Modelling of LH2 transfer operations with engineering tools

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UK Research and Innovation

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Outline

- Introduction to DISCHA engineering tool
- Tool features
- Recent Validation
  - Emptying of an LH2 tank due to boil-off
  - Self pressurization of LH2 tanks
- Tank to tank transfer simulations
  - Filling of an LH2 truck from a stationary tank at 2 and 5 bars

Introduction

- DISCHA tool for
  - Physical properties at single phase and two-phase conditions
  - Discharge calculations
  - Tank to tank transfer calculations
- DISCHA development / validation in previous EC projects
  - NET-Tools

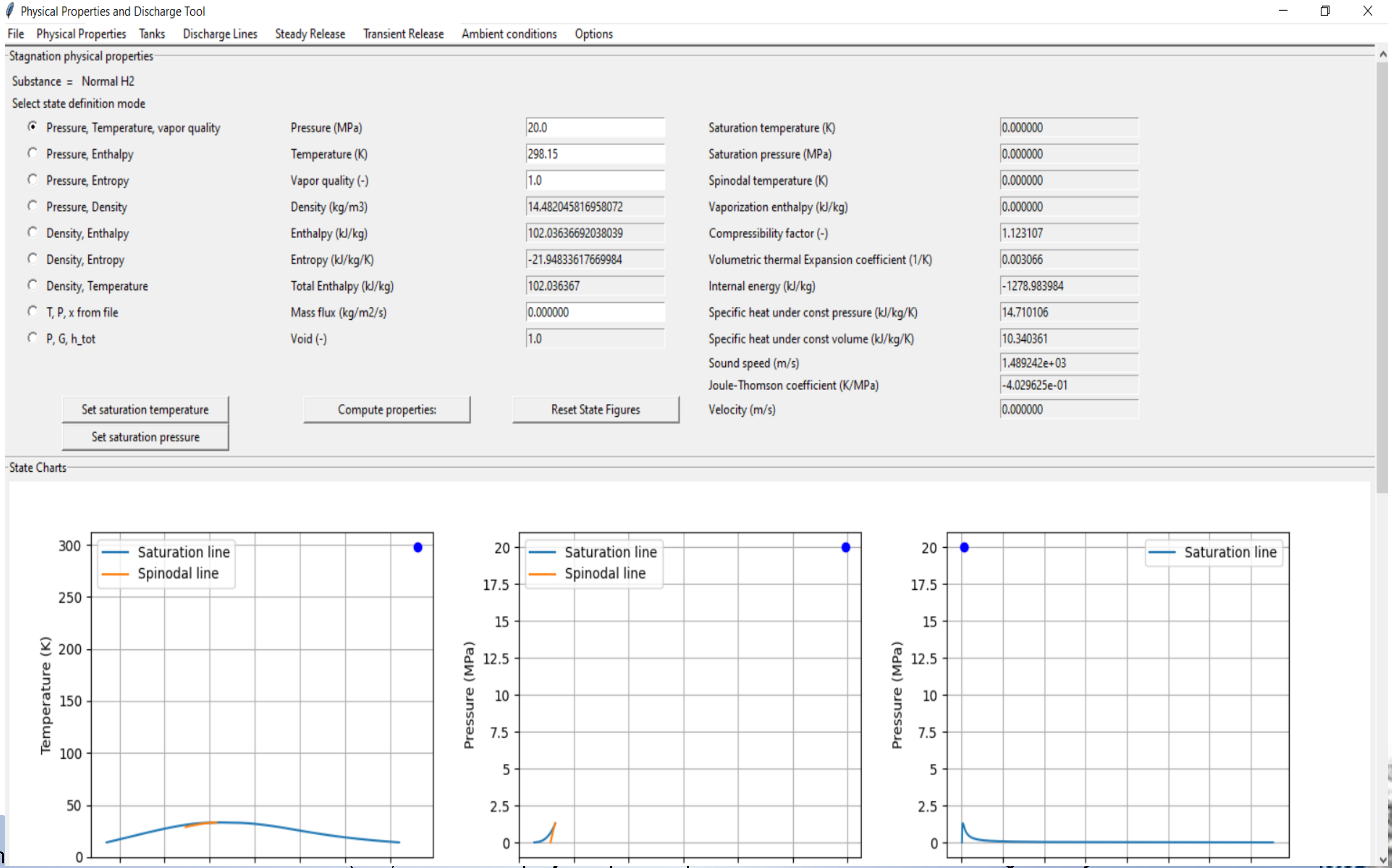
    NET-Tools_Venetsanos
  - PRESLHY

    PRESLHY_Venetsanos.mp4 PRESLHY_Venetsanos.pdf
  - HyTunnel-CS

    HyTunnel-CS_D4.4.pdf

DISCHA features

- GUI (Python), Main code (Fortran)



Stagnation physical properties

Substance = Normal H2

Select state definition mode

● Pressure, Temperature, vapor quality
○ Pressure, Enthalpy
○ Pressure, Entropy
○ Pressure, Density
○ Density, Enthalpy
○ Density, Entropy
○ Density, Temperature
○ T, P, x from file
○ P, G, h_tot

Pressure (MPa) 20.0
Temperature (K) 298.15
Vapor quality (-) 1.0
Density (kg/m3) 14.482045816958072
Enthalpy (kJ/kg) 102.03636692038039
Entropy (kJ/kg/K) -21.94833617669984
Total Enthalpy (kJ/kg) 102.036367
Mass flux (kg/m2/s) 0.000000
Void (-) 1.0

Saturation temperature (K) 0.000000
Saturation pressure (MPa) 0.000000
Spinodal temperature (K) 0.000000
Vaporization enthalpy (kJ/kg) 0.000000
Compressibility factor (-) 1.123107
Volumetric thermal Expansion coefficient (1/K) 0.003066
Internal energy (kJ/kg) -1278.983984
Specific heat under const pressure (kJ/kg/K) 14.710106
Specific heat under const volume (kJ/kg/K) 10.340361
Sound speed (m/s) 1.489242e+03
Joule-Thomson coefficient (K/MPa) -4.029625e-01
Velocity (m/s) 0.000000

DISCHA features

- Substances
  - Normal H_2, Para-H_2, CH_4, CO_2, H_2O, NH_3, O_2, N_2, He
- EoS
  - Helmholtz free energy, SRK, PR, RKMC, Abel-Noble, Ideal gas
- Two-phase modelling
  - Ideal mixture of liquid and vapor phase
  - HEM
  - HRM, DEM mainly for H_2O
- Various input modes for thermodynamic state definition
  - Pressure + temperature + vapor quality
  - Pressure + (enthalpy or entropy or density or internal energy)
  - Density + (internal energy or entropy)
  - …

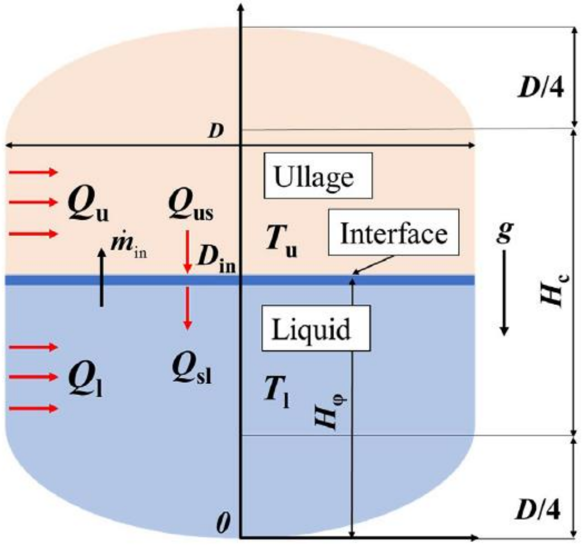
DISCHA features

- Discharge / tank to tank transfer calculations
  - Arbitrary network of tanks connected by transfer lines.
  - A transfer line either connects 2 tanks or connects a tank with the ambient environment
  - No direct connection between different lines (branches).

