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A CFD comparison of interfacial phase change models for boil-off, self-pressurisation and thermal stratification in LH2 storage tanks

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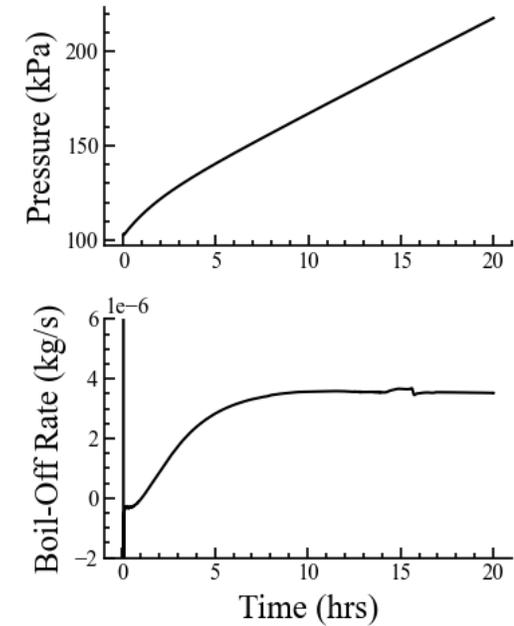
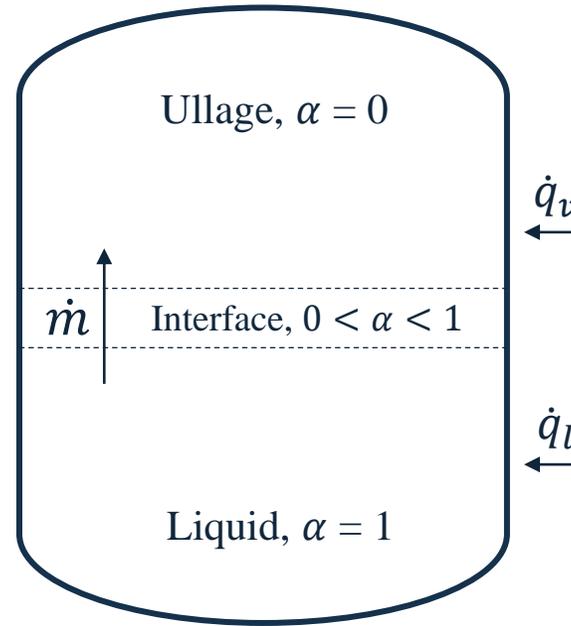
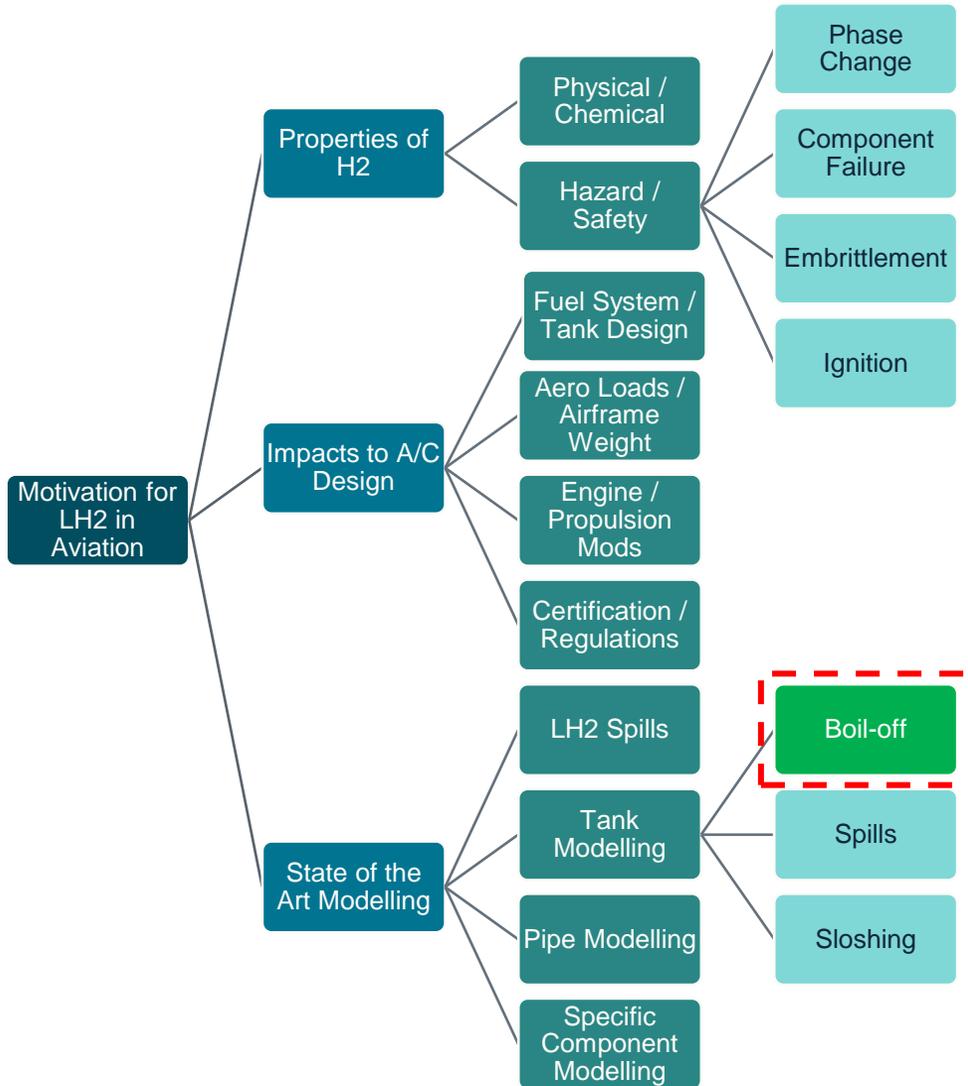


Motivation

- Enabling Net-Zero Transport: Decarbonising hard-to-electrify sectors such as aviation, maritime, and heavy-duty road transport.
- Overcoming Storage Challenges: Boil-off, thermal stratification, structural integrity under dynamic conditions
- Bridging Knowledge Gaps: Critical need for high-fidelity data and validated models to support the design, optimisation, and certification.



