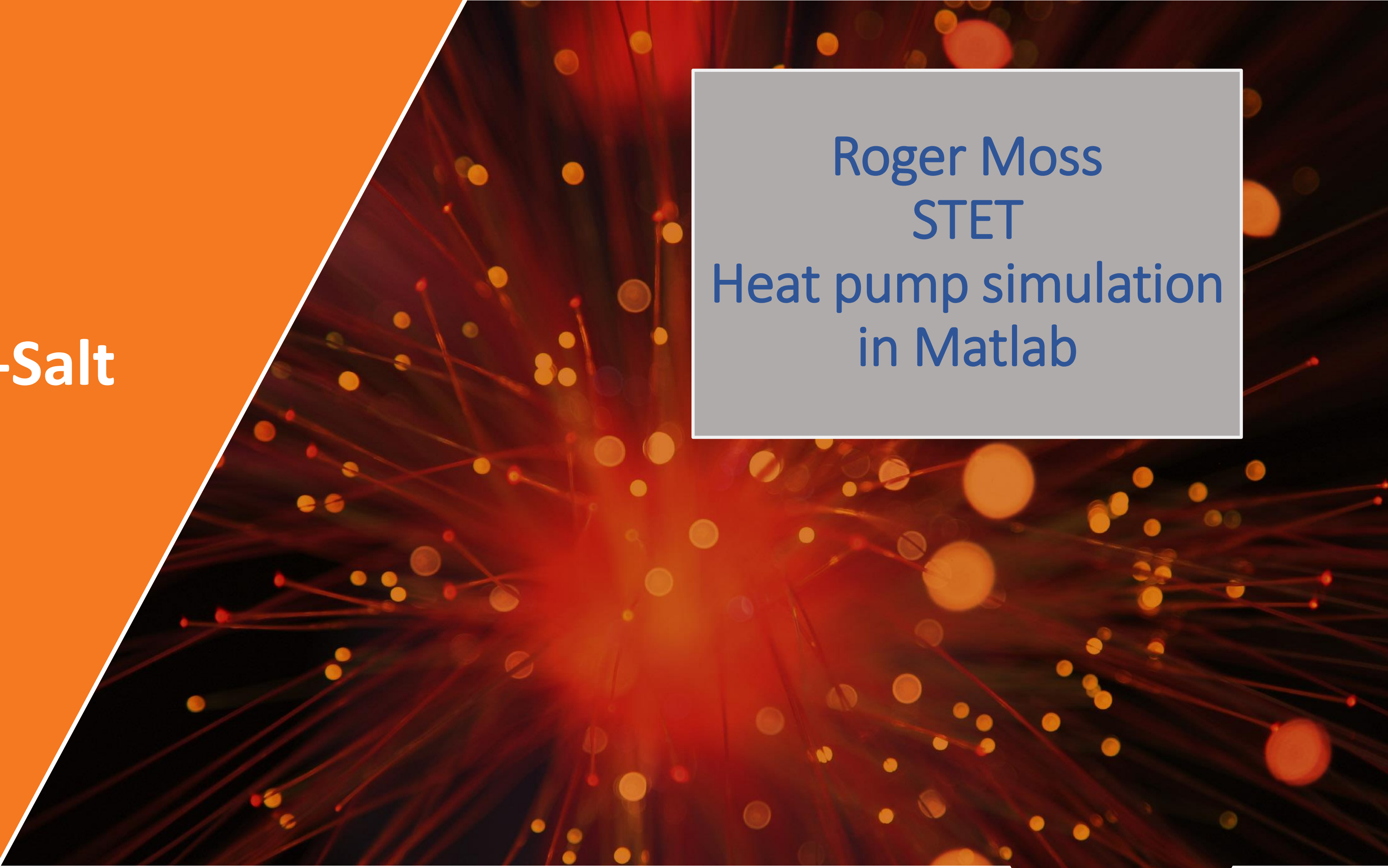
MI meeting

3rd June 2021

Session 3 - Ammonia-Salt Research at Warwick



Roger Moss
STET
Heat pump simulation in Matlab

STET MISSION INNOVATION

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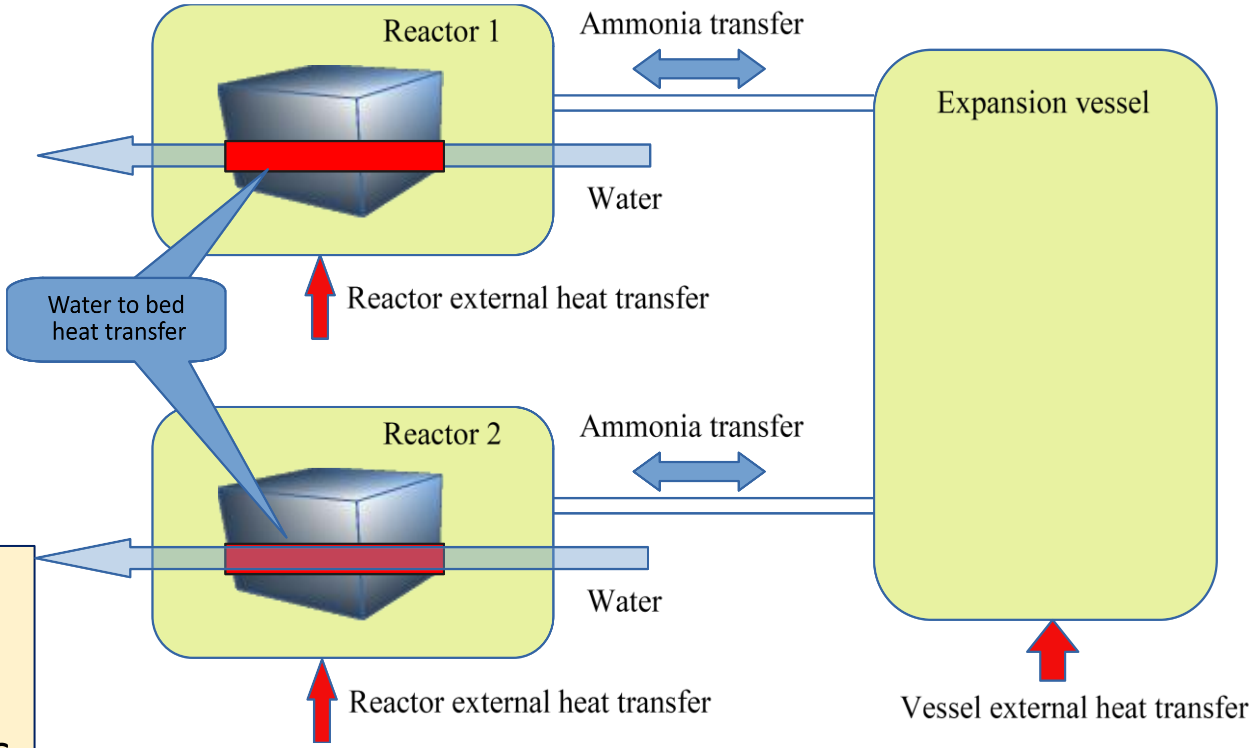
Ammonia/salt adsorption code development

Simulation code:

- 1, 2 or more reactors
- Cuboid or cylindrical 2D grid
- ENG + 1 or more salts per reactor
- Driven by temperature versus time water flows (heat transfer coefficient).
- Models heat transfer, reaction rate, ammonia transfer through ENG



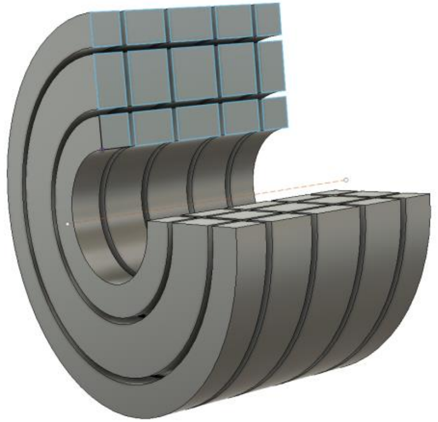
Output viewer:

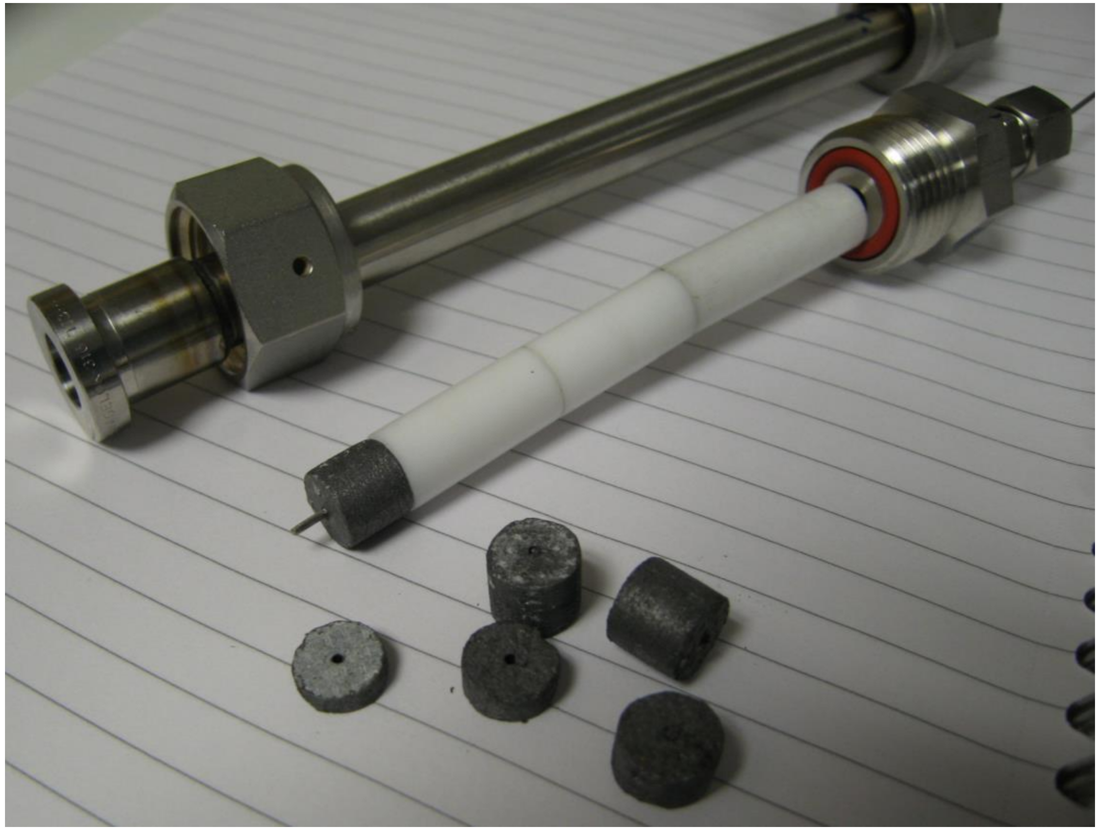
- Separate window for each reactor
- Time history for area mean or spot parameters
- Animated 2D grid surfaces
- Experimental comparisons