DISCHA features

- Tank modelling
  - Single zone
    - Liquid and vapor phases share the same (sat) temperature
    - Transient mass and energy equations for the entire tank volume.
  - Multizone
    - Two distinct volumes (liquid below, vapor above) separated by one interface
    - Liquid phase subcooled or saturated
    - Vapor phase superheated or saturated
    - Liquid-Vapor Interface saturated
    - Various models for evaporation/condensation through the interface
    - Transient mass and energy equations for the vapor phase
    - Transient mass and energy equations for the liquid phase
  - Wall heat transfer
    - Time-dependent energy equation within tank walls.
    - Different material layers within tank walls

Tank conservation equations



Single zone

$$V\frac{d\rho}{dt} = \dot m_{in} - \dot m_{out} \qquad V\frac{d\rho u}{dt} = \dot m_{in} h_{tot,in} - \dot m_{out} h_{tot,out} + \dot q A$$

Multizone zone (Wang et al. 2022)

$$\frac{d\rho_L V_L}{dt} = \dot m_{L,in} - \dot m_{L,out} \boxed{-\dot m_{LV}} \qquad \frac{d\rho_L V_L u_L}{dt} = \left[\dot m_{in} h_{tot,in} - \dot m_{out} h_{tot,out} + \dot q A\right]_L \boxed{+\dot q_{SL} A_S - \dot m_{LV} h_{sat,L}}$$

$$\frac{d\rho_V V_V}{dt} = \dot m_{V,in} - \dot m_{V,out} \boxed{+\dot m_{LV}} \qquad \frac{d\rho_V V_V u_V}{dt} = \left[\dot m_{in} h_{tot,in} - \dot m_{out} h_{tot,out} + \dot q A\right]_V \boxed{-\dot q_{VS} A_S + \dot m_{LV} h_{sat,V}}$$

$V_L + V_V = V$ Volume constraint

Wang H.R. et al., Modeling and thermodynamic analysis of thermal performance in self-pressurized liquid hydrogen tanks, IJHE, 47 (2022)

Evaporation/Condensation model

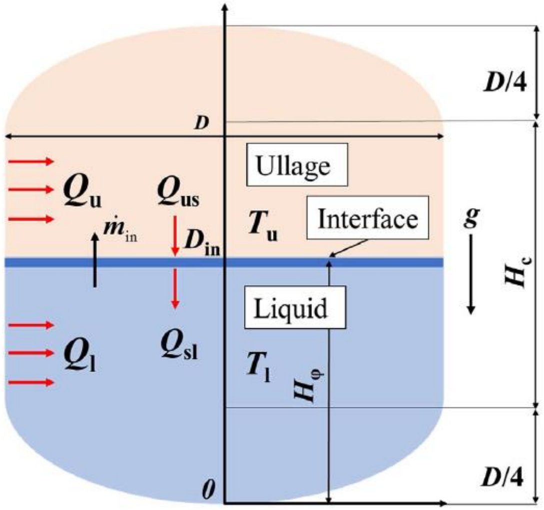
$$\boxed{\dot{q}_{VS} - \dot{q}_{SL} = \dot{m}_{LV}\left(h_{sat,V} - h_{sat,L}\right)}$$

$$\dot{q}_{VS} = K_V a_{VS}\left(T_V - T_{Sat}\right) \qquad \dot{q}_{SL} = K_L a_{SL}\left(T_{Sat} - T_L\right)$$

$$Nu_{VS} \equiv \frac{a_{VS} D}{\lambda_{VS}} = 0.27 Ra_{VS}^{1/4}$$ Mc Adams

$$Nu_{SL} \equiv \frac{a_{SL} D}{\lambda_{SL}} = 2.5\left\{\ln\left\{1.0 + \frac{2.5}{0.527 Ra_{SL}^{0.2}}\left(1.0 + \left(\frac{1.9}{\mathrm{Pr}_{SL}}\right)^{0.9}\right)^{2/9}\right\}\right\}^{-1}$$ Nellis & Klein

$$K_V = K_L = 0.1$$ Account for non-equilibrium



Wang H.R. et al., Modeling and thermodynamic analysis of thermal performance in self-pressurized liquid hydrogen tanks, IJHE, 47 (2022)

DISCHA features

- Discharge/transfer line modelling
  - Conservation equations
    - Steady state momentum and energy balance
    - Line resistance, area change, wall heat transfer both for single phase and two-phase conditions
    - Transient internal energy equation within pipe walls.
  - Choked flow
    - Calculated using general Possible-Impossible-Flow (PIF) algorithm
    - Discretization along discharge line is necessary (refine grid near pipe exit !!!)
    - Mach = 1 at exit is an output result not a BC
  - Fictitious nozzle
    - 7 available models

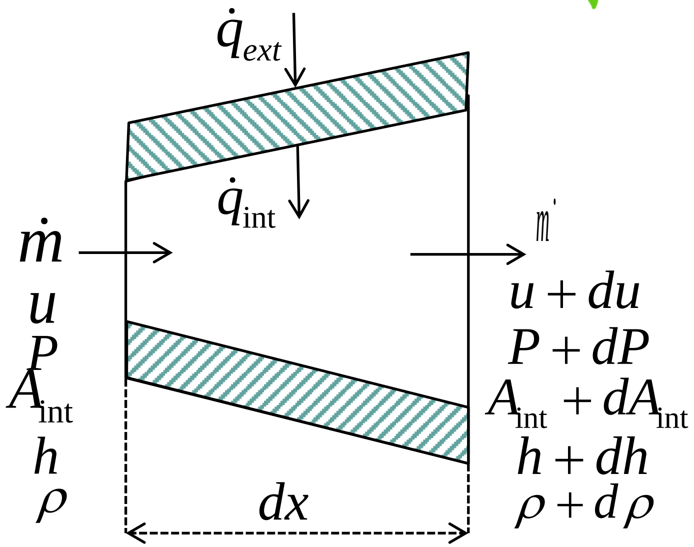
Line modeling

Pipe steady state equations:

$$\rho u A_{\text{int}} = \dot{m} = ct$$

$$\rho u du = -dP - \frac{\rho u^2 dx}{2}\left(\frac{f_D}{D_{\text{int}}} + \frac{K}{L}\right)$$

$$\rho u d\left(h + \frac{u^2}{2}\right) = \dot{q}_{\text{int}} \frac{4dx}{D_{\text{int}}}$$