Motivation

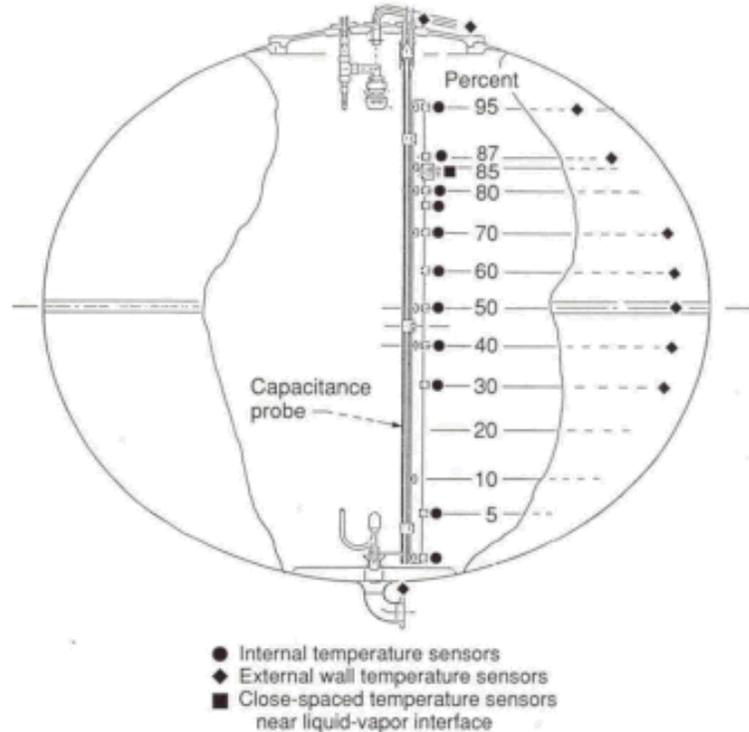


- When a cryogenic liquid e.g. LN2 or LH2, is stored in a tank, ambient heat can cause the liquid to vaporize in a process called **boil-off**
- This raises the internal **pressure** of the tank, requiring appropriate venting
- As well as this many issues are coupled to this e.g.
 - Increased complexity in design and storage
 - Fuel loss > Direct economic loss
 - Operational issues > Refuel duration, Maintenance etc
 - Environmental & Safety

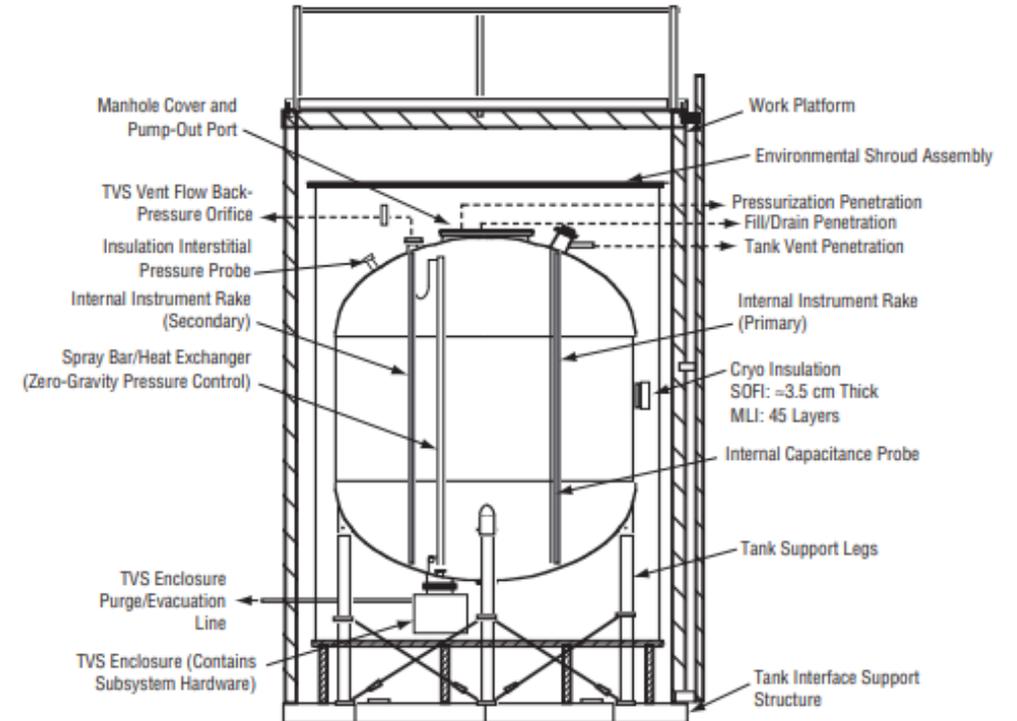
A Fundamental Problem Associated with LH2 Storage



NASA Benchmark Cases



(a) K-Site Tank 1991 [1, 2]
2 Different Experiments at different heats (2.0 and 3.5 W/m²)



(b) MHTB Tank 2000s [3]
3 Different Experiments at 3 different fills (25%, 50% & 90%)



CFD Tank Modelling

Governing Equations: Volume of Fluid (VoF)

$$\frac{\partial(\alpha_l)}{\partial t} + \nabla \cdot (\alpha_l \mathbf{u}) = S_{\alpha_l} - \frac{\alpha_l D\rho_l}{\rho_l Dt} - \frac{1}{\rho_l} \nabla \cdot (\alpha_l \rho_l \mathbf{v}_{d,l})$$