- ➢ Ability to model ENG pellets

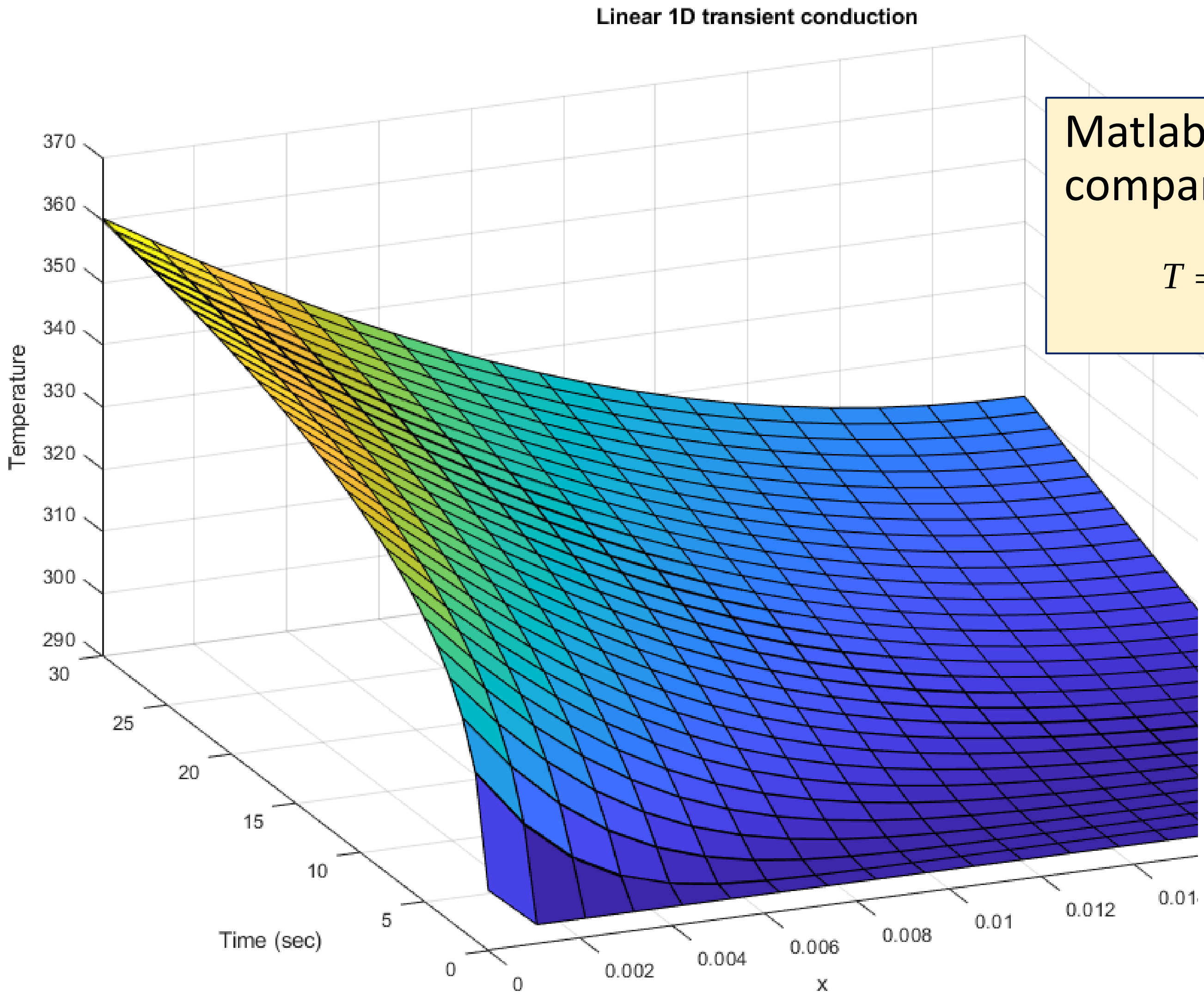
e.g. Cycling Rig and LTJ - external heating, internal thermocouple.

- ➢ Can also model internal heating e.g. “kebab” of ENG with central tube.



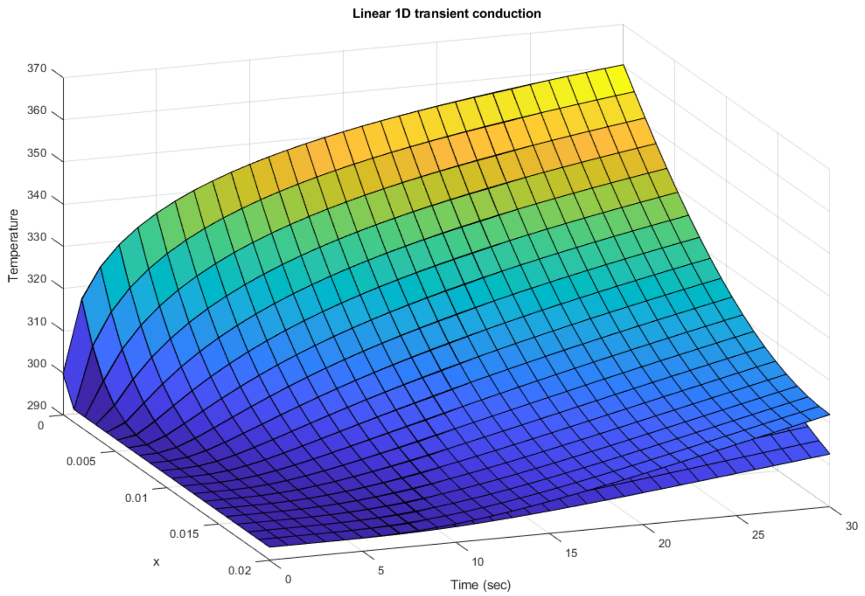


Conduction equation validation



Matlab solution with a step in water temperature compared with the semi-infinite analytical solution

$$T = T_2 + (T_1 - T_2)\left[\operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right) - e^{\left(\frac{hx}{k}+\frac{\alpha h^2 t}{k^2}\right)}\operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}}+\frac{h\sqrt{\alpha t}}{k}\right)\right]$$



Ammonia transport through ENG

Matrix solution of a resistance network

Assume Darcey's law $Q = \frac{Ak}{\mu}\frac{dP}{dx}$ for cell-to-cell transport.