Extra resistances (fittings)

Friction

Wall heat transfer
Omitted in this work

DISCHA validation

Emptying of an LH2 tank due to boil-off

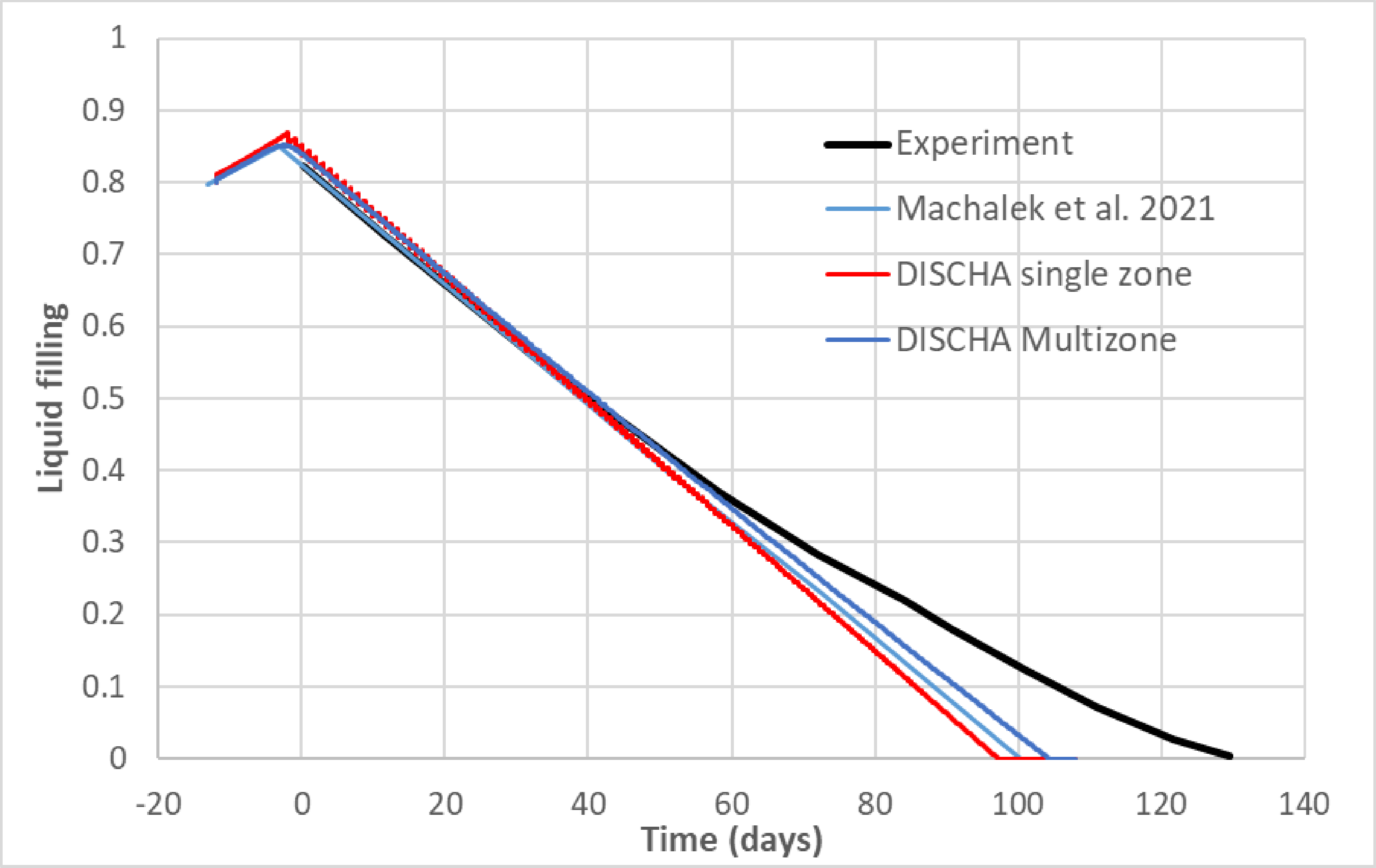
Emptying of an LH2 tank due to boil-off

- Experiments
  - From Lawrence Livermore National Laboratories, see also Machalek et al., ICHS-9, 2021.
- System
  - Tank
    - Vertical cylindrical tank 2 m diameter, 3.97 m height, 12.47 m^3 volume.
    - 11.1 mm inner steel + 50.8 mm MLI vacuum + 8.3 mm outer steel walls
    - 80% initial LH2 fill
  - Line
    - 5 mm PRV, opens at 3.1 bar and closes at 2.9 bar

Material	Inner steel	MLI	Outer steel
Conductivity	3	2e-4	15
Specific heat	25	0.1	450
Density	8050	0.1	8050

Machalek et al., Influence of non-equilibrium conditions on liquid hydrogen storage tank behavior, 9th Int. Conf. on Hydrogen Safety, 21-23 Sept. 2021, Edinburgh, UK

Emptying of an LH2 tank due to boil-off

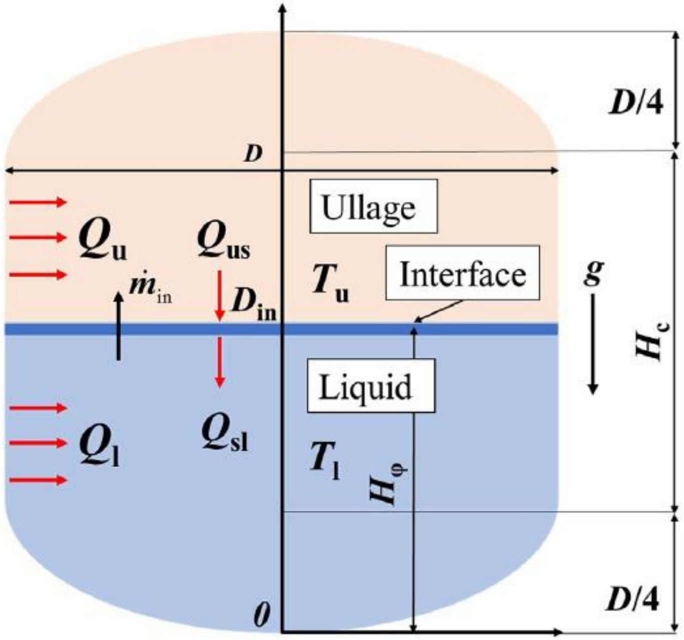


DISCHA validation

Self pressurization of LH2 tanks

Self-pressurization of LH2 tanks

- Experiments
  - NASA multipurpose hydrogen test bed (MHTB) tank experiments see Hastings et al., (2003) and related modeling by Wang et al. (2022).
- System
  - Tank volume 18.09 m^3,
  - tank diameter D = 3.05 m
  - Cylindrical height H_c = 1.525 m
  - No venting



Hastings et al., Spray bar zero-gravity vent system for on orbit liquid hydrogen storage. NASA TM-12926 (2003)

