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A condensation model based on Greens Function solution of heat transfer equation at GH2-LH2 interface

3rd workshop on safety of cryogenic hydrogen transfer technologies
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Contents

Background

- Task definitions in ELVHYS Agreement
  - WP3: LH2 transfer facilities performance
  - Subtask 3.3: Theoretical support to the LH2 transfer tests and protocols

- Condensation blocking phenomenon had been observed in practice of LH2 transfer into closed vessels

- It turned out that, condensation blocking at the GH2-LH2 interface dominates the efficiency of LH2 transfer

Motivation of this work

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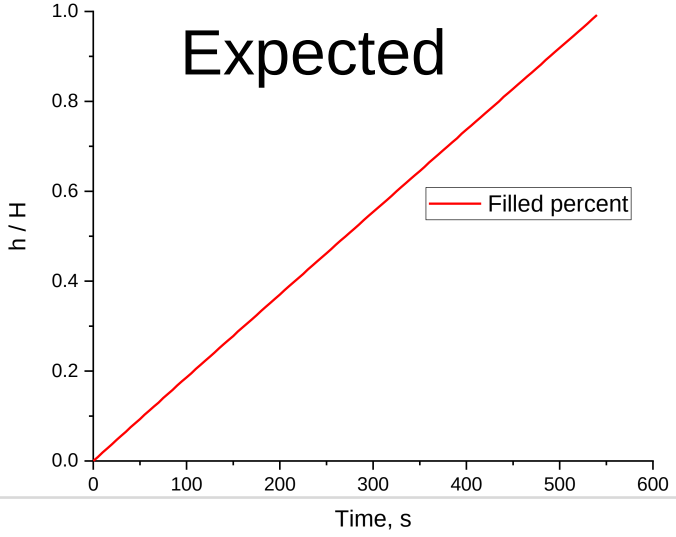
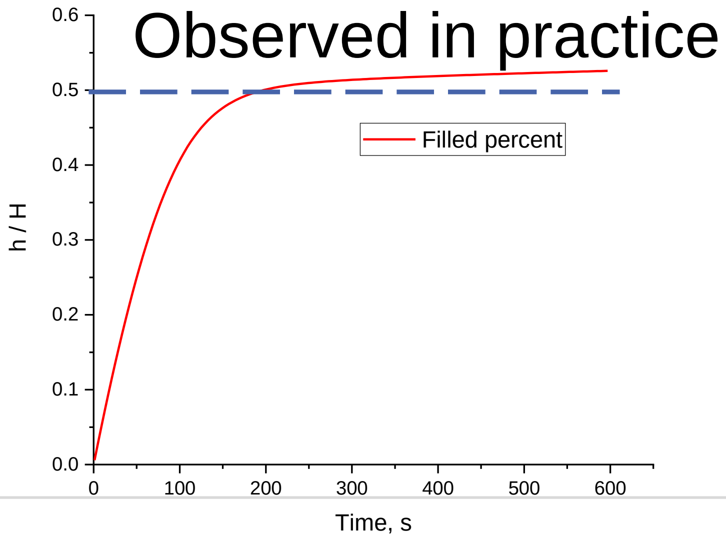
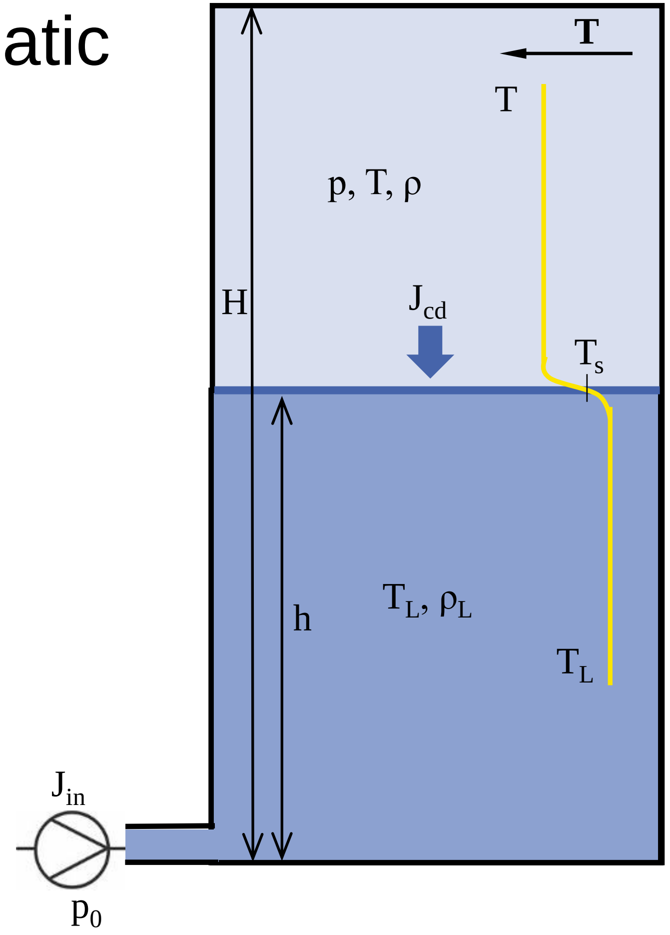
- To understand condensation blocking phenomena thoroughly
- To model condensation blocking properly
- Venting of the LH2 receiving tank is a reasonable way to alleviate condensation blocking
  - The design of a suitable venting system, e.g., nozzle diameter and timing of venting, relies on proper condensation model and thus proper simulation of the filling process
- The developed condensation model will be verified against experimental data, which can be supplied by DLR and/or KIT through LH2 transfer tests