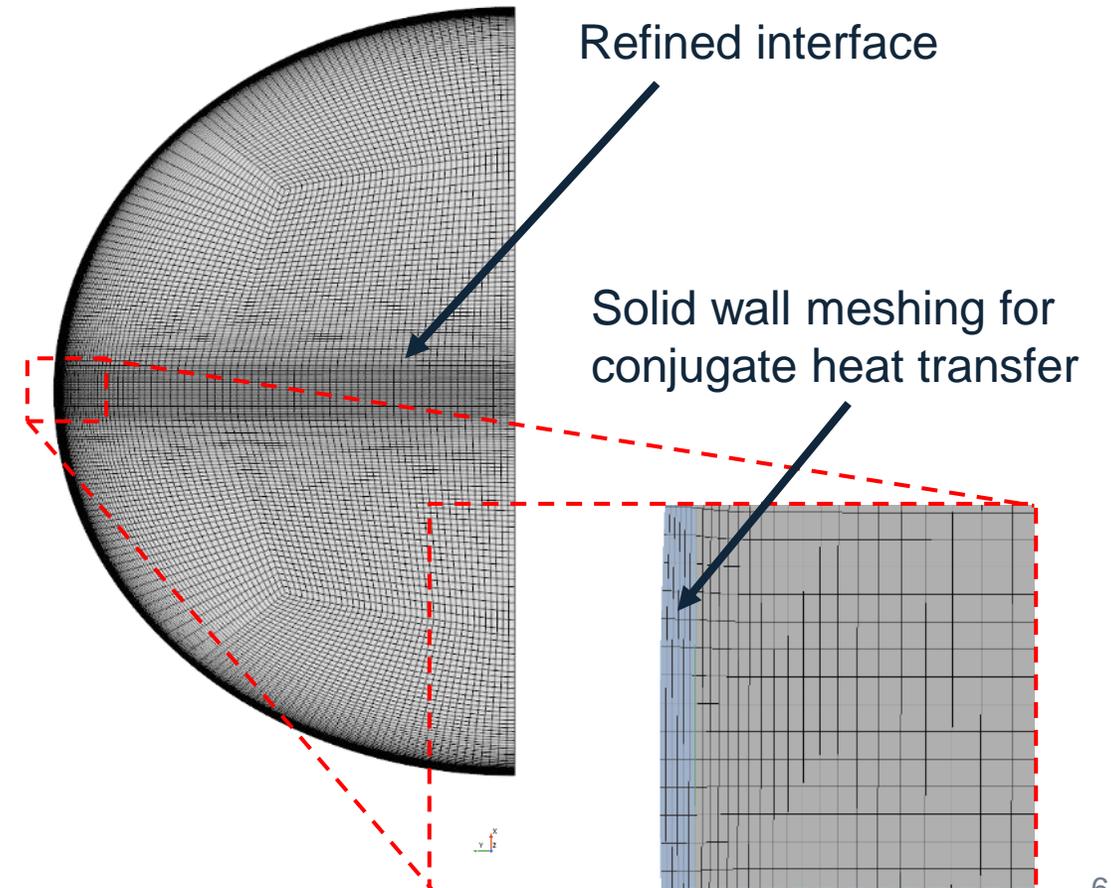
$$\alpha_v = 1 - \alpha_l$$

$$\frac{\partial(\rho)}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S_{\alpha_l} \rho_l + S_{\alpha_v} \rho_v$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = \nabla \cdot (k \nabla T) + \rho \mathbf{g} \cdot \mathbf{u} + S_W + S_E$$

Mesh Generation



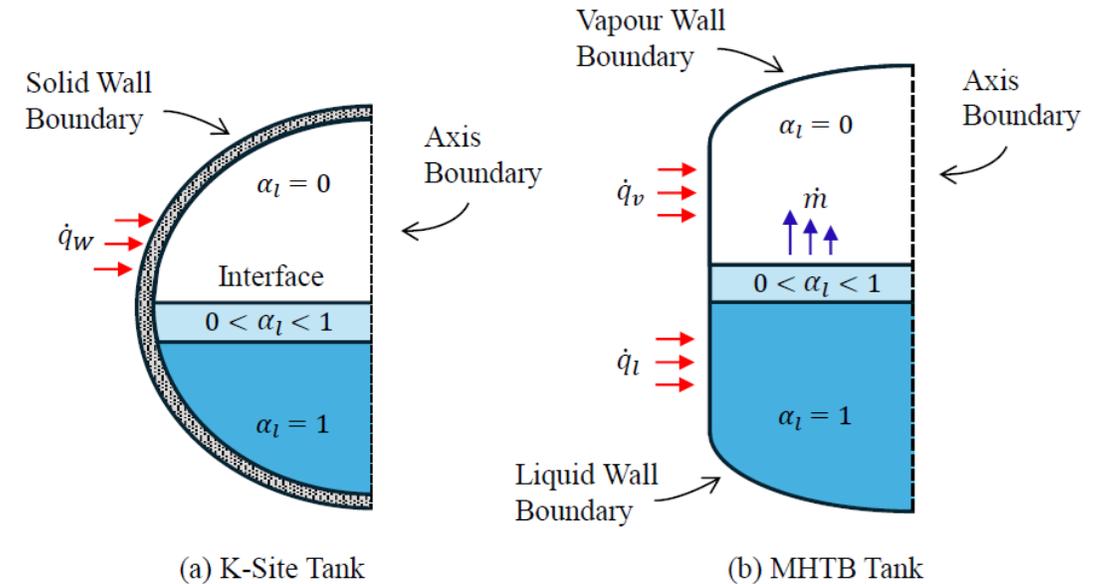


CFD Tank Modelling

Initial Conditions

- MHTB tank – Isothermal conditions used – lack of experimental data
- K-Site tank – Stratified temperature condition from Hasan and Van-Dresar experiment [1].