Wang H.R. et al., Modeling and thermodynamic analysis of thermal performance in self-pressurized liquid hydrogen tanks, IJHE, 47 (2022)

Self-pressurization of LH2 tanks

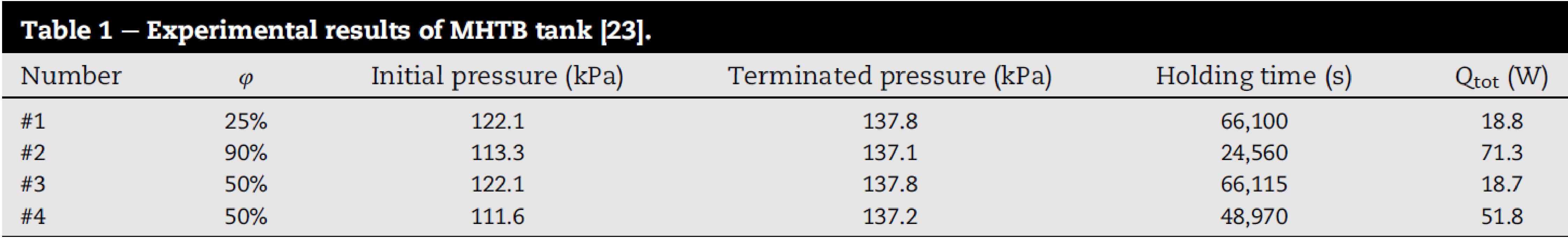
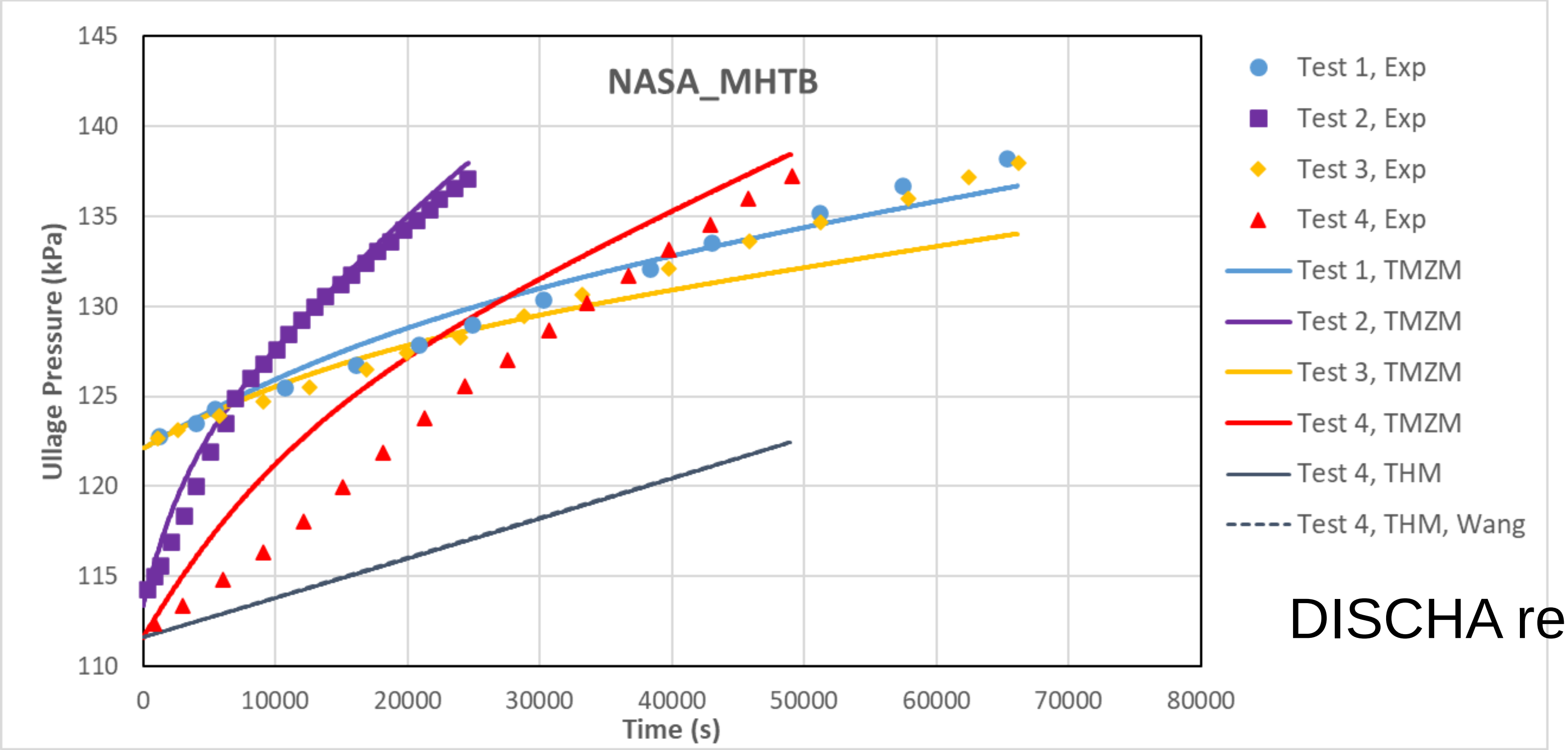


Table 1 – Experimental results of MHTB tank [23].

Number	φ	Initial pressure (kPa)	Terminated pressure (kPa)	Holding time (s)	Q_{tot} (W)
#1	25%	122.1	137.8	66,100	18.8
#2	90%	113.3	137.1	24,560	71.3
#3	50%	122.1	137.8	66,115	18.7
#4	50%	111.6	137.2	48,970	51.8