Permeability $k \approx 2 \times 10^{-12}$ m²

Volume flow rate $Q_1 = T_1 \frac{k}{\mu} p_1$ etc

$q_1 = Q_1 - Q_2 + Q_{13} - Q_{14}$ etc

(assume constant density & viscosity).

Column vectors $\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{Q}$:

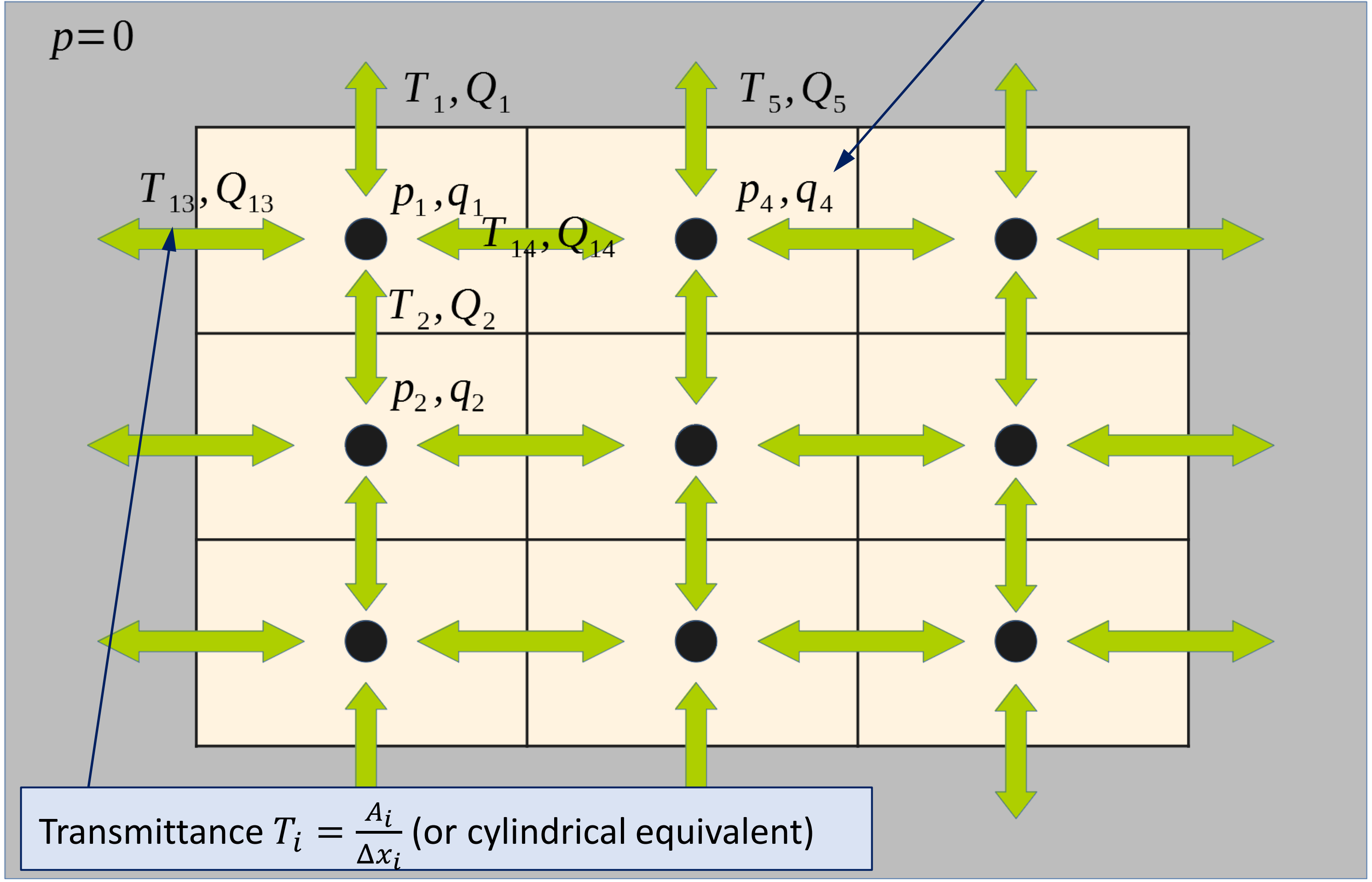
$$\boldsymbol{JQ} = \boldsymbol{q},\ \boldsymbol{Q} = \frac{k}{\mu}\boldsymbol{Tp}.$$