Boundary Conditions



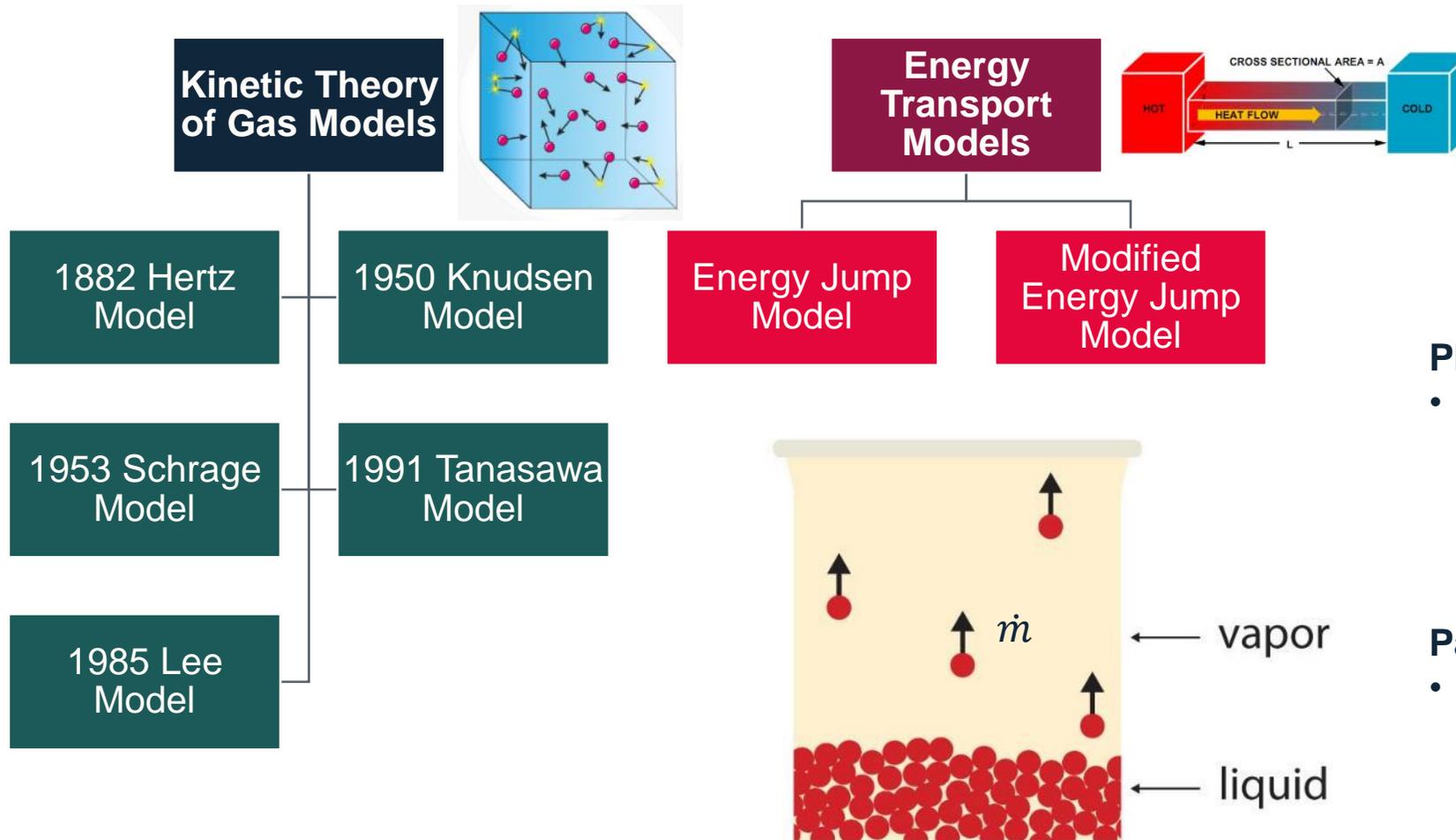
$$q_w = 2.00, 3.50 \text{ W/m}^2$$
$$q_v = 0.45, 0.90, 0.97 \text{ W/m}^2$$
$$q_l = 0.85, 2.08, 2.17 \text{ W/m}^2$$

Haoren [7]



Phase Change Modelling

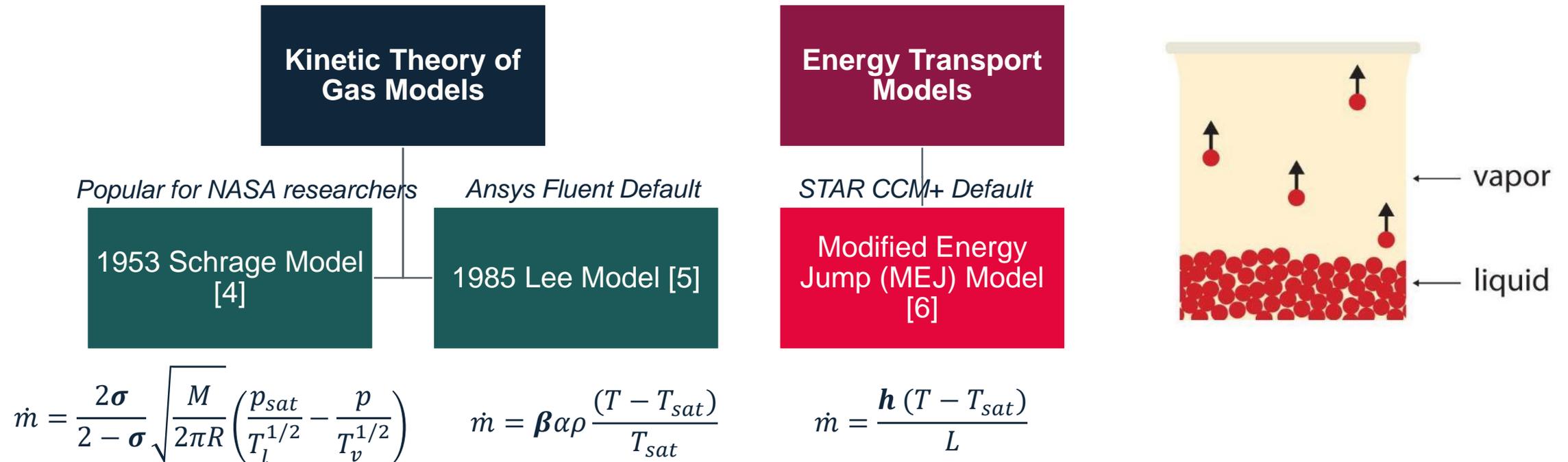
- Two branches of interfacial phase change modelling:





Phase Change Modelling

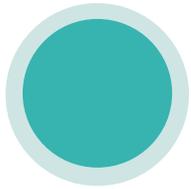
- We chose to study the following popular phase change models in a parametric study:



- Each model has its own characteristic coefficient



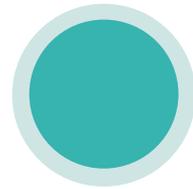
Phase Change Model Comparison



Modified Energy Jump (MeJ) Model

$$\dot{m} = \frac{h(T - T_{\text{sat}})}{L}$$

$$h = \frac{kC\lambda}{l} \cdot Ra^n$$

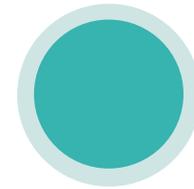


Lee Evaporation/Condensation Model

$$(8) \quad \dot{m} = \begin{cases} \beta\alpha_l\rho_l \frac{T - T_{\text{sat}}}{T_{\text{sat}}}, & \text{for } T > T_{\text{sat}} \\ \beta\alpha_v\rho_v \frac{T - T_{\text{sat}}}{T_{\text{sat}}}, & \text{for } T < T_{\text{sat}} \end{cases}$$

(9)

$$\beta = \sigma \sqrt{\frac{M}{2\pi RT_{\text{sat}}}} \cdot \frac{L\rho_l}{\rho_l - \rho_v} \quad (11)$$



Schrage Kinetics Model

$$(10) \quad \dot{m} = \frac{2\sigma}{2 - \sigma} \sqrt{\frac{M}{2\pi R}} \left(\frac{p_l}{T_l^{0.5}} - \frac{p_v}{T_v^{0.5}} \right) \quad (12)$$

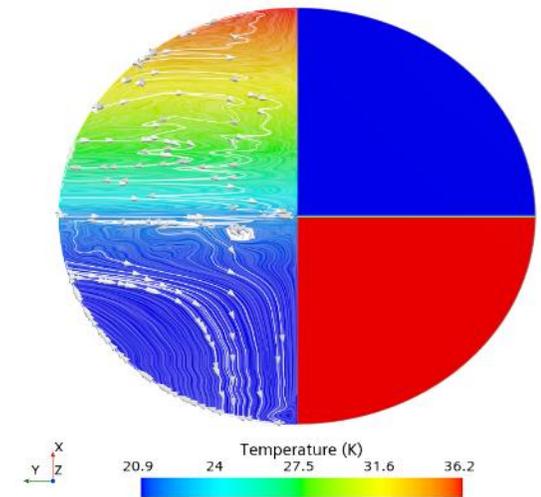
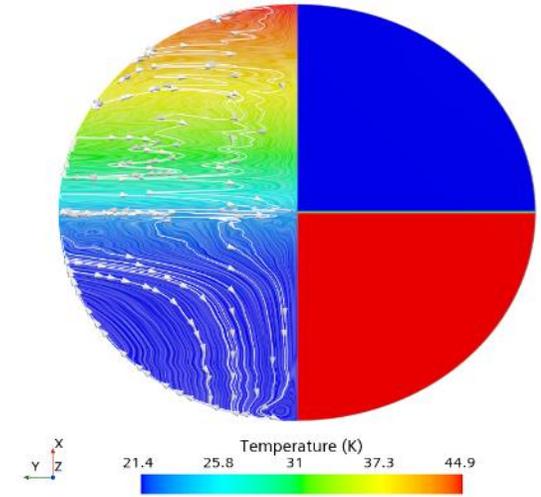
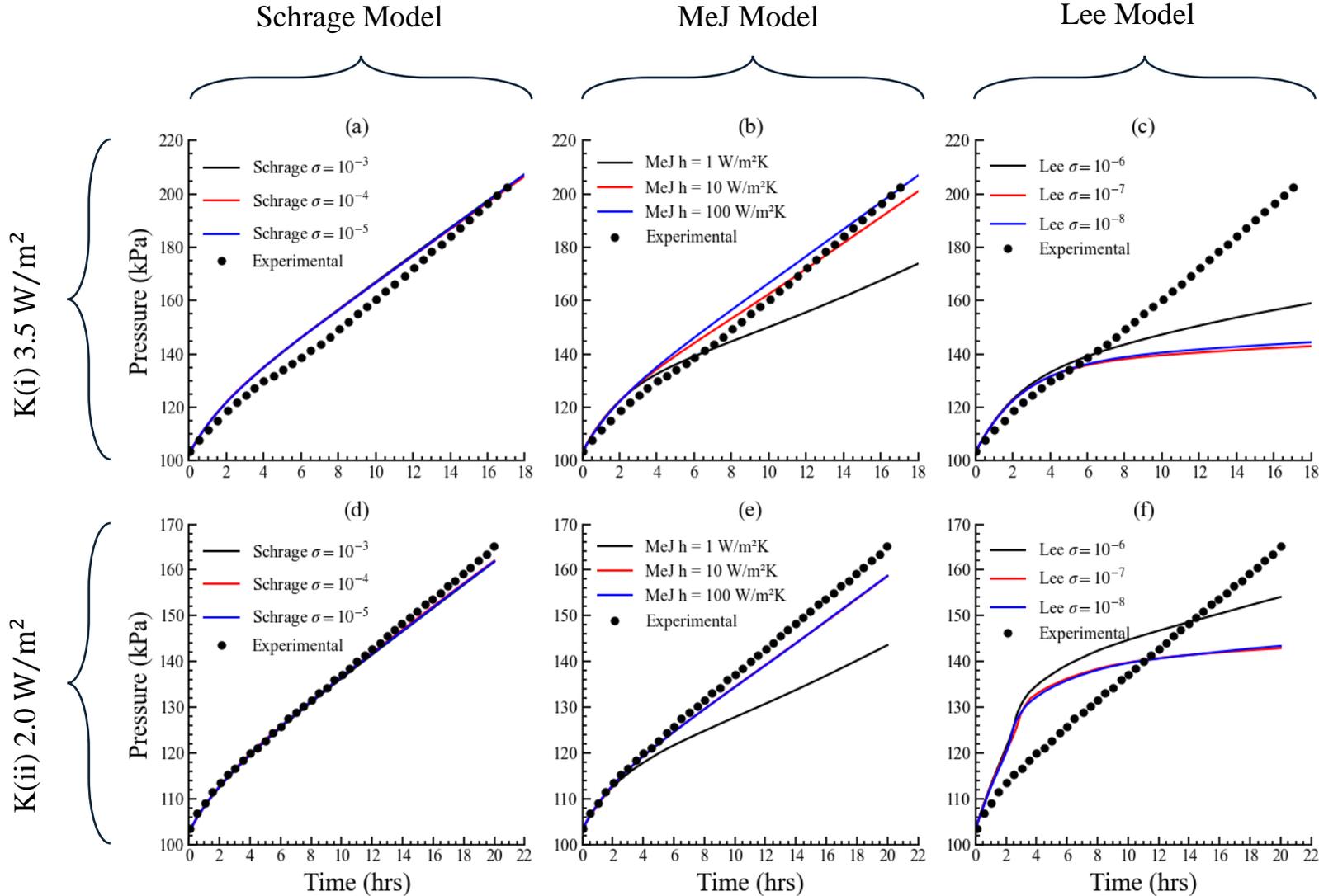
Each model has its own characteristic coefficient