$$\frac{\dot{q}_V}{\dot{q}_L} = 0.5$$



DISCHA results

Tank to tank transfer

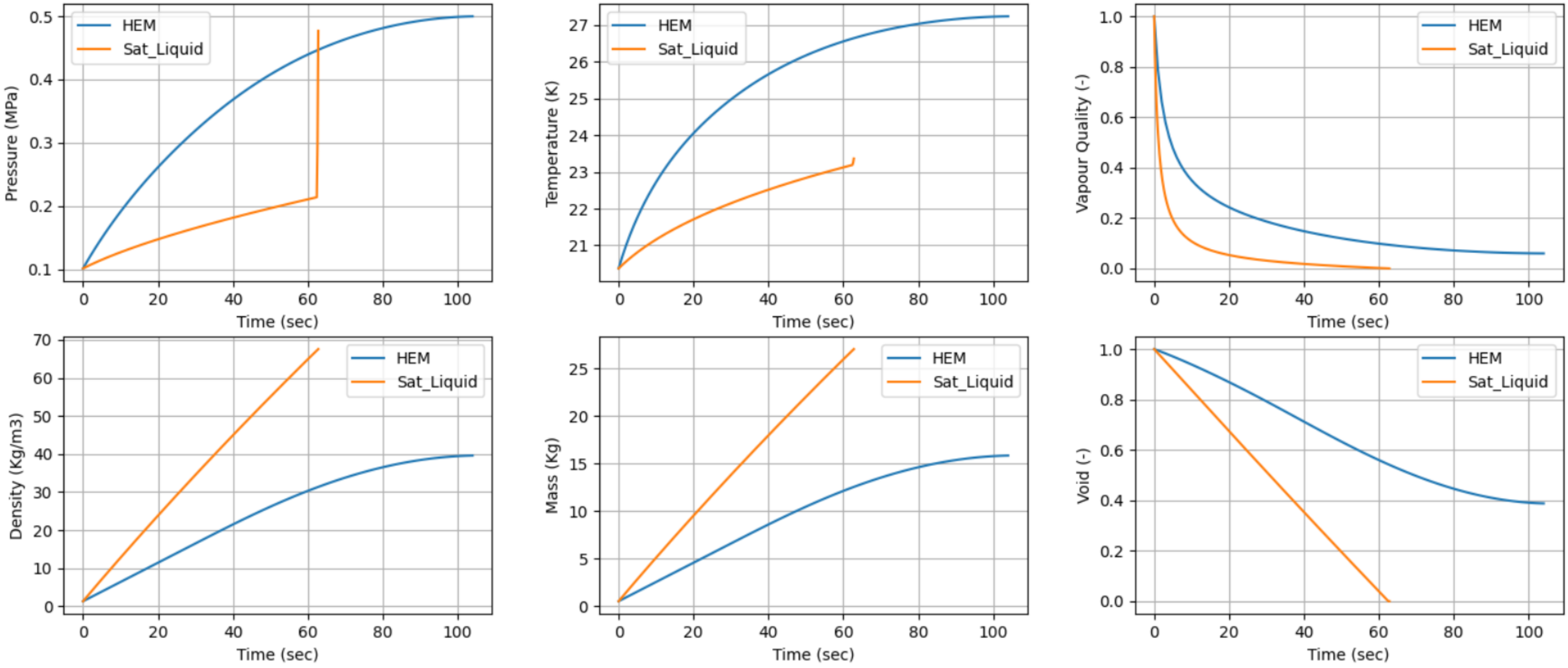
Filling of an LH2 truck from a stationary tank

Tank to tank transfer

- System Components:
  - Supply tank 12 m^3 (2 or 5 bars, sat LH_2)
  - Transfer line (30 m, 2.54 cm) + (5 cm, 10mm) nozzle
  - Receiving tank 0.4 m^3 (1 atm, sat GH2) without vent
  - All components are considered adiabatically isolated.
- Models:
  - Constant pressure for supply tank (2 or 5 bars abs.)
  - HEM or Sat_Liquid for transfer line
  - Single zone or Multizone for receiving tank