Condensation blocking (1/2)

- LH2 tank: no vent, vacuum insulated, almost adiabatic
- LH2 inflow: $J_{in} = k\,(p_0 - p)$
- Condensation rate: J_{cd}
- Expected filling time is ~ 10 min
- In reality it takes longer than 2100 min (1.5 days)

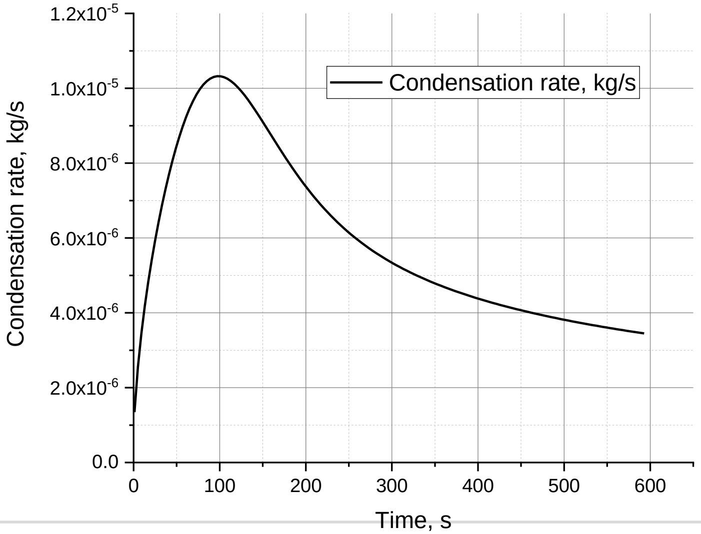


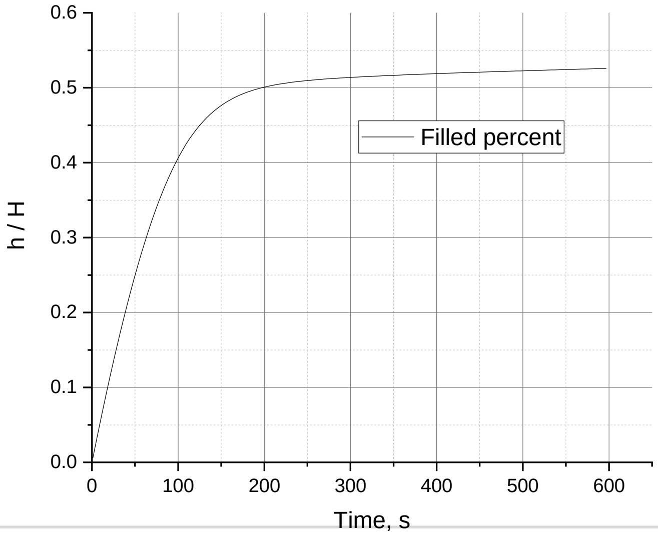


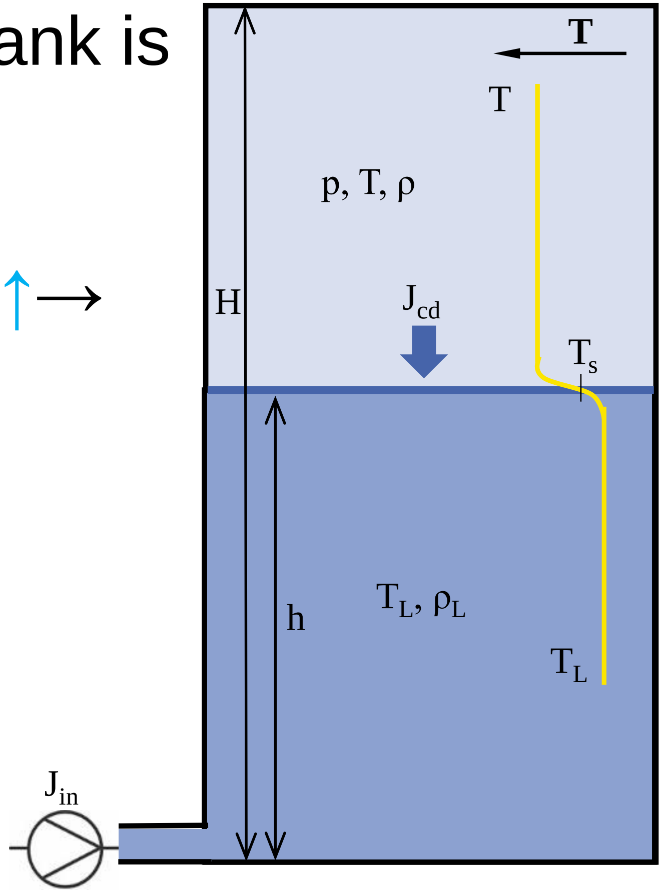


Condensation blocking (2/2)