Phase Change Model	Model Coefficient	Units	Values		
MeJ	h	W/m ² ·K	1.0*	10.0	100.0
Lee	σ	–	1e-6*	1e-7	1e-8
Schrage	σ	–	1e-3*	1e-4	1e-5

- We conducted a parametric study on each of the model's coefficients for each experiment
- 5 experiments, 3 phase change models, 3 coefficient variations = **45 total simulations**

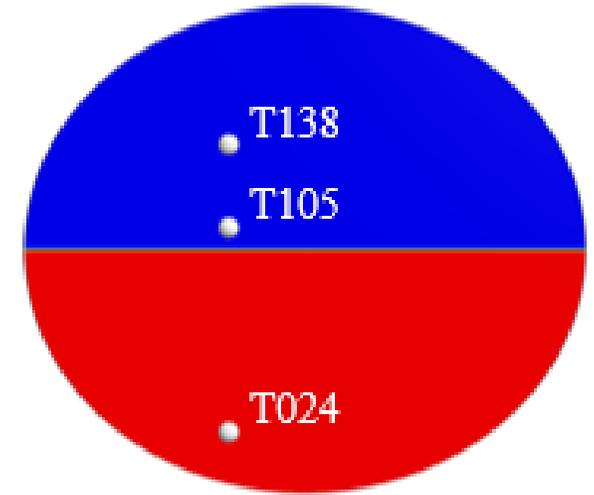
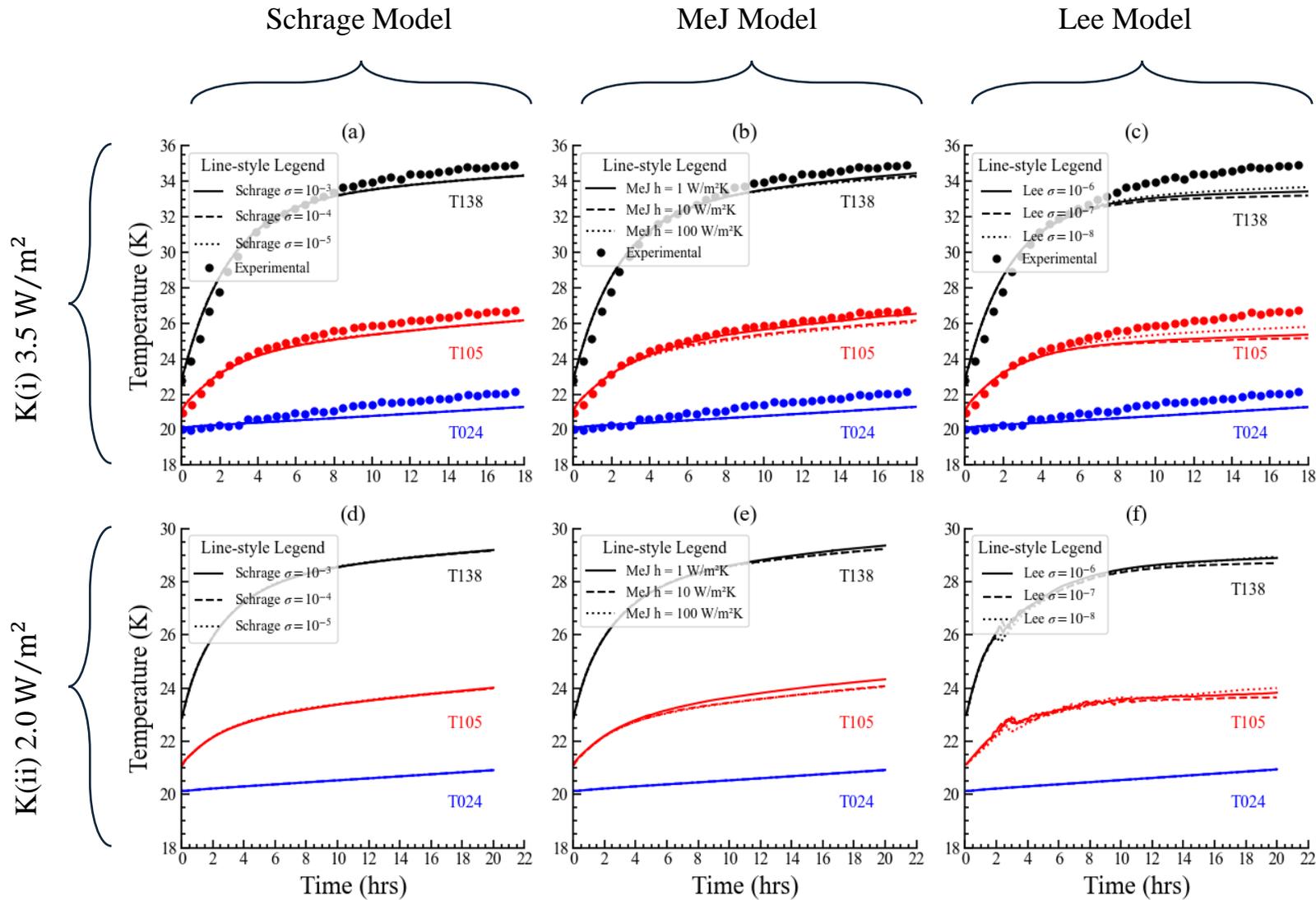