5 bars, single zone

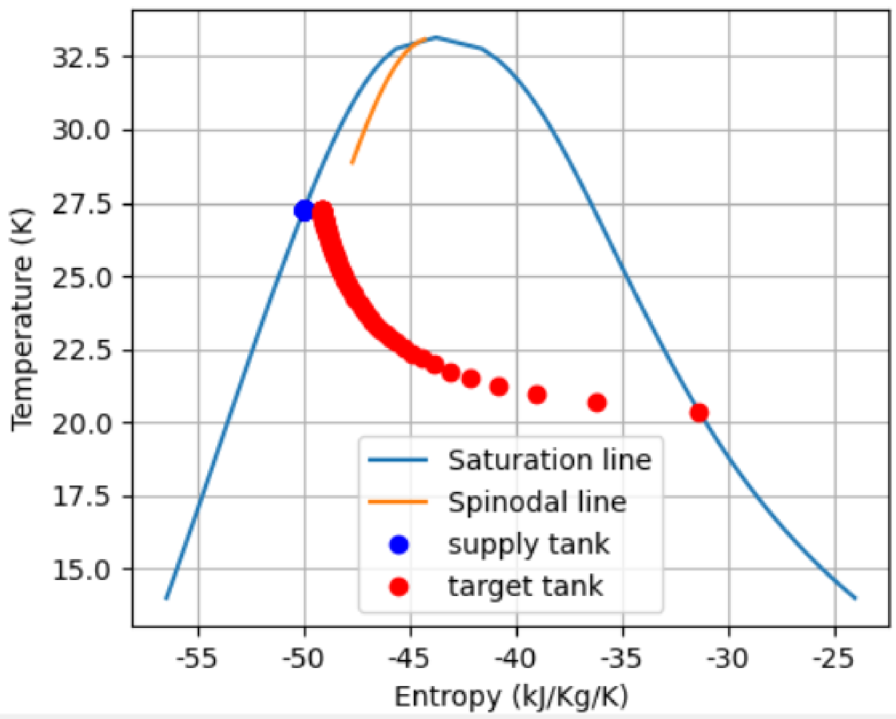
Predicted conditions in receiving tank



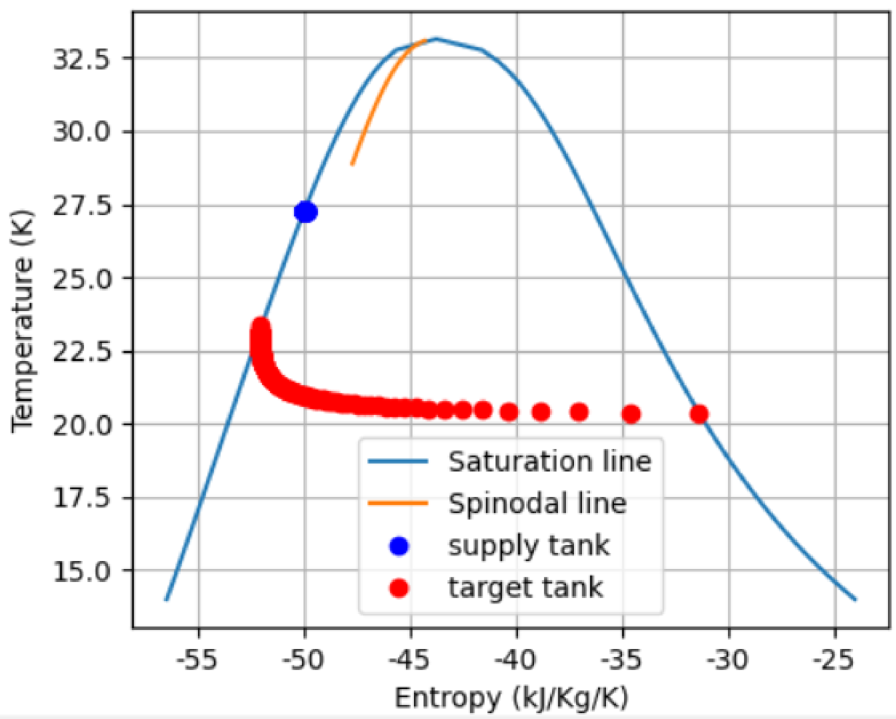
5 bars, single zone

Filling path on the TS chart

HEM

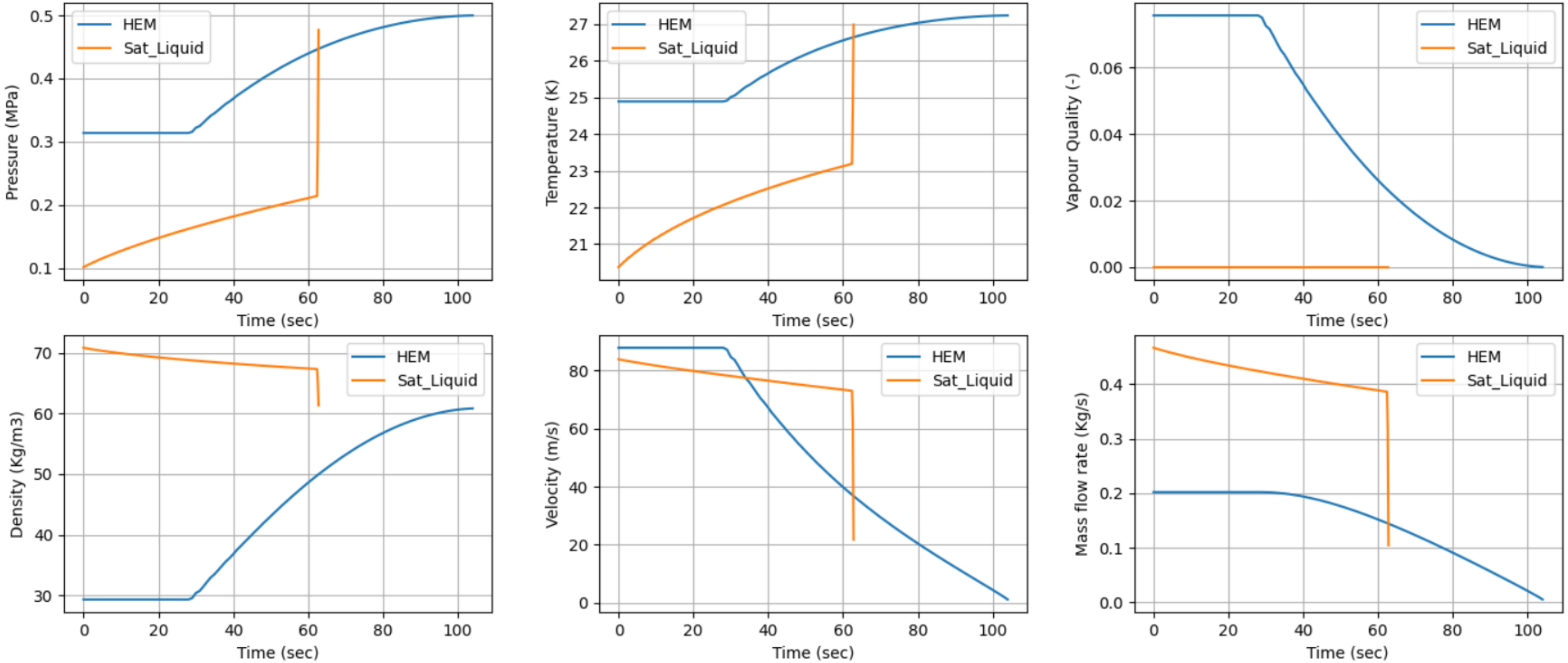


Sat_Liquid



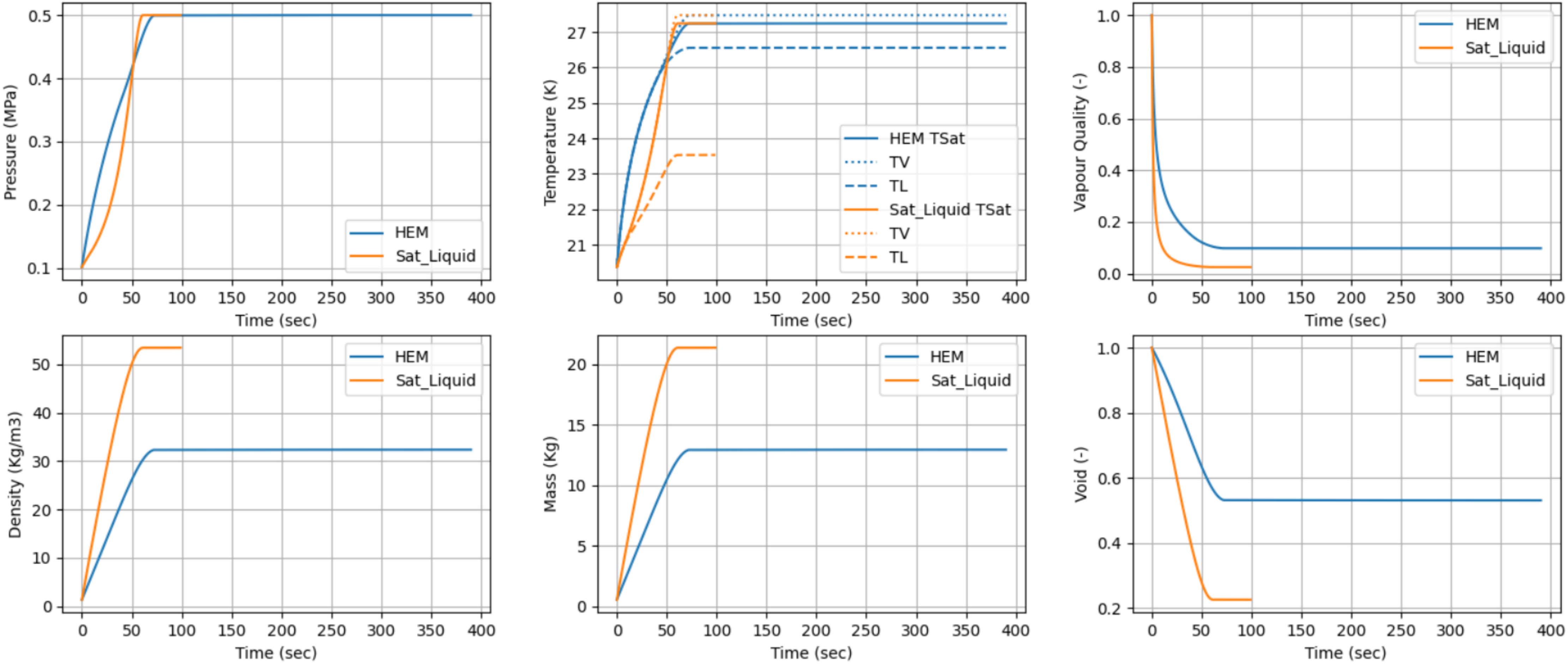
5 bars, single zone

Predicted conditions at transfer line exit



5 bars, Multizone

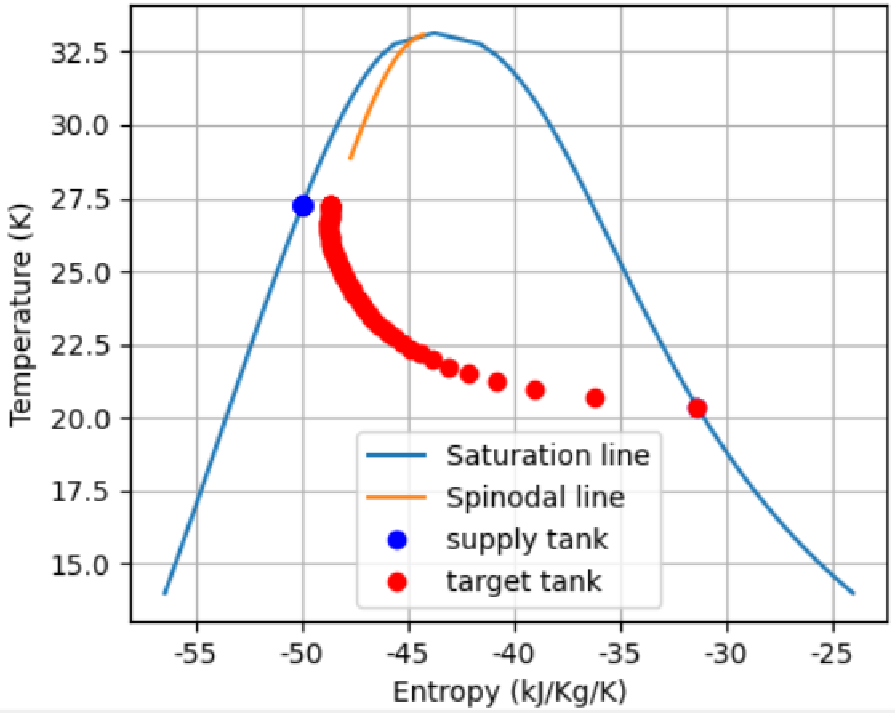
Predicted conditions in receiving tank



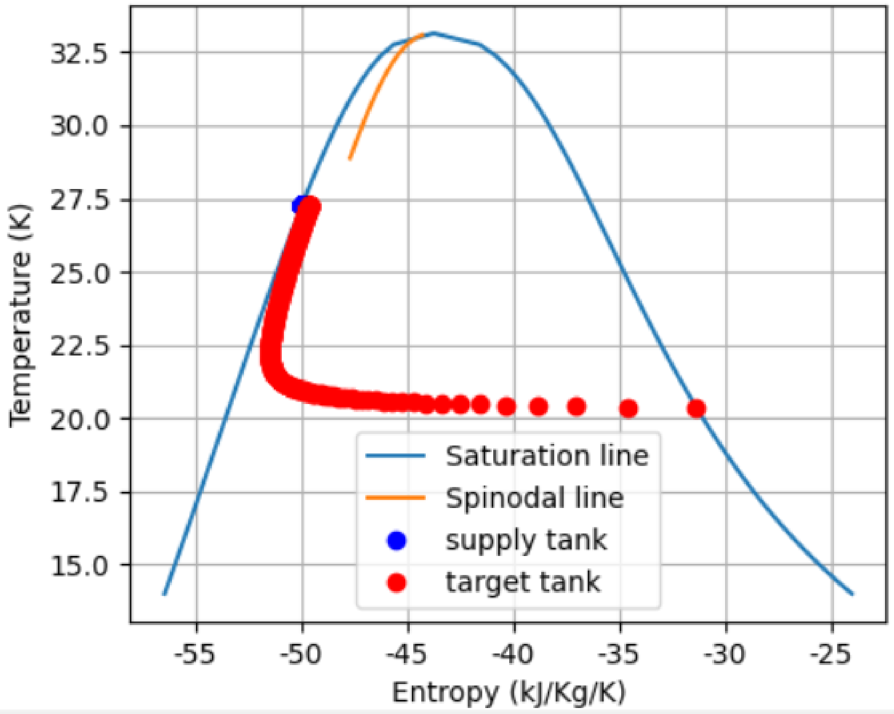