- Condensation rate starts to decay while ~ 40% of tank is filled
- Decaying condensation rate is called “blocking”
- Condensation blocking: → vapor accumulates → p↑→ T↑ → vaporization↑ → net flux of condensation ↓







Dynamics of filling process

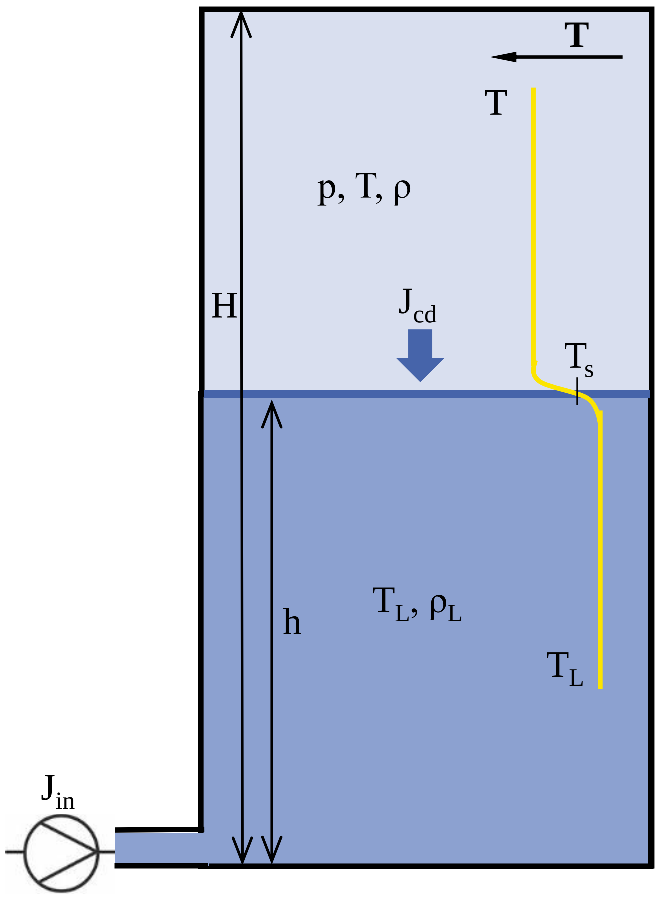
$$\left\{\begin{aligned} \frac{�h}{��} &= \frac{��� + ���}{���} \\ \frac{��}{��} &= \frac{�}{�(� - h)}\left(\frac{���}{��} - \frac{���}{�}\right) \\ \frac{��}{��} &= \frac{��}{���(� - h)}\left(\frac{���}{��} - \frac{���}{�}\right) \end{aligned}\right.$$

(Liquid mass equation)

(Vapor mass equation)

(Internal energy change equals to compression work)

- Assumptions:
  - Incompressible LH2, i.e., $��$ is constant
  - Ideal gas (GH2): $� = ���$
  - $� \ll ��$
  - $��� = �(�_0 - �)$, e.g., $�_0 = 3\ ���, � = 10^{-7} ��/(�� \cdot �)$
- Needed model: $��� = ?$



Traditional model of condensation (1/2)

- Well-known Hertz-Knudsen-Schrage relation

$$\square_{\square\square} = \frac{2\square}{2-\square}\cdot\frac{\square}{\sqrt{2\square\square}}\cdot\left(\frac{\square_{\square}}{\sqrt{\square_{\square}}} - \frac{\square}{\sqrt{\square}}\right)(0<\square<1)$$

$\square, \square$ of bulk vapor, responsible to condensation

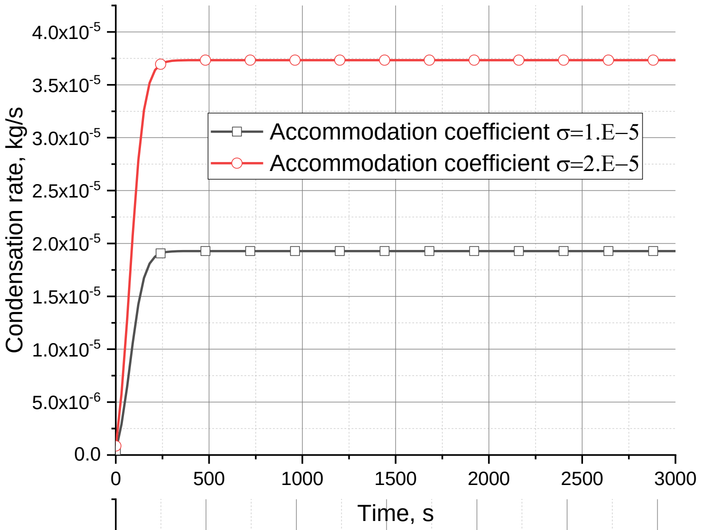
$\square_{\square}, \square_{\square}$ at interface, responsible to vaporization