K-Site Pressurisation Results





K-Site Thermal Stratification Results



(a) K-Site



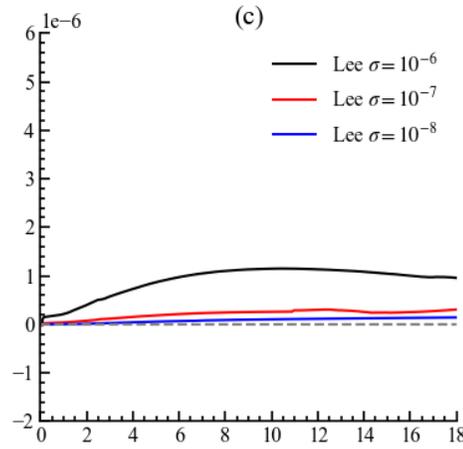
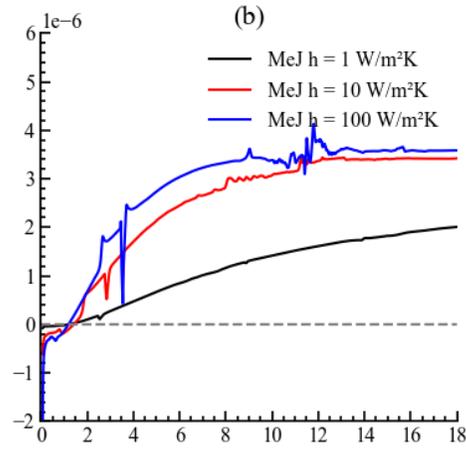
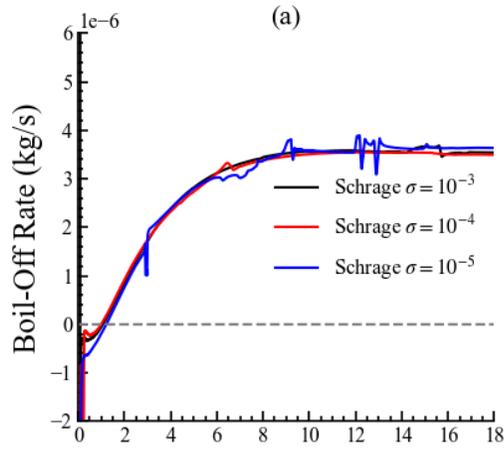
K-Site Boil-Off Analysis

Schrage Model

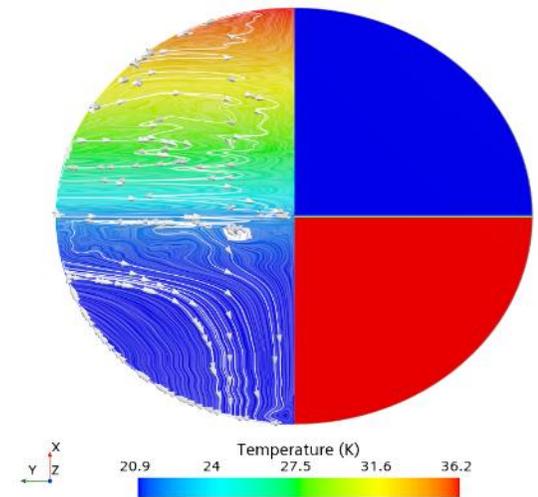
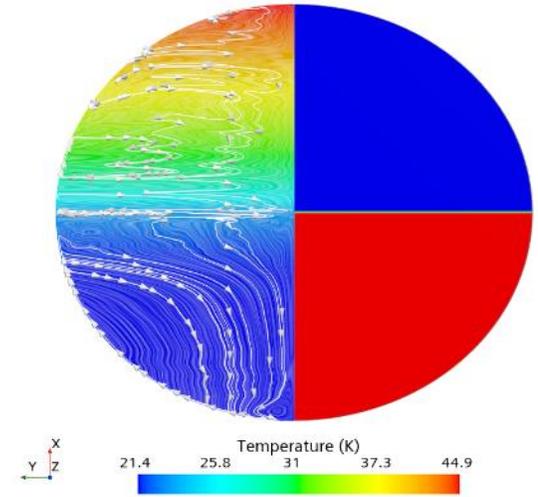
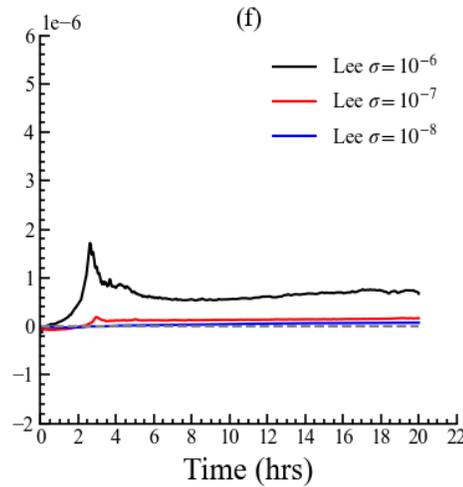
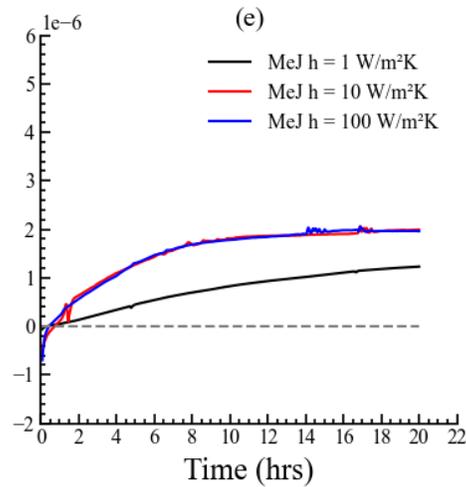
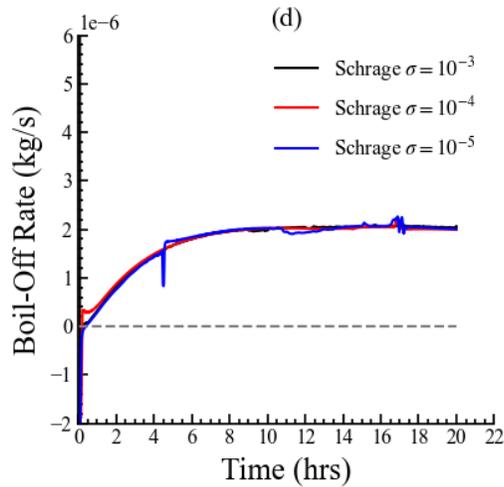
MeJ Model