5 bars, Multizone

Filling path on the TS chart

HEM

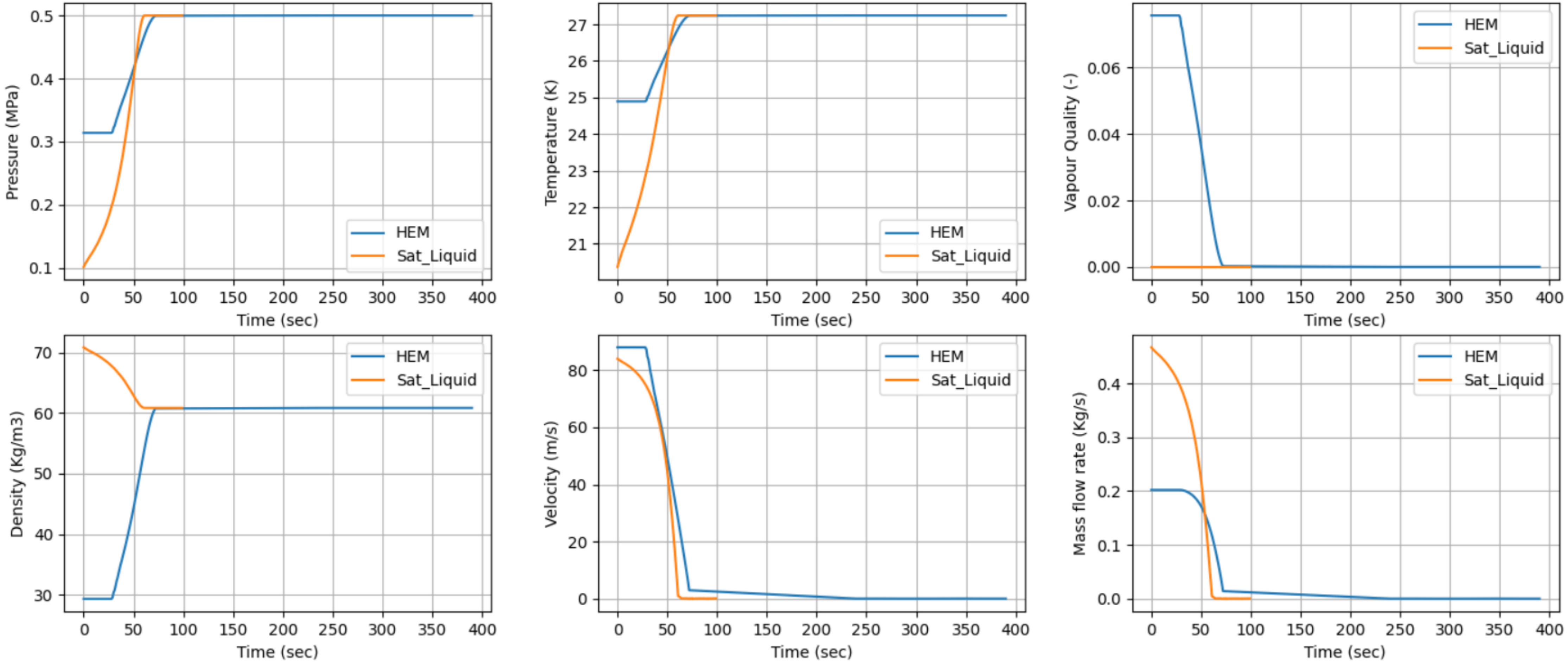


Sat_Liquid



5 bars, Multizone

Predicted conditions at transfer line exit

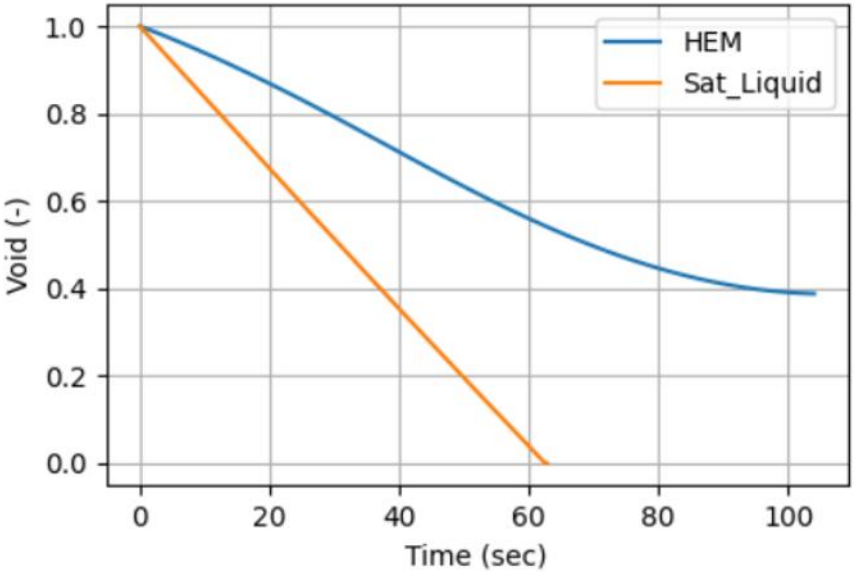


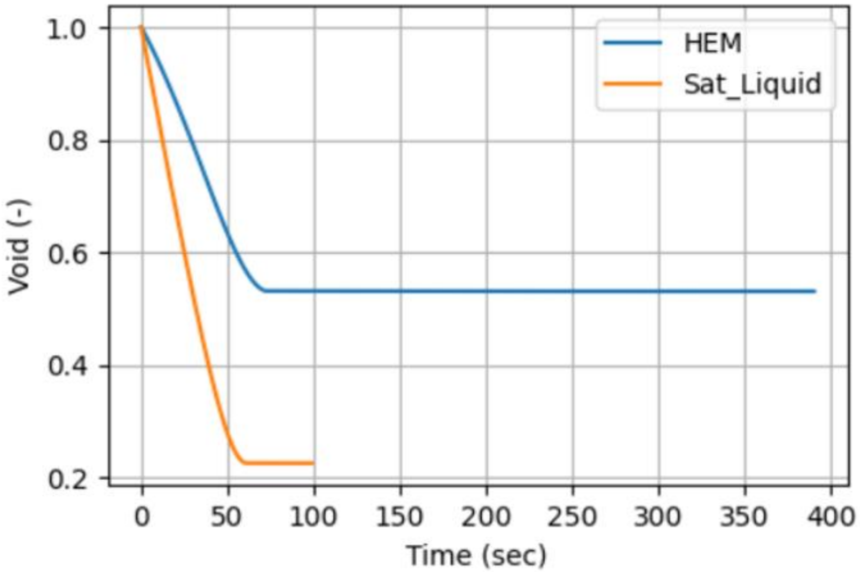
Predicted conditions in receiving tank

Single zone

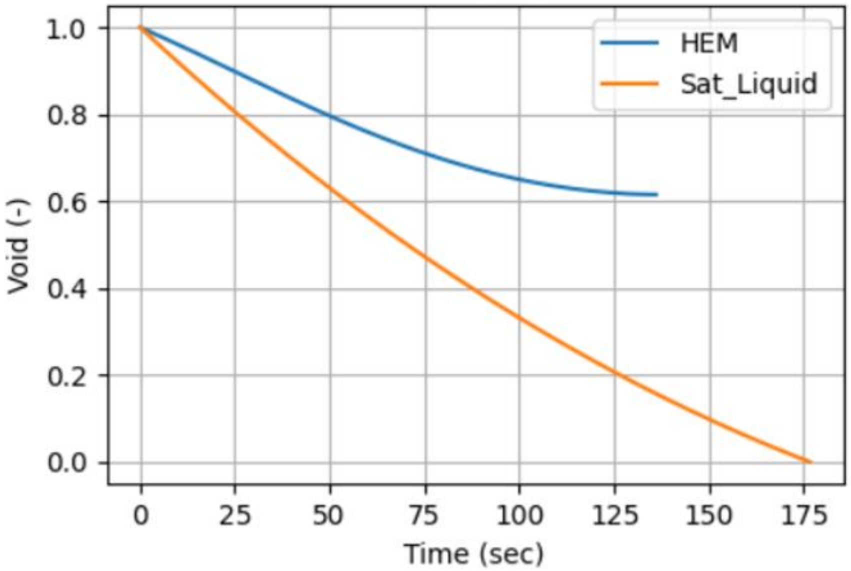
Multi-zone

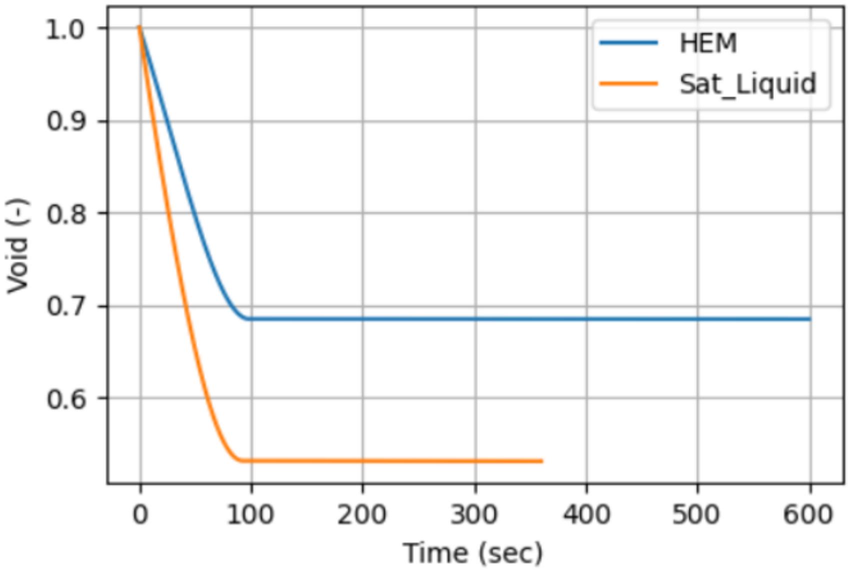
5 bars





2 bars





Conclusions

- DISCHA validation
  - Reasonable agreement against LLNL LH2 boiloff tests and NASA MHTB pressurization tests
- Tank to tank transfer simulations
  - Non-vented pressure filling can be blocked (never reach 100% fill). Happens always with HEM.
  - Multizone model gives lower tank fill compared to single zone
  - Saturated liquid in transfer line gives higher fill compared to HEM
  - Higher pressure gives generally larger fills

Acknowledgments

ELVHYS

Thank you for your attention

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