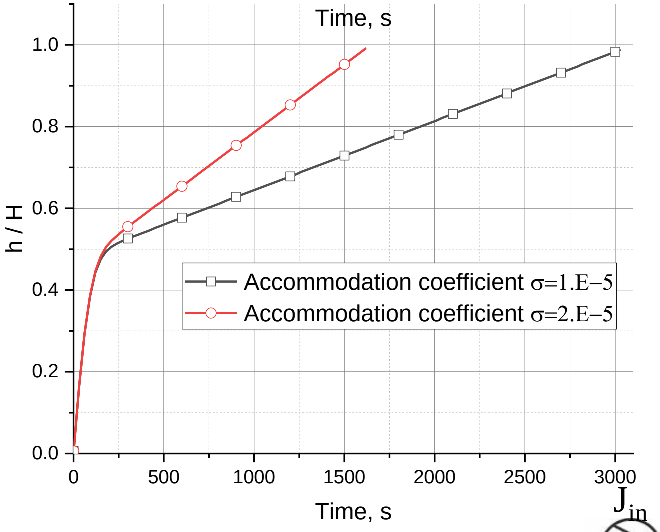
- Derived from molecular statistical mechanics
- $\square_{\square\square}$ depends solely on thermo-dynamic states of vapor and liquid and the accommodation coefficient $\square$
- Implicit assumption: latent heat is transferred away from the interface in a sufficiently fast speed. I.e., thermal accumulation is not considered
- Suitable to equilibrium or quasi-equilibrium state of a vapor/ liquid system

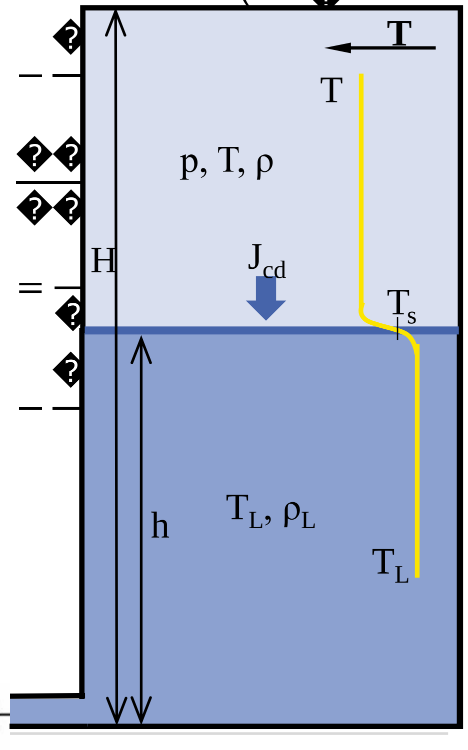
- *Can it explain the condensation blocking phenomenon in case of LH2?*

Traditional model of condensation (2/2)

- Assumptions
  - Saturation at the gas/ liquid interface: ��, ��
  - Pure vapor of H_2: � = ��
  - Ideal gas law: � = ���
- Dynamics equations were solved for condensation rate and filling level
- Result: Condensation blocking does not occur, no matter what value is taken for the accommodation coefficient "�"
- Conclusion: The equilibrium-based condensation model does not work for the dynamic LH2 filling process
- *� varies by orders of magnitude in literatures, there is no clear definition*







Heat-flux-based condensation model

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- What's happening on interface during the filling process?
  phase change →latent heat →heat up interface →heat transfer to liquid
- If heat transfer is sufficiently fast, the interface temperature is maintained at a relatively low level, condensation is maintained without "blocking", like filling water into a closed vessel.
- However, if heat transfer is not fast enough, the interface temperature increases, vaporization is enhanced and net condensation rate drops, until vaporization rate compensates condensation rate. Then net condensation is stopped, like "blocking"

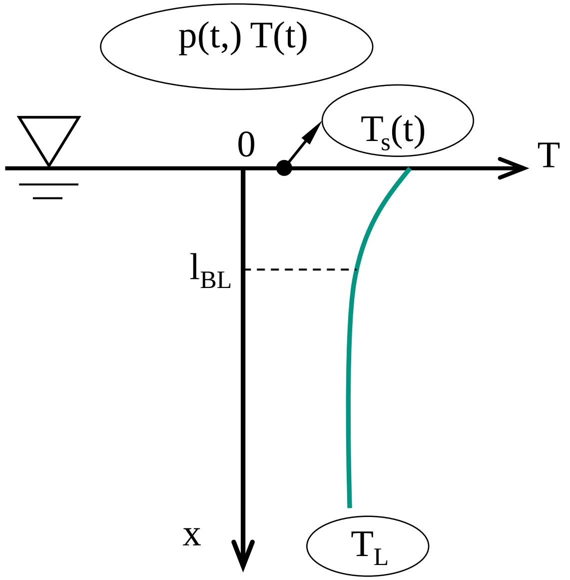
- Latent heat of condensation from phase change is the major heat source for heat transfer from interface to liquid. Thus, condensation rate can be determined by heat transfer flux

Greens function solutions for heat flux at interface (1/3)

- Assumptions
  - Both vapor and liquid at interface are in saturated state
  - Saturation temperature $T_s(t)$ is determined by partial pressure of vapor $p_s(t)$
  - If no other incondensable gas like He is present, $p_s(t) = p(t)$, bulk gas pressure
  - Initial temperature of liquid: $T_L = 20$ K, pressure is 1 bar

- Fourier equation with boundary value (Type I)

$$\begin{cases} \frac{??}{??} - ? \cdot \frac{?^2 ?}{??^2} = 0 \\ ?(?, 0) = ?_? \\ ?(0, ?) = ?_?(?) \end{cases} \qquad \left(? \equiv \frac{?_?}{?_? ?_?} \right)$$



