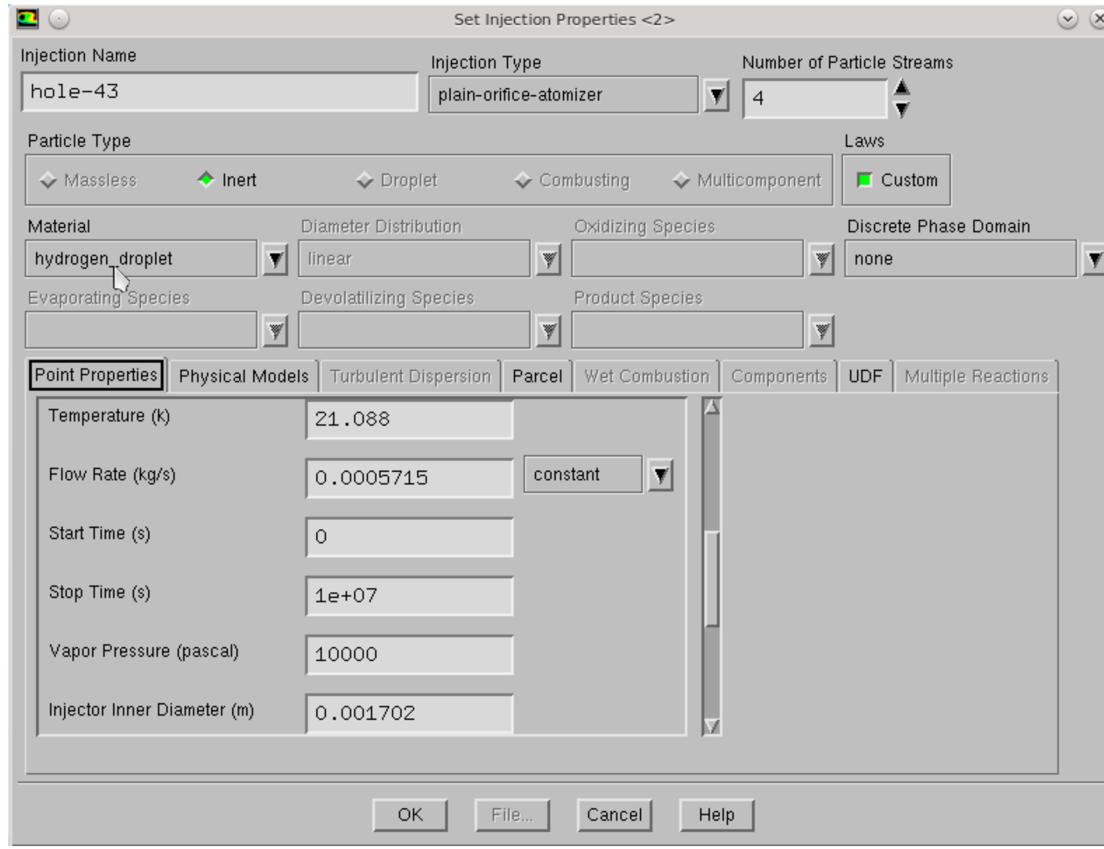
Computational Model Description: Boundary Conditions



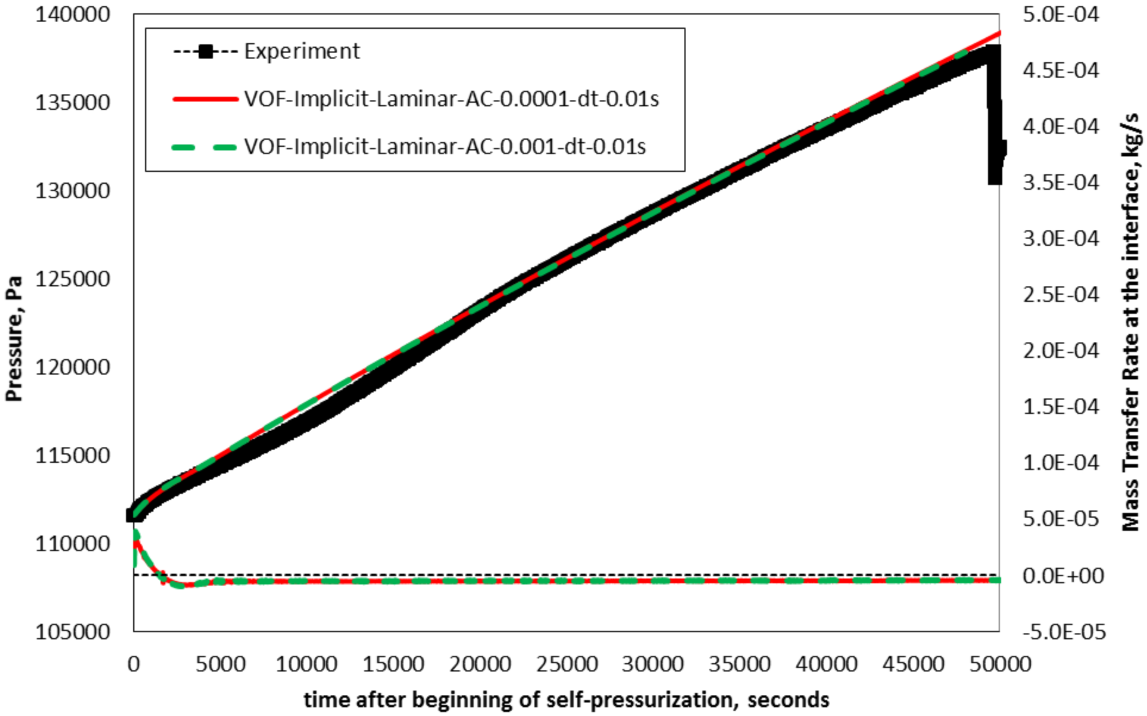
Computational Model Description: Injection Setup

- Injection type: **plain-orifice atomizer** with 4 particle streams per injection
- **Inert particle** (coupling with continuous phase for mass transfer done in the UDF)
- **Standard parcel release method** (releases one parcel per injection stream, calculates number of particles based on the mass flow rate of the particle stream)
- Injection material is **liquid hydrogen** with **constant properties** at T=21.088K
- **Two-way coupling** with continuous phase; unsteady particle tracking with flow time step
- Particle **breakup** model
- **Spherical** drag law model
- **Variable flow rate** based on experimental data
- Injector inner diameter = 0.001702 m
- Orifice length = 0.000711 m
- Turbulent dispersion of particles: **Discrete Random Walk model**