Solve:

$$\boldsymbol{p} = \frac{\mu}{k}(\boldsymbol{JT})^{-1}\boldsymbol{q}$$

$$\boldsymbol{Q} = \boldsymbol{T}(\boldsymbol{JT})^{-1}\boldsymbol{q}$$

Cell adsorption & desorption rates q from the reaction rate equation.



Energy equations

Energy equation for each cell:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \dot{Q}_{in} + \dot{W}_{in} + \sum \dot{m}_{in,j} h_j$$

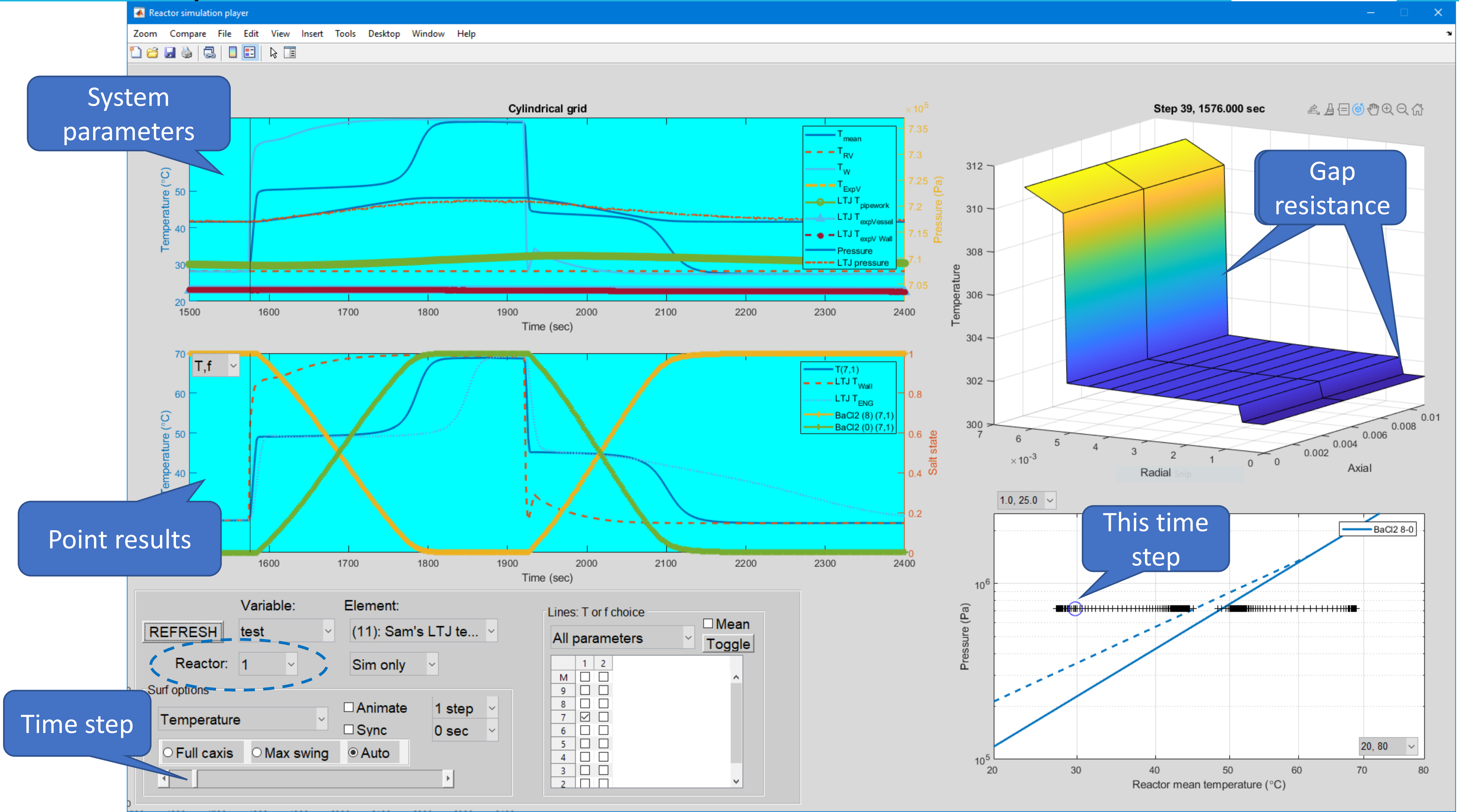
$$\sum_{cell} (mc_v) \frac{\mathrm{d}T}{\mathrm{d}t} + \Delta U_{ads} \left. \frac{\mathrm{d}m}{\mathrm{d}t} \right|_{NH_3,ads} = \dot{Q}_{conduction} + \sum \dot{m}_{in,j} h_j$$