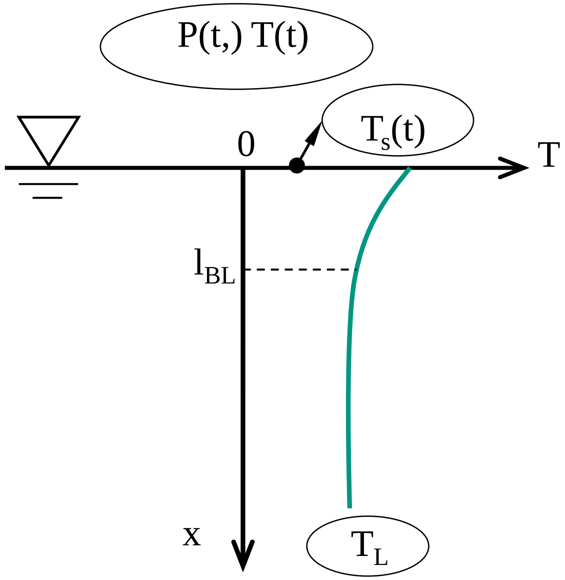
Greens function solutions for heat flux at interface (2/3)

- Greens Function solution of T

$$T(x,t)=T_L\cdot erf\left(\frac{x}{\sqrt{4\cdot D\cdot t}}\right)+\frac{1}{\sqrt{4\cdot\pi\cdot D}}\cdot\int_0^t T_s(\tau)\cdot\frac{x\cdot e^{\frac{-x^2}{4\cdot D\cdot(t-\tau)}}}{(t-\tau)^{\frac{3}{2}}}\,d\tau$$

- Greens Function solution of ∇T

$$\frac{?}{?}(x,t)=T_L\cdot\frac{2}{\sqrt{4\cdot\pi\cdot D\cdot t}}\cdot e^{\frac{-x^2}{4\cdot D\cdot t}}+\frac{1}{\sqrt{4\cdot\pi\cdot D}}\cdot\int_0^t\frac{T_s(\tau)}{(t-\tau)^{\frac{3}{2}}}\cdot\left(1-\frac{2\cdot x^2}{4\cdot D\cdot(t-\tau)}\right)\cdot e^{\frac{-x^2}{4\cdot D\cdot(t-\tau)}}\,d\tau$$



Greens function solutions about heat flux at interface (3/3)

- In ideal case,

$$�|_{�=0} = �_{�} \cdot \frac{��}{��}|_{�=0}$$

Unfortunately, due to mathematical singularity at origin (boundary), value of GF solution at $� = 0$ is not valid or not defined

- As a compromise, heat flux at $� = �_{�h}$ can be determined by using GF solution

$$�|_{�=�_{�h}} = �_{�} \cdot \frac{��}{��}|_{�=�_{�h}}$$

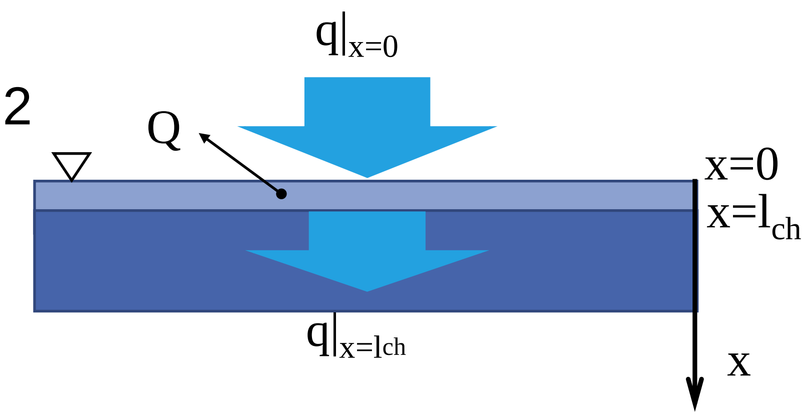
where,

$�_{�h}$ - length scale determined by $�_{�h} = \sqrt{� \cdot �_{�h}}$

$�_{�h}$ - relaxation time of filling, e.g., 0.1 s, $�_{�h}$ ~ 0.1 mm for LH2

- According to energy conservation,

$$�|_{�=0} = �|_{�=�_{�h}} + \frac{�}{�} = �_{�} \cdot ��_{�h}� \cdot \left[�\left(\frac{�_{�h}}{2}, � + ��\right) - �\left(\frac{�_{�h}}{2}, �\right)\right]$$



- If $\frac{�}{�} \ll �|_{�=�_{�h}}$, $�|_{�=0} \approx �|_{�=�_{�h}}$

Condensation blocking in dynamic LH2 filling process (1/3)

$$\begin{cases} \frac{�h}{��} = \frac{�_{��} + �_{��}}{�_{�}�} \\ \frac{��}{��} = \frac{�}{�(� - h)}\left(\frac{�_{��}}{�_{�}} - \frac{�_{��}}{�}\right) \\ \frac{��}{��} = \frac{��}{�_{�}�(� - h)}\left(\frac{�_{��}}{�_{�}} - \frac{�_{��}}{�}\right) \end{cases}$$

$$�_{��} \approx � \cdot \frac{�|_{�=�} �_h}{h_{�}} = \frac{� \cdot �_{�}}{h_{�}} \cdot \frac{��}{��}|_{�=�}$$