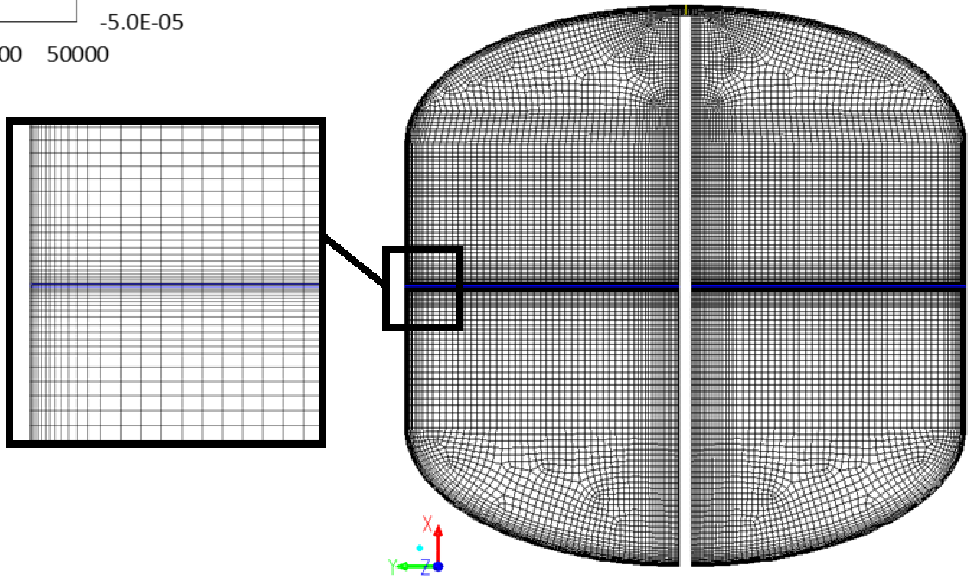


CFD Results:
MHTB Tank Self-Pressurization

CFD Results: MHTB Tank Self-Pressurization - Accommodation Coefficient Effect

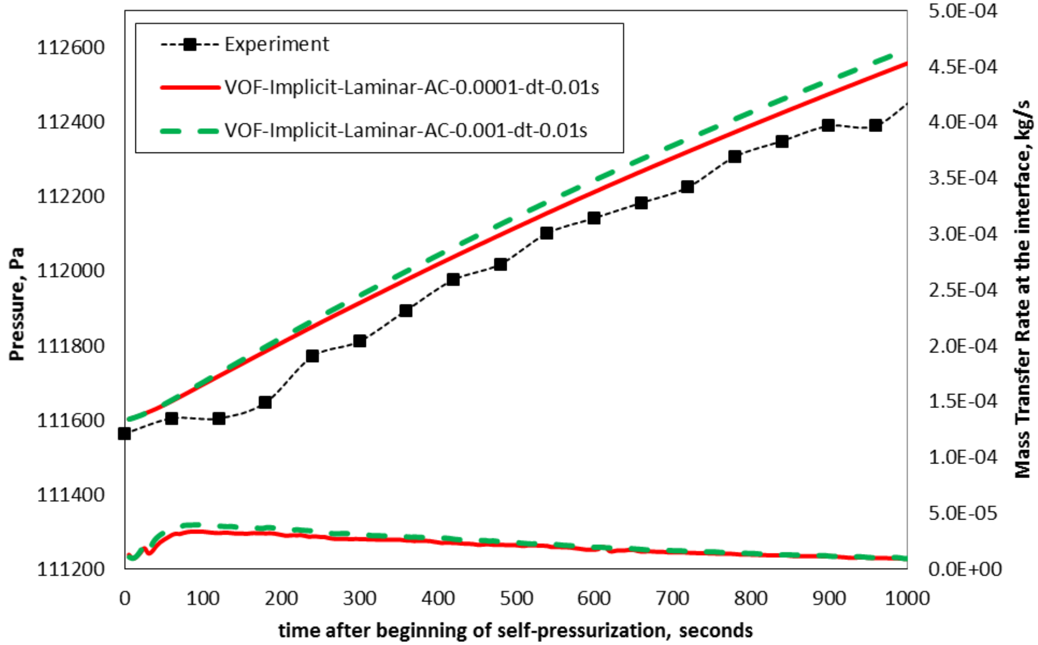


Medium Grid: 9,246 cells

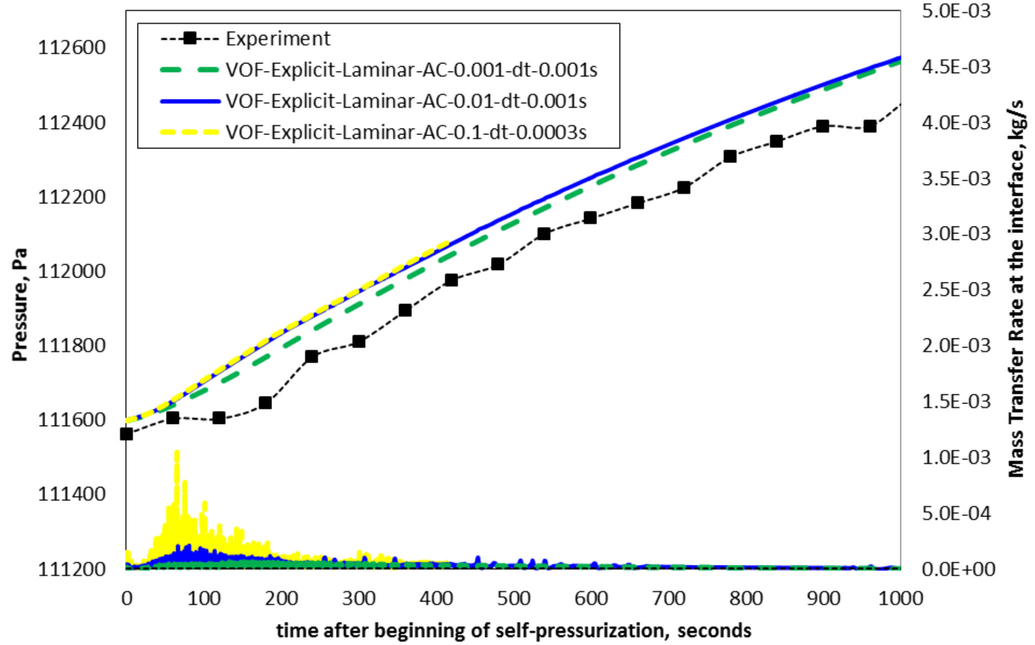


CFD Results: MHTB Tank Self-Pressurization - Accommodation Coefficient Effect

Implicit VOF

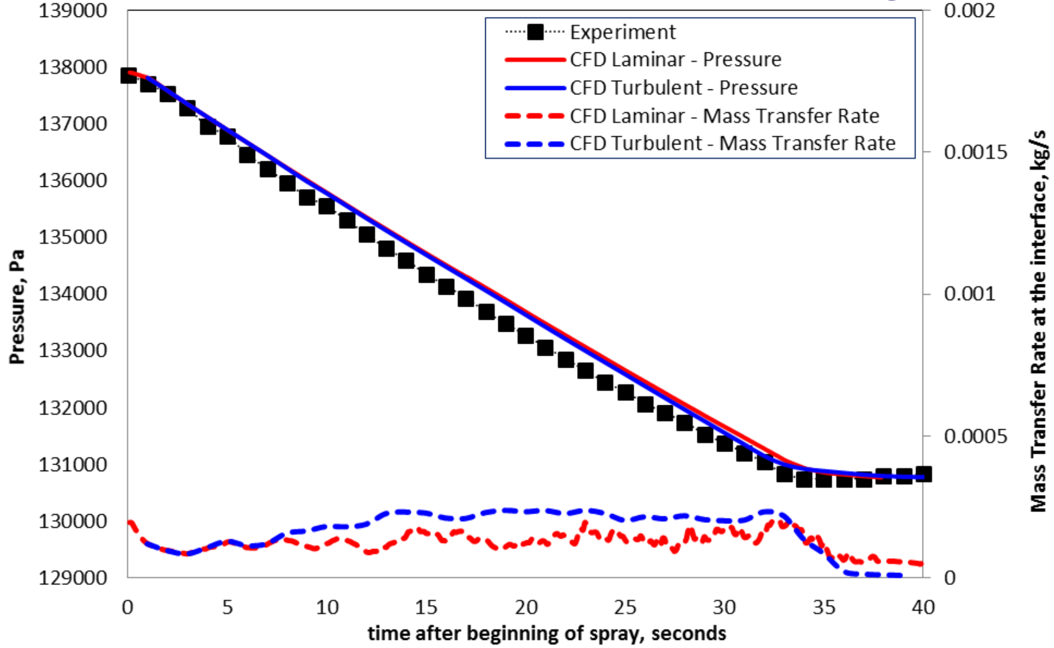


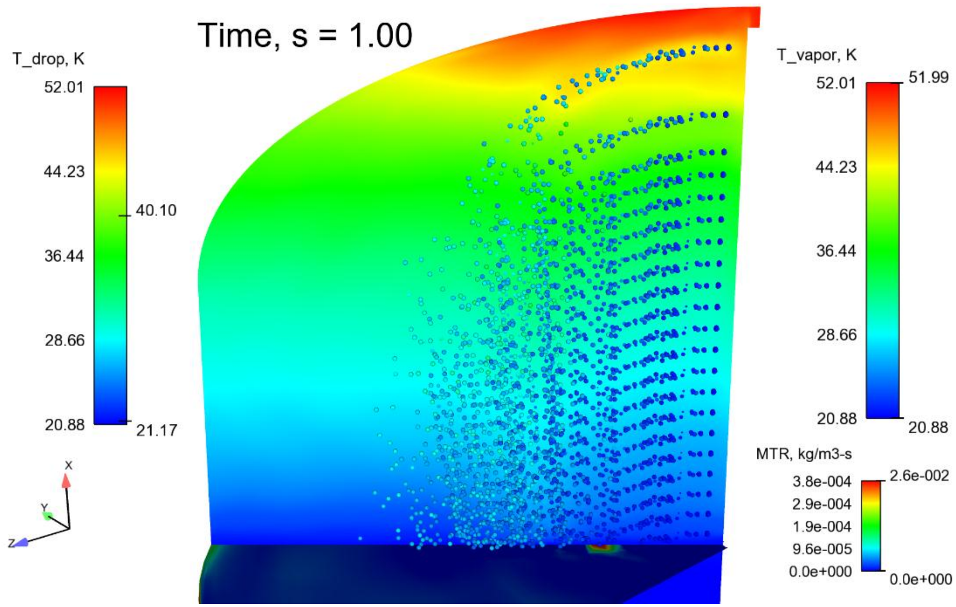