$$\therefore \sum_{cell} (mc_v) \frac{\mathrm{d}T}{\mathrm{d}t} + \Delta H_{ads} \left. \frac{\mathrm{d}m}{\mathrm{d}t} \right|_{NH_3,ads} \approx \dot{Q}_{conduction} + \sum \dot{m}_{in,j} c_p \Delta T_j$$

Energy equation for reactor vessel and its gas:

$$\sum_{reactor} (mc_v) \frac{\mathrm{d}T}{\mathrm{d}t} = \dot{Q}_{water} + \dot{Q}_{ENG} + \sum \dot{m}_{in,j} c_p \Delta T$$

Output viewer



LTJ comparisons (1) – desorption, matching pressure rise

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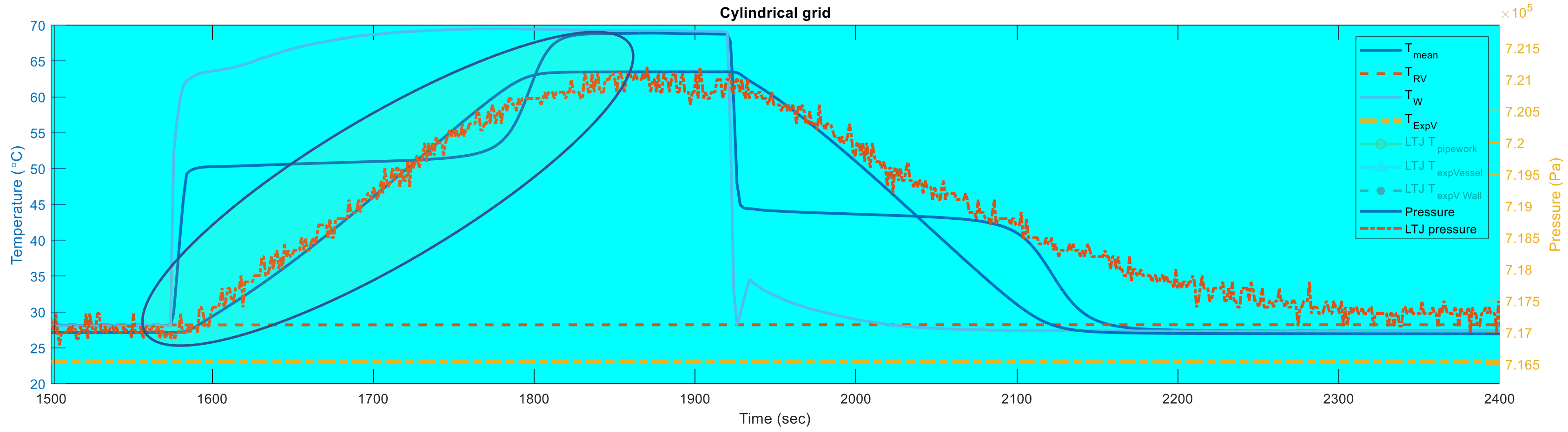
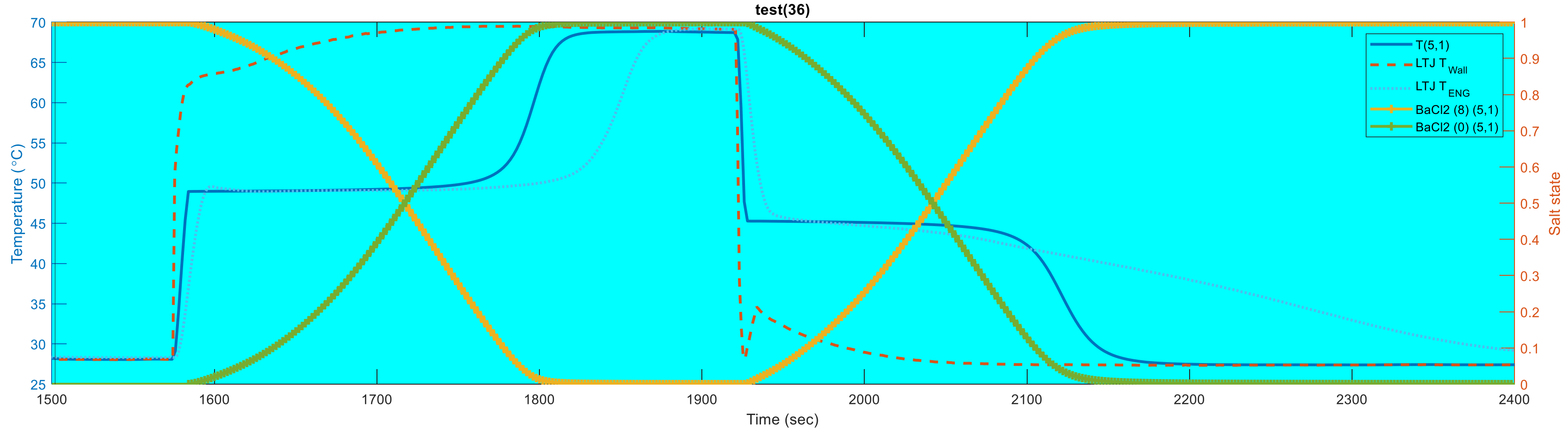