Lee Model

$K(i)$ 3.5 W/m²

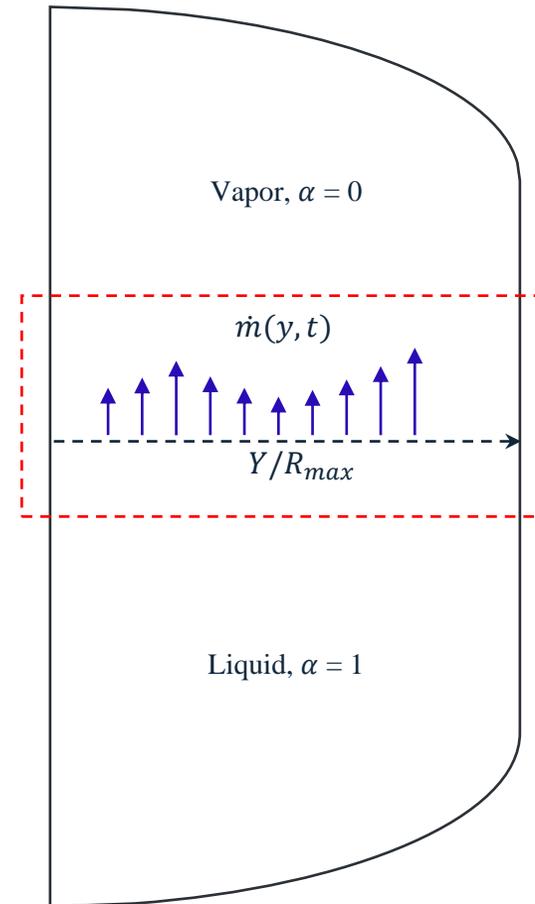
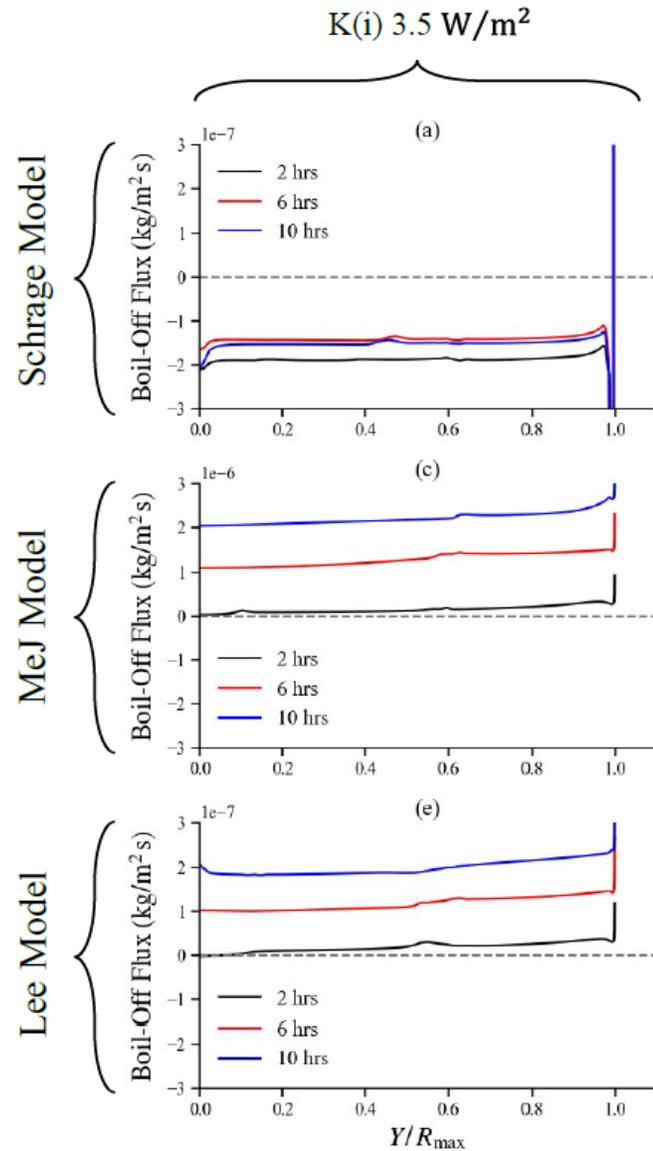


$K(ii)$ 2.0 W/m²





K-Site Boil-Off Analysis





Conclusions

- Modelling Framework: A robust user-defined framework was developed in STAR-CCM+ to simulate LH2 self-pressurisation, boil-off, and thermal stratification, enabling comparative assessment of interfacial phase change models.
- Schrage model: Most accurate and stable across all cases; optimal performance with a coefficient of 10^{-3}
- Modified Energy Jump (MeJ): Accurate when heat transfer coefficients are well-specified. Sensitivity analysis recommended for new cases.
- Lee model: Least accurate, prone to divergence unless thermal expansion dominates.



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