Explicit VOF



CFD Results:
Cooling of MHTB tank using Spray

CFD Results: Cooling of MHTB Tank using Spray - Effect of Turbulence Modeling





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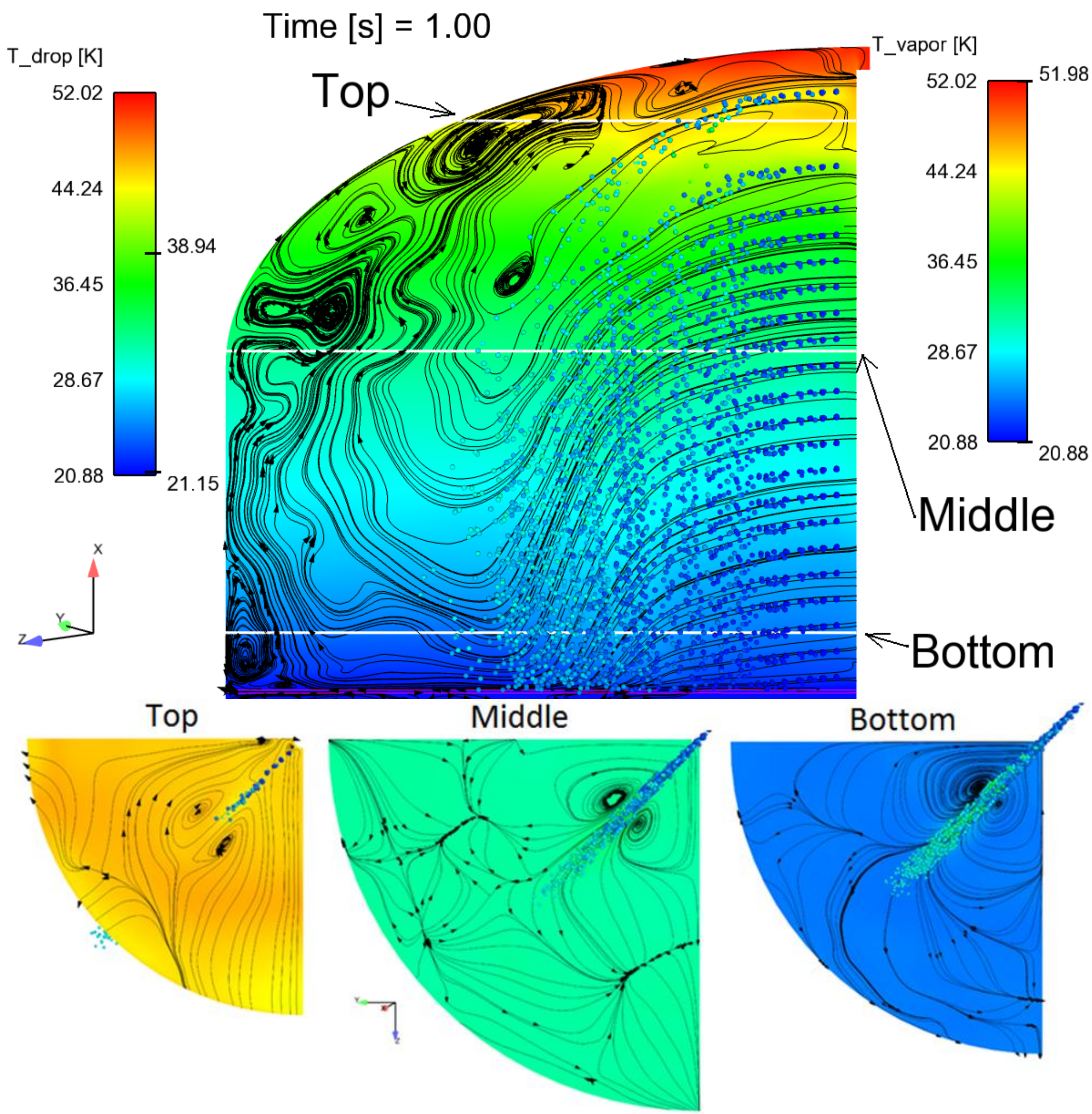
CFD Results: Cooling of MHTB Tank using Spray - Results of the Turbulent VOF Model



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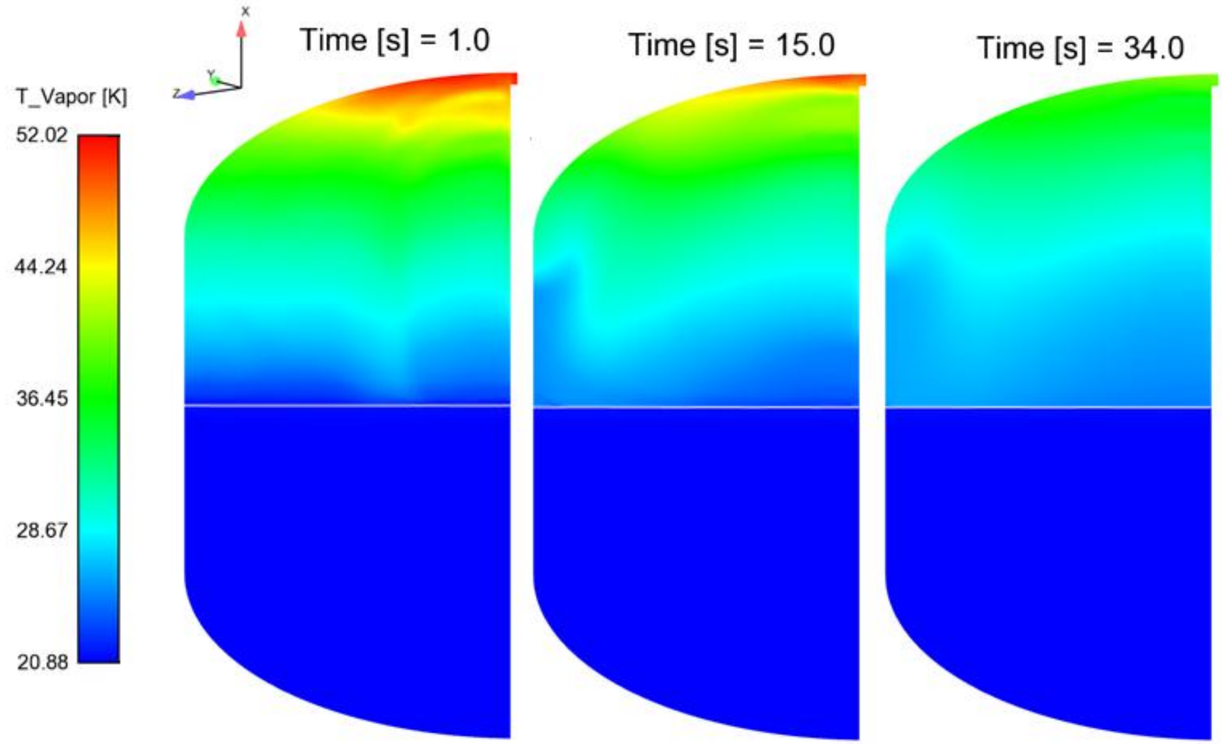

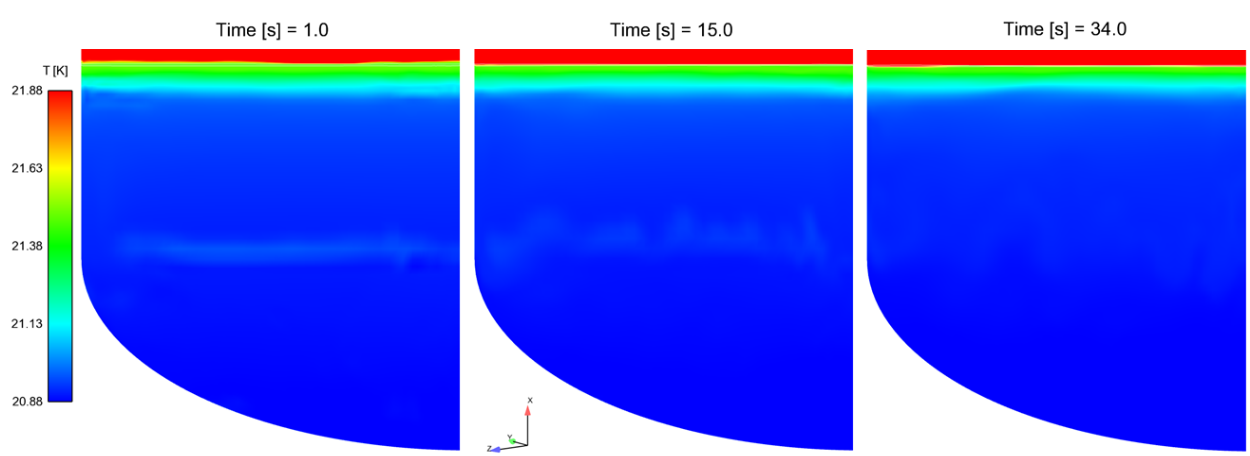

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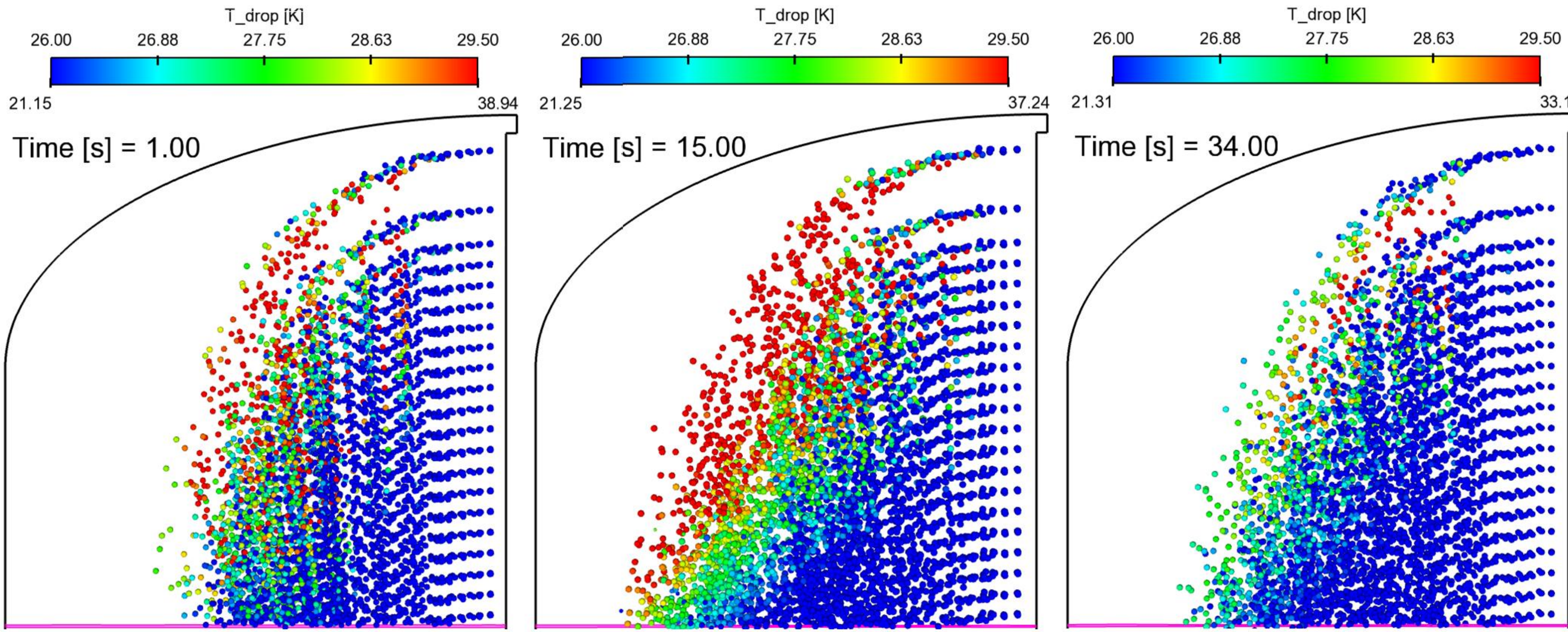
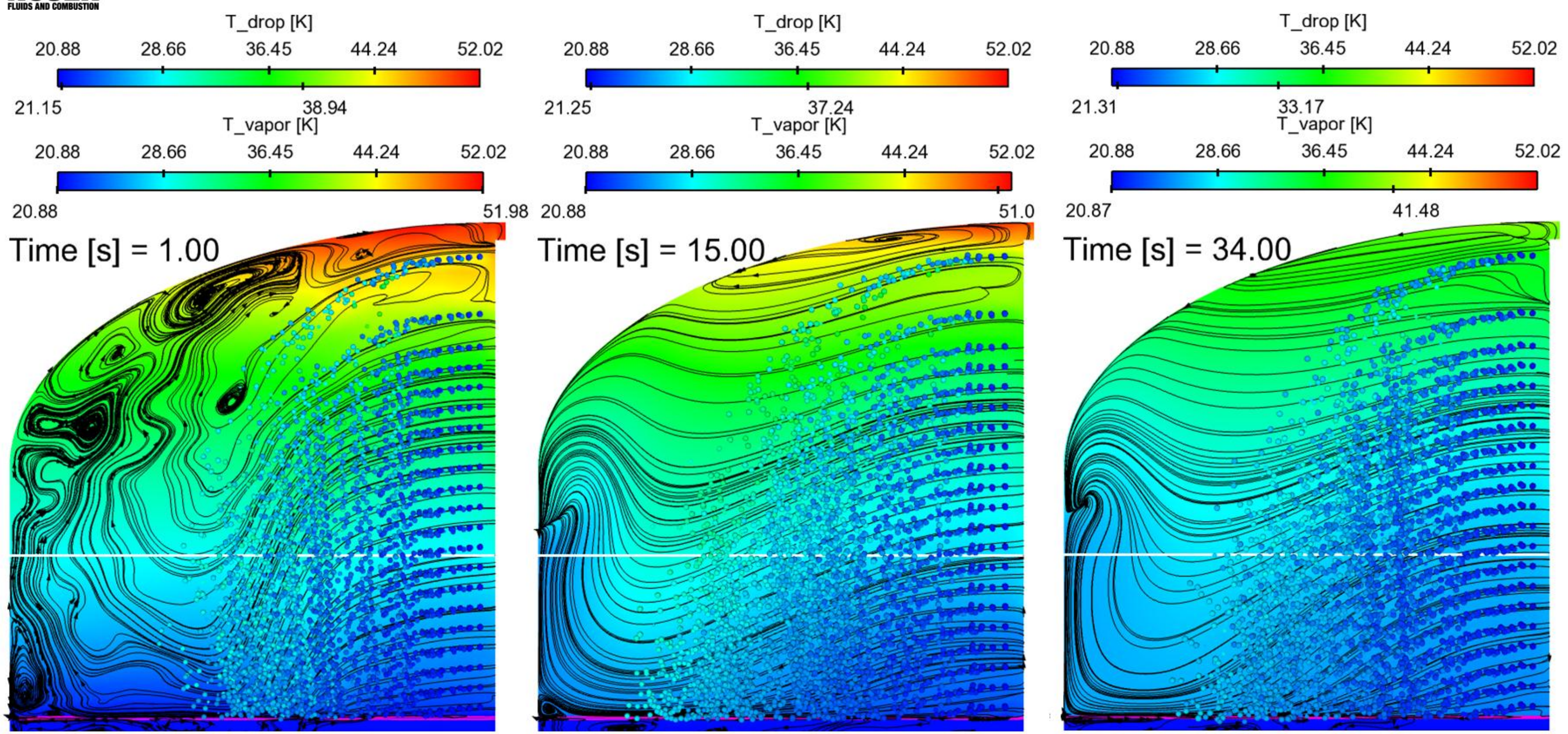