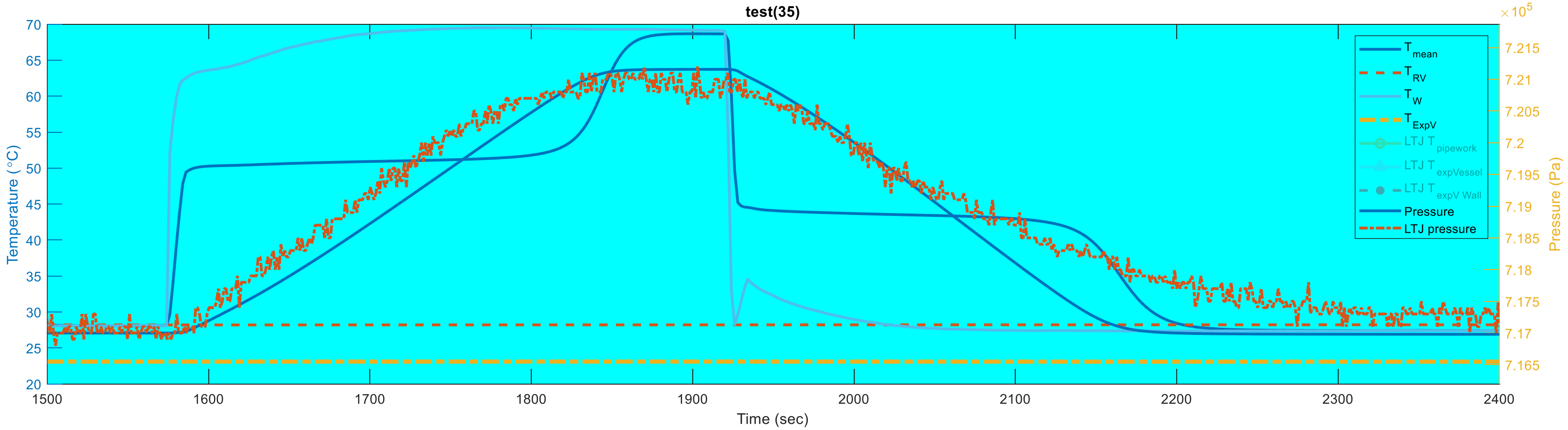
Sam's $BaCl_2$ at 7 bar, modelled with inner & outer gap.

90% of salt content.