$$= \frac{� \cdot �_{�}}{h_{�}}$$

$$T_L \cdot \frac{2}{\sqrt{4 \cdot \pi \cdot D \cdot t}} \cdot e^{\frac{-l_{ch}^2}{4 \cdot D \cdot t}} + \frac{1}{\sqrt{4 \cdot \pi \cdot D}} \cdot \int_0^t \frac{T_s(\tau)}{(t-\tau)^{\frac{3}{2}}} \cdot \left(1 - \frac{2 \cdot l_{ch}^2}{4 \cdot D \cdot (t-\tau)}\right) \cdot e^{\frac{-l_{ch}^2}{4 \cdot D \cdot (t-\tau)}} \, d\tau$$

where, $�_{�}(�) = �\left(�_{�}(�)\right) = �(� \cdot �(�) \cdot �(�))$, in case of pure vapor

$$�_{��} = �(�_0 - �)$$

- Three unknowns $h(�)$, $�(�)$, $�(�)$ and three ODEs form a closed time dependent equation system
- The convolution integral can NOT be computed in a straightforward way, because every individual value at a given time is always related to the historic evolution in the whole time range
- It has to be handled by numerical iterations over the whole filling time, which is not addressed in the present presentation

Condensation blocking in dynamic LH2 filling process (2/3)

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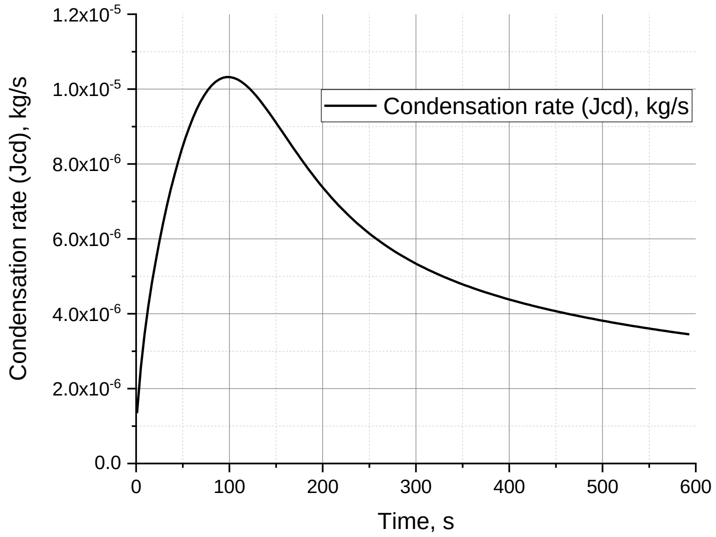
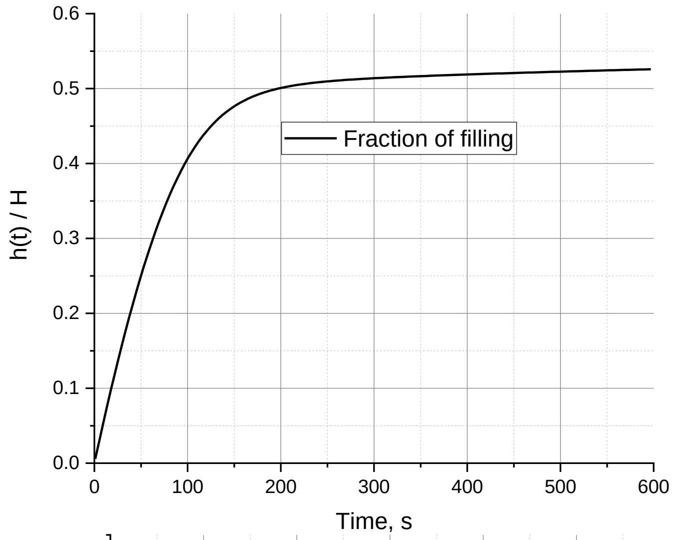
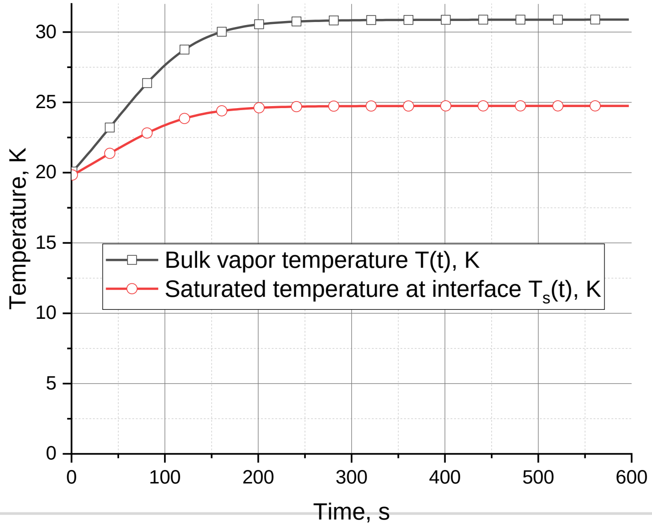
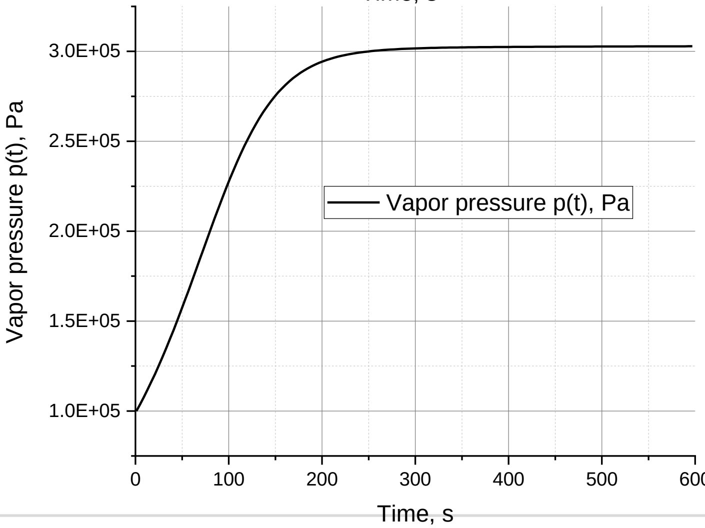
- Condensation blocking is reproduced in a perfect agreement with practice
- Due to the condensation blocking, it needs 1,5 days to fill the closed vessel with LH2
- Core of the simulation work is the Greens Function-solution-based condensation model
- The convergence of the solutions has been proven