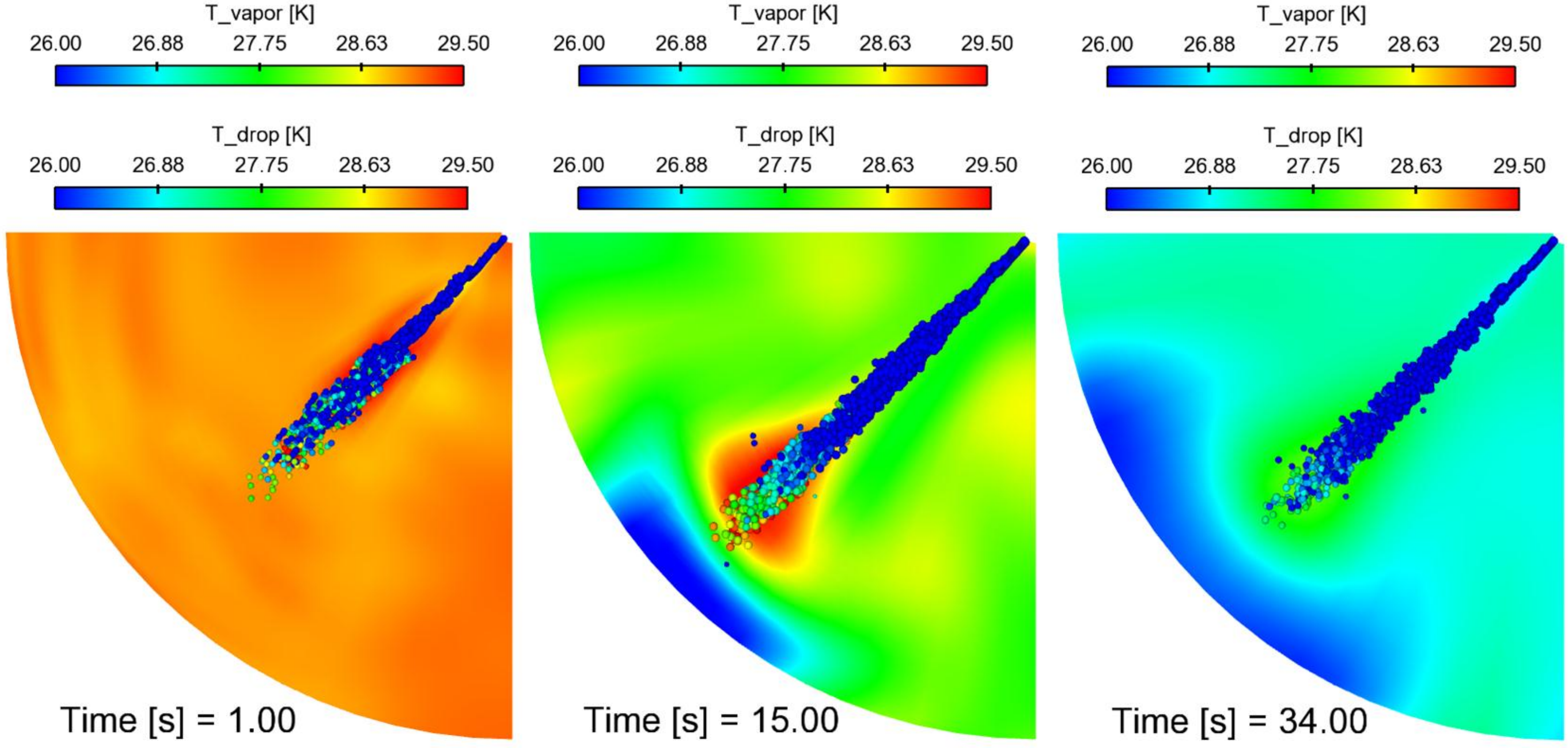
Droplet and temperatures at the center plane of injections

CFD Results: Cooling of MHTB Tank using Spray - Results of the Turbulent VOF Model



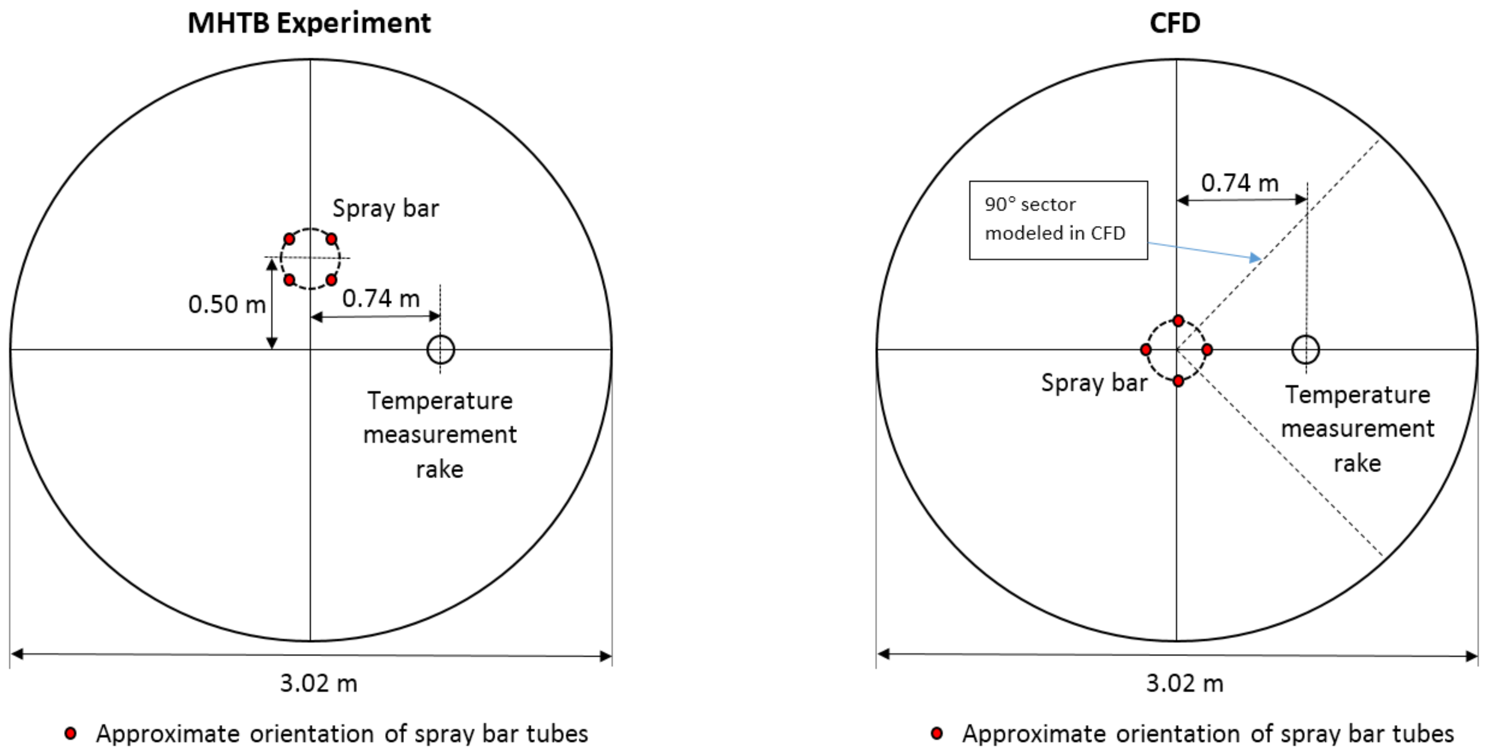
Droplet and vapor temperatures and streamlines at the center plane of injections

CFD Results: Cooling of MHTB Tank using Spray - Results of the Turbulent VOF Model



Temperature at the horizontal plane in the vapor

CFD Results: Cooling of MHTB Tank using Spray - Results of the Turbulent VOF Model



Location of the spray bar relative to the temperature measurement rake

CFD Results: Cooling of MHTB Tank using Spray - Results of the Turbulent VOF Model

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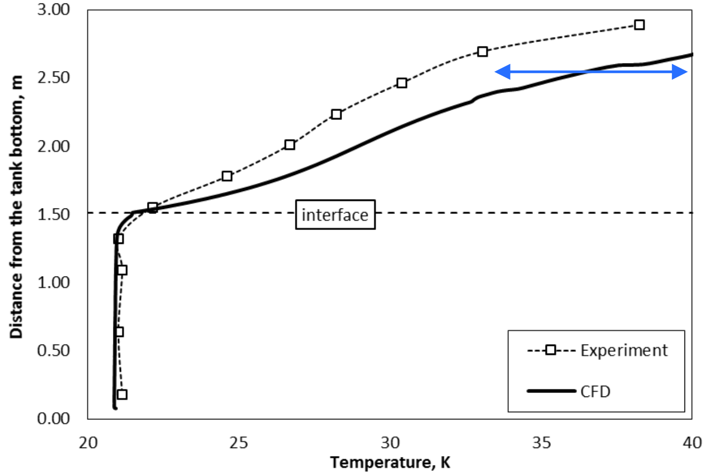

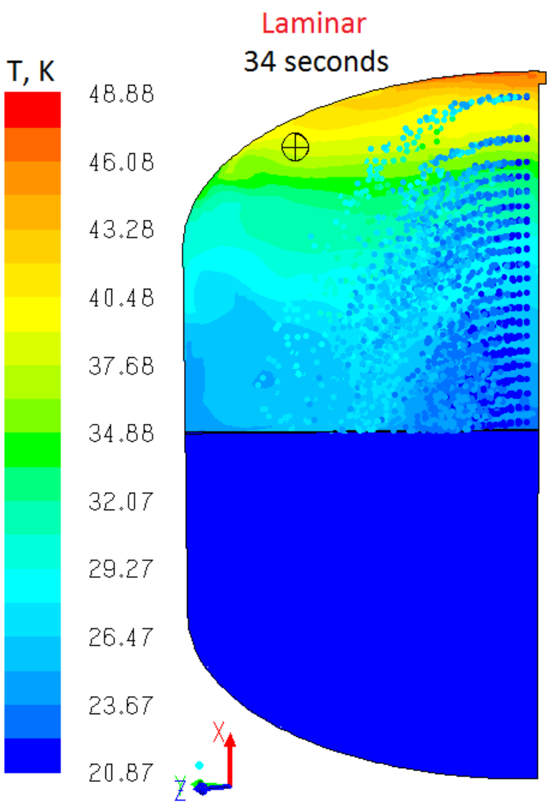

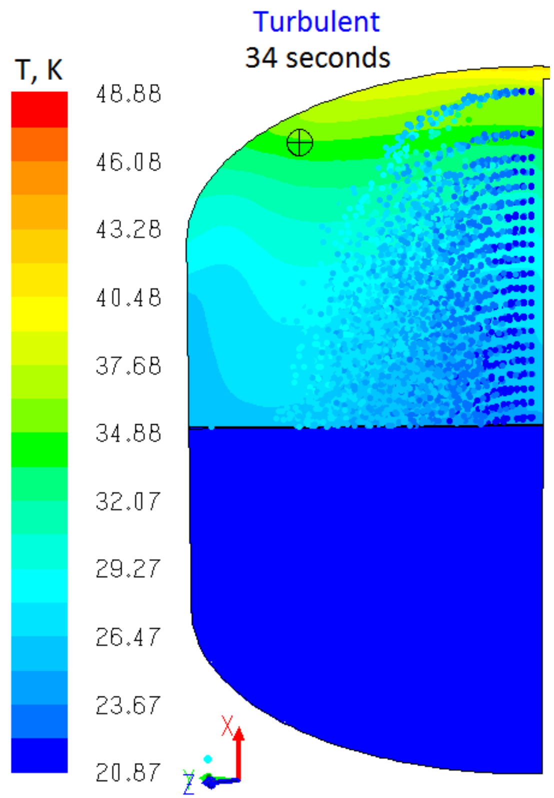

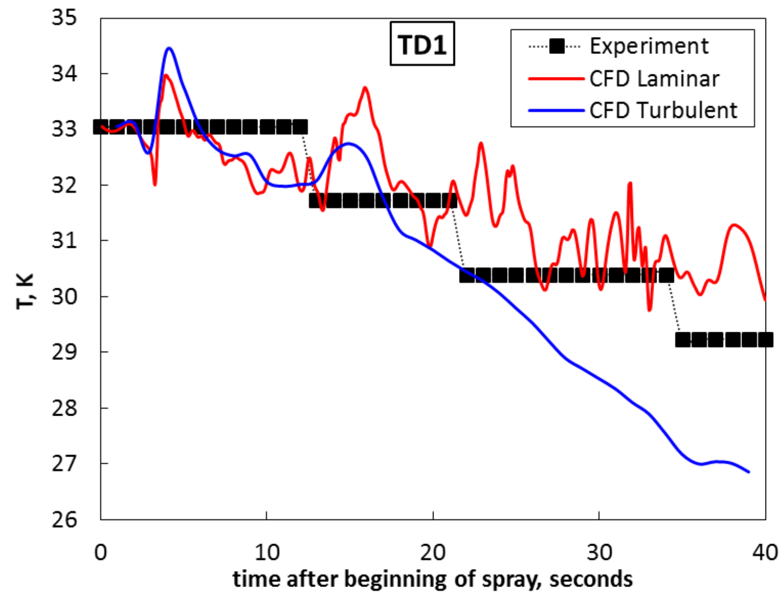

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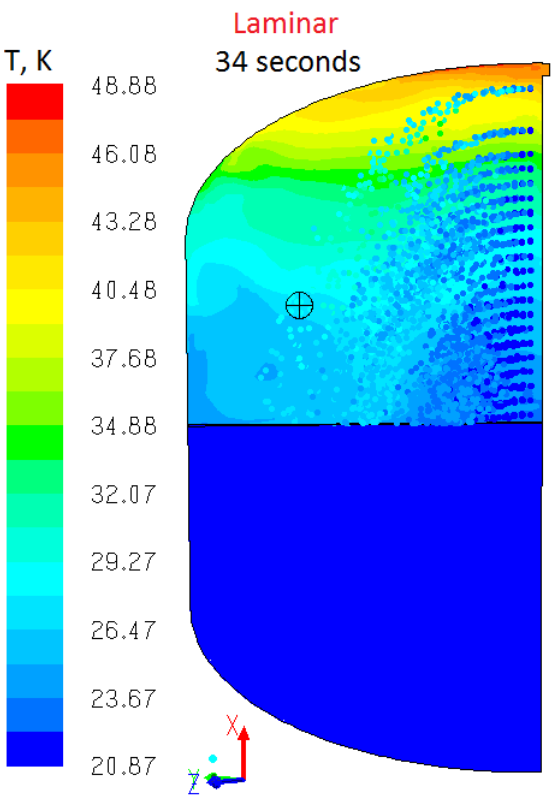

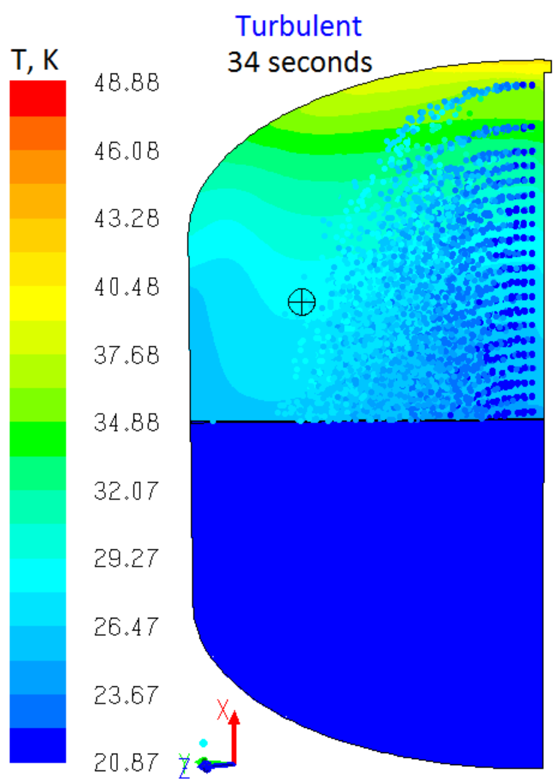

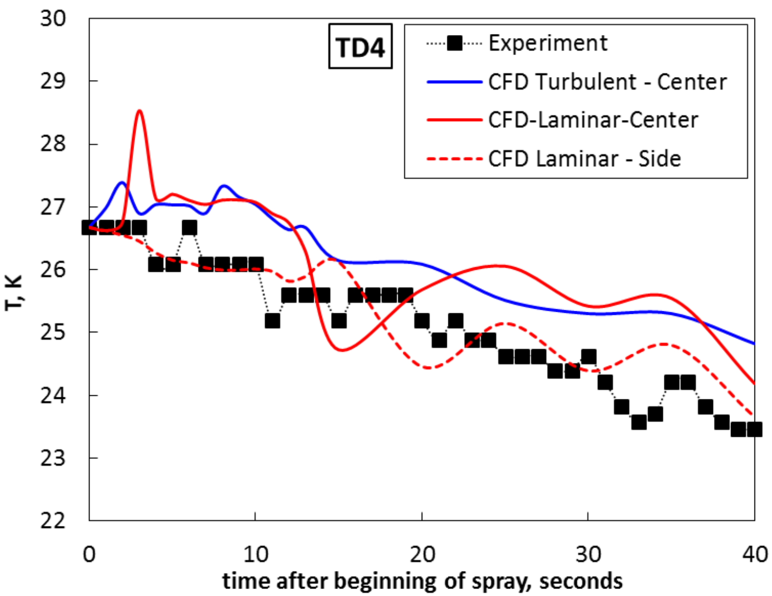

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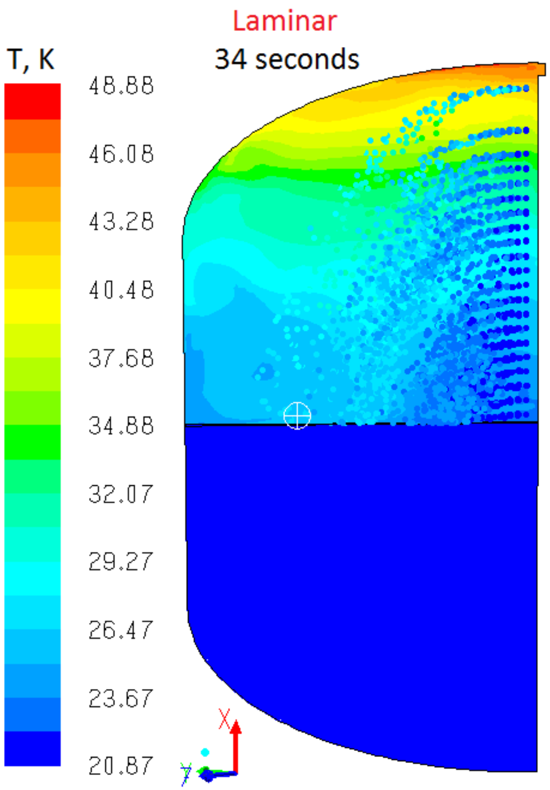

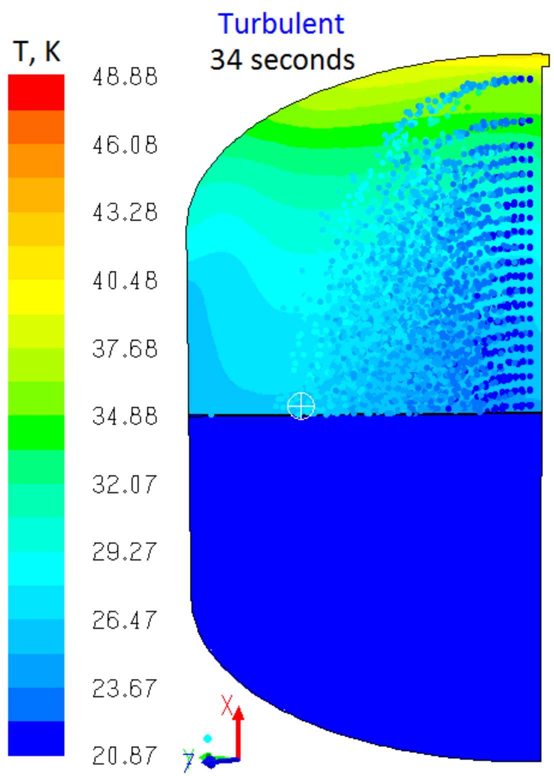

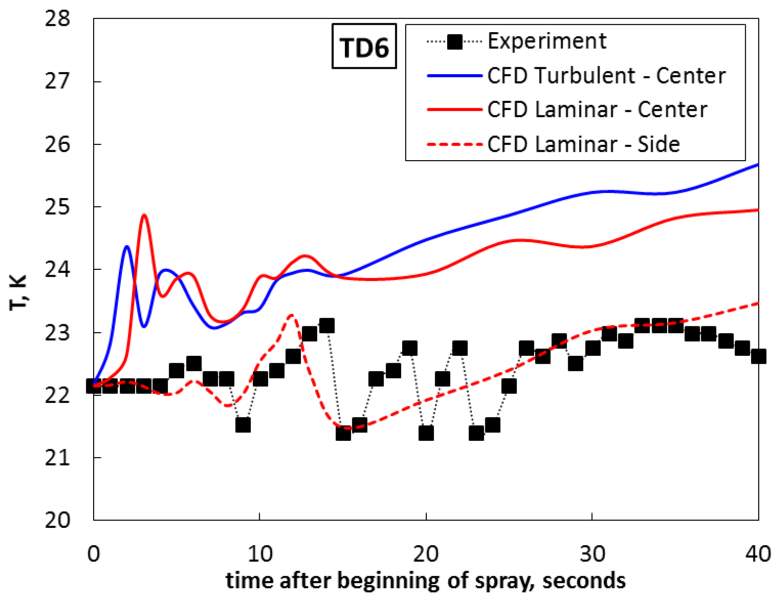

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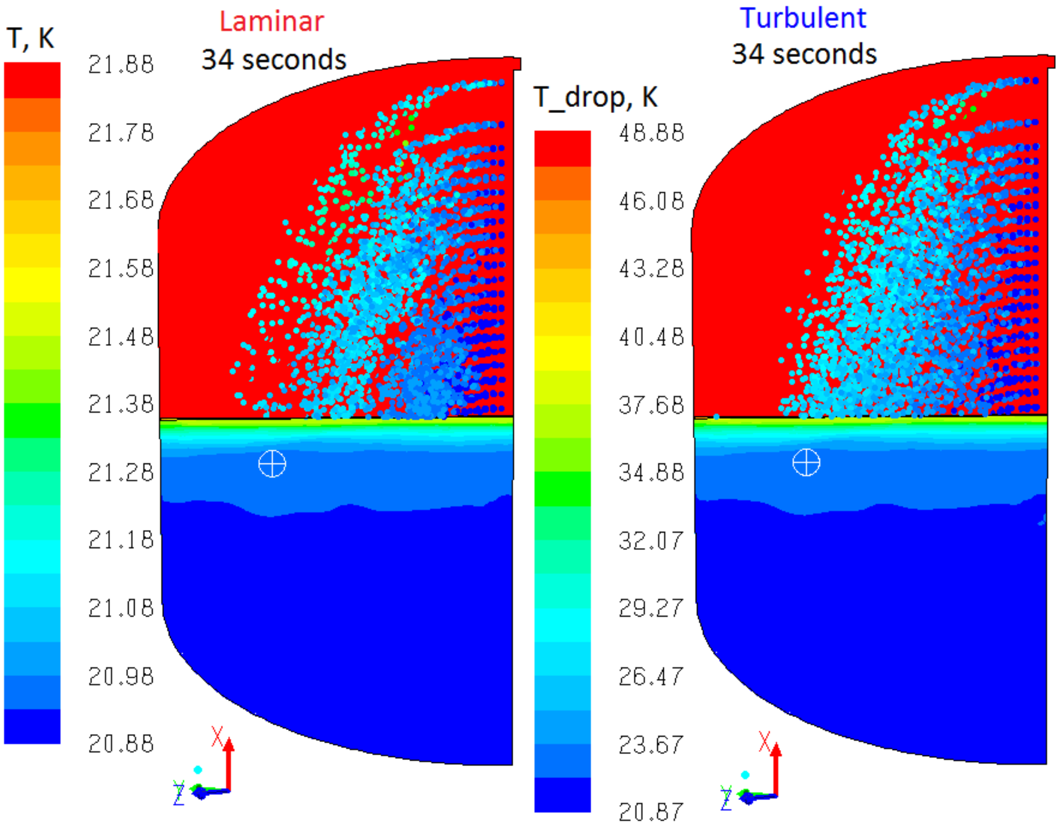

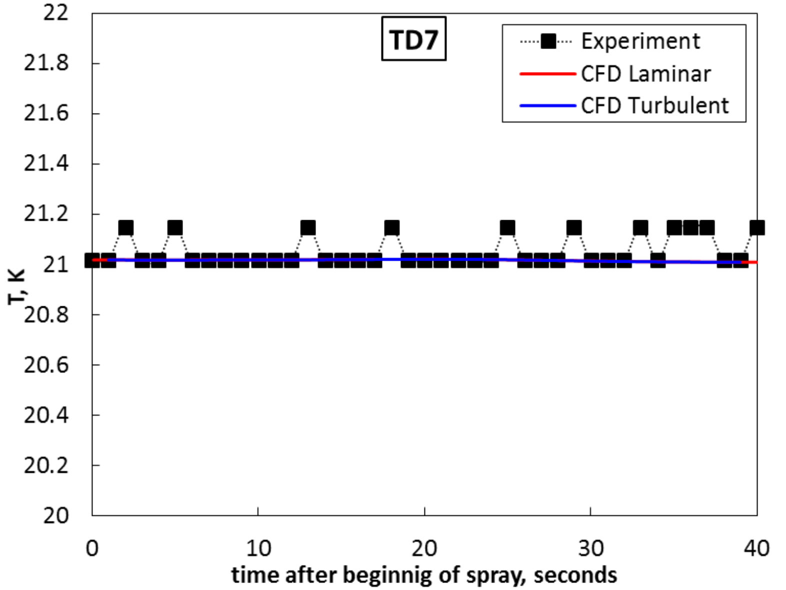

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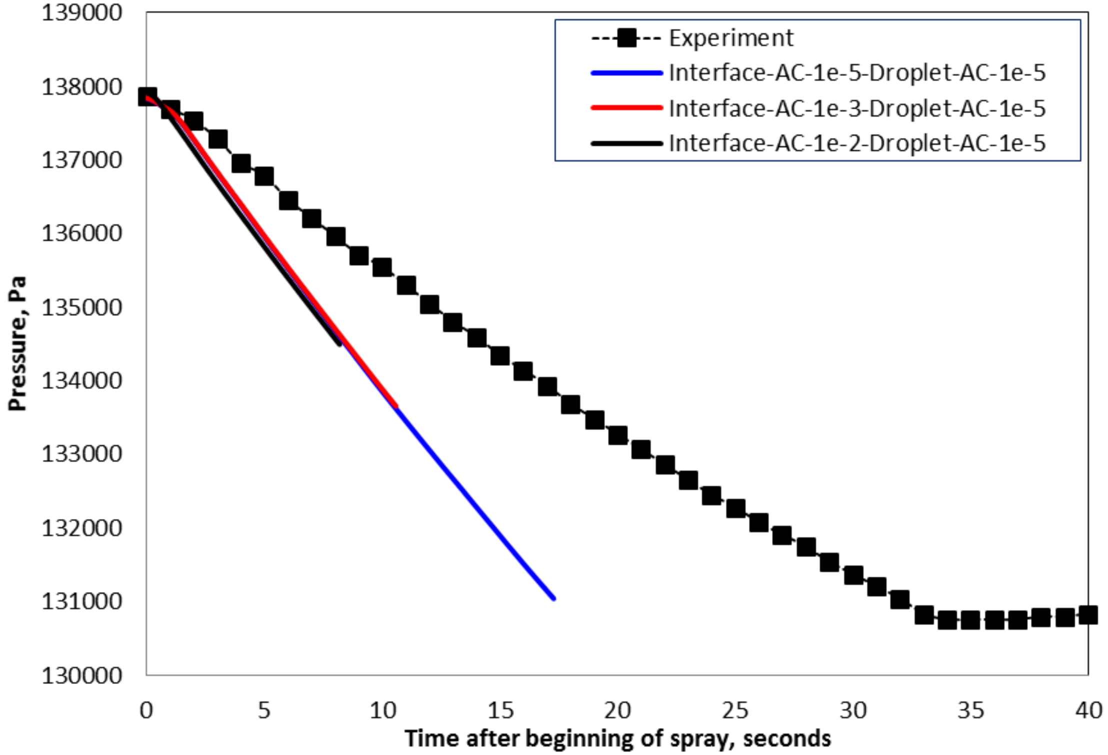

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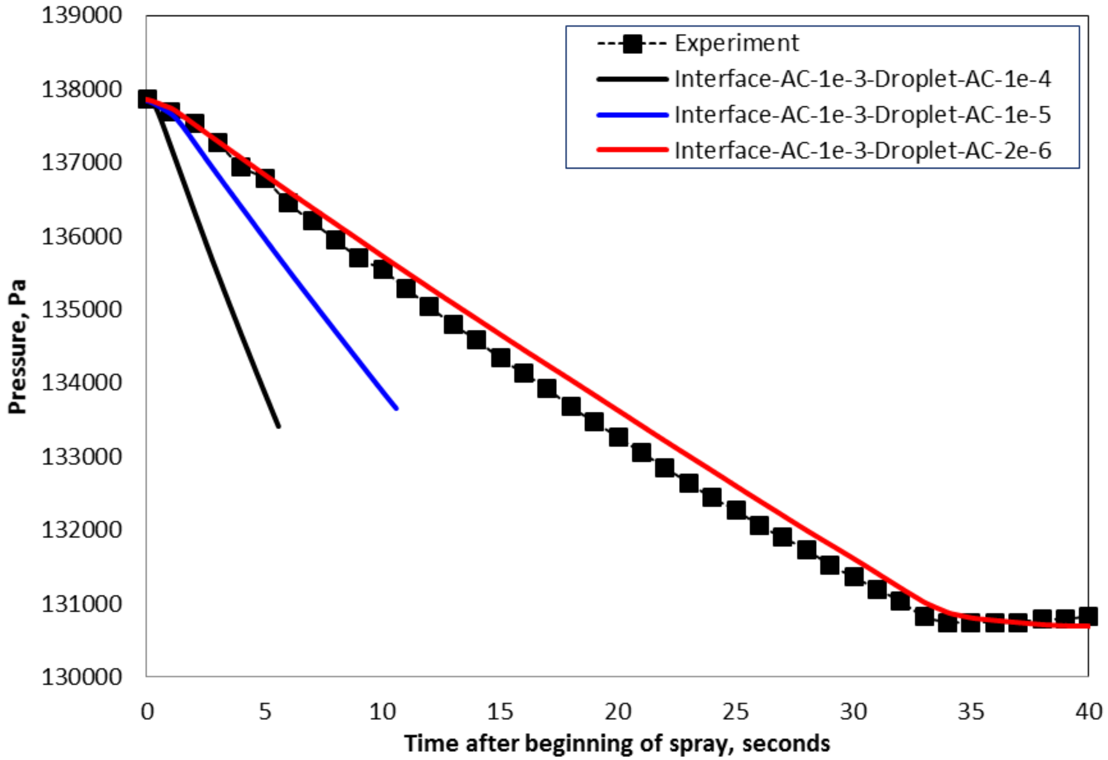

Conclusions

Self-Pressurization

- A CFD model was developed for modeling self-pressurization of MHTB tank using **compressible VOF** model with custom model for mass transfer between liquid and vapor phases.
- Varying accommodation coefficient from 0.1 to 0.0001 had very little effect on the tank pressure predictions. Explicit VOF model allowed use of larger value of accommodation coefficient with a need to reduce time step size when the highest value was used

Spray Cooling

- A CFD model was developed for simulating spray cooling of MHTB tank using **compressible VOF** with **Lagrangian Spray** model.
- The laminar and turbulent VOF models resulted in very similar tank pressures that agree well with experimental data.
- The droplets reduce temperature and promote mixing in the vapor region via heat and mass exchange during spray. Temperature of the droplets increases when they travel in the vapor towards the interface. Passage of the droplets creates a hot spot in the areas of higher droplet concentration in the middle of the vapor region.
- Droplet accommodation coefficient had significant effect on the tank pressure decrease with the higher values resulting in faster pressure drops

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