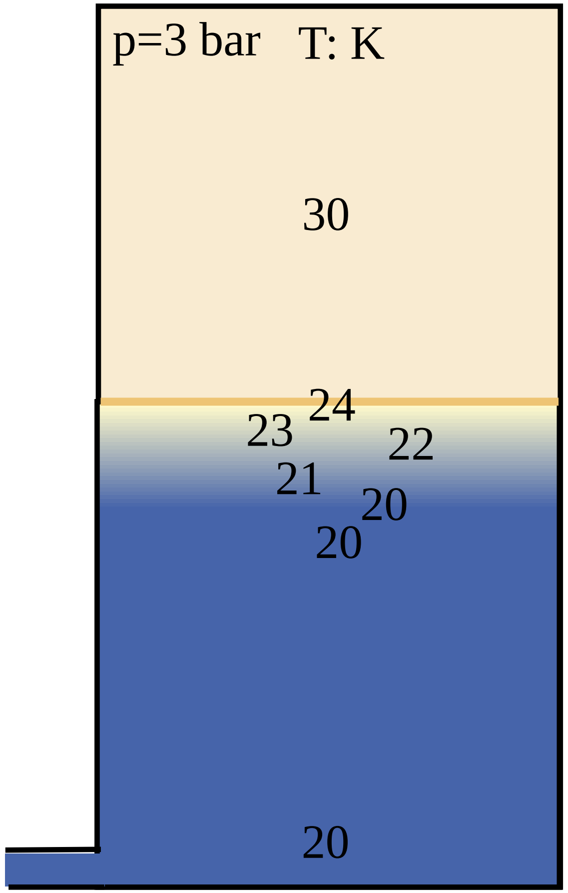




Condensation blocking in dynamic LH2 filling process (3/3)

Heat transfers at the vapor/liquid interface,

- Radiation: ignorable
- Forced convection: no
- Natural convection: no, because of the vertically stratified temperature distribution with a higher temperature on the top and the lowest on the bottom of the vessel
- Thermal conduction from vapor to the interface is ignored owing to
  - Explicit heat is far less than latent heat of phase change
  - Thermal conductivity of vapor is far less than that of liquid

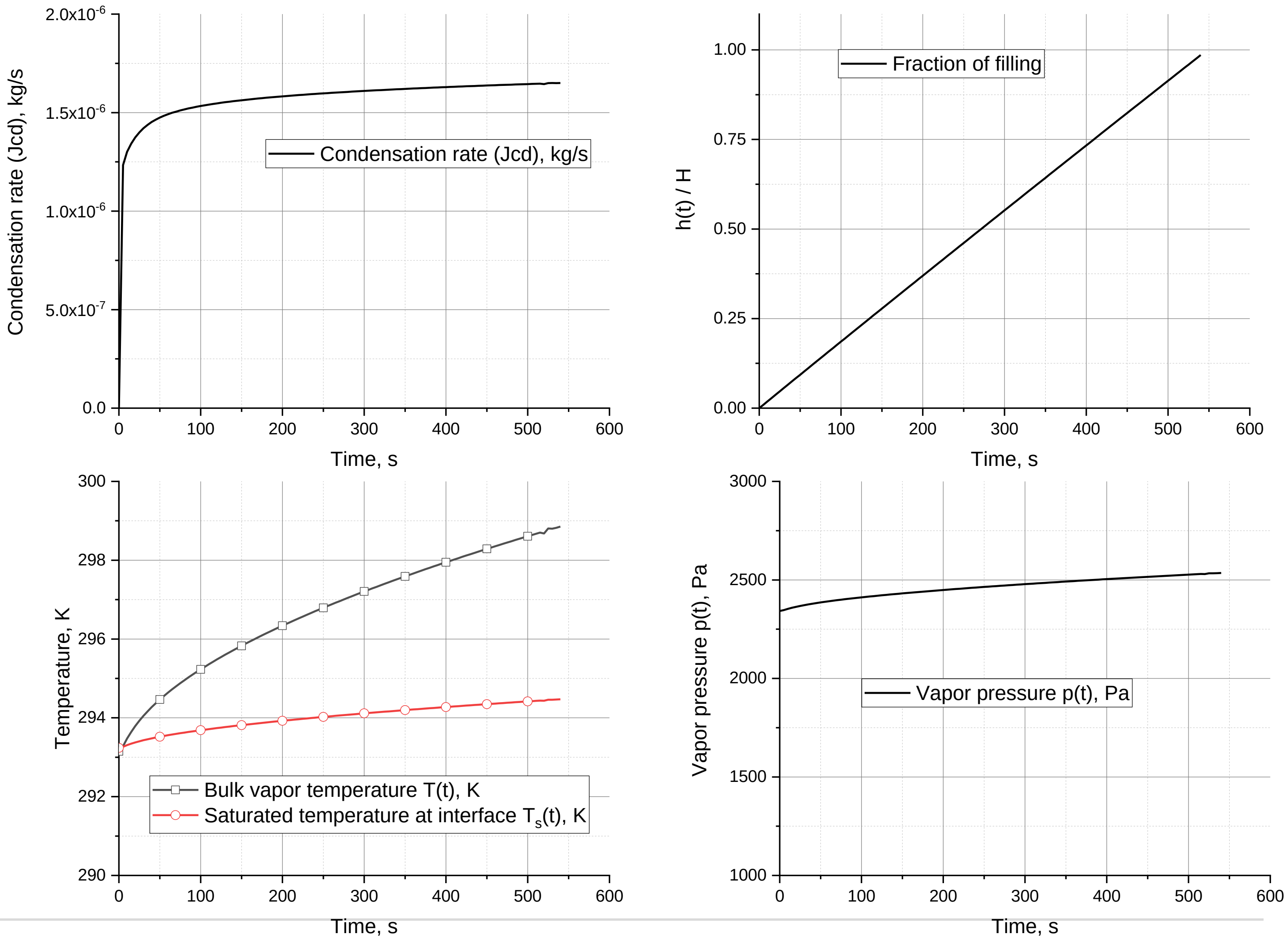


Therefore,

- **Latent heat** released from condensation is almost the only major source of heat. This is the foundation of the heat-flux-based condensation model

Comparison to water filling process

- Same procedure has been applied to water filling with water/steam properties
- As expected, water level increases almost linearly. Vessel is filled up in ~ 550 s
- Condensation rate increases monotonically without “blocking”
- Steam vapor pressure shows slight increase, only a little pressurization occurs



Reasons for condensation blocking during LH2 filling (1/2)

- Obviously, the special thermo-dynamic properties of LH2 determine the condensation feature with “blocking”

- Open question: which properties dominate the phenomenon of condensation blocking ?

$$\dot{?}_{??} = \frac{??}{h_{?}} \cdot \left(T_L \cdot \frac{2}{\sqrt{4 \cdot \pi \cdot D \cdot t}} \cdot e^{\frac{-l_{ch}^{2}}{4 \cdot D \cdot t}} + \frac{1}{\sqrt{4 \cdot \pi \cdot D}} \cdot \int_{0}^{t} \frac{T_s(\tau)}{(t-\tau)^{\frac{3}{2}}} \cdot \left(1 - \frac{2 \cdot l_{ch}^{2}}{4 \cdot D \cdot (t-\tau)}\right) \cdot e^{\frac{-l_{ch}^{2}}{4 \cdot D \cdot (t-\tau)}} \, \mathrm{d}\tau \right)$$

Reasons for condensation blocking during LH2 filling (2/2)

- Comparison of LH2 (sat.@20 K, 10^5 Pa) and water (sat.@293 K, 2340 Pa)

	Thermal conductivity of liquid, λ_l, W/(m·K)	Initial saturation temperature, T_s, K	Latent heat at saturation temperature, h_{lv}, kJ/kg	Length scale of thermal diffusion $L_{th} = \sqrt{\alpha \cdot t_{th}}$, L_{th}, m	Initial inflow mass flux of liquid, $\dot{m}_{in}$, kg/(m²·s)	Newly proposed dimensionless number, $\frac{h_{lv} \cdot L_{th} \cdot \dot{m}_{in}}{\lambda_l \cdot T_s}$
H2	0.1	20	450	1.2E-4	0.4	11
H2O	0.6	293	2450	1.2E-4	1.9	3

$$NN = \frac{h_{lv} \cdot L_{th} \cdot \dot{m}_{in}}{\lambda_l \cdot T_s}$$

- Can it be a general criterion for condensation blocking in filling process? E.g., if $NN > NN_{critical}$, then condensation blocking would occur.
- Further tests needed, e.g., is it relevant to density ratio btw. vapor and liquid?

Conclusions

- Traditional condensation model (HKS relation) is not able to explain the condensation blocking phenomenon occurring in the dynamic process of LH2 filling into a none-vented vessel

- Instead, using the Greens Function solution of heat conduction equation, a new heat-flux-based condensation model is proposed, which can explain the condensation blocking effectively

- A dimensionless number is proposed to judge if condensation blocking occurs in fluid filling processes. However, more fluids like liquid O_2, N_2, He, etc., need to be tested in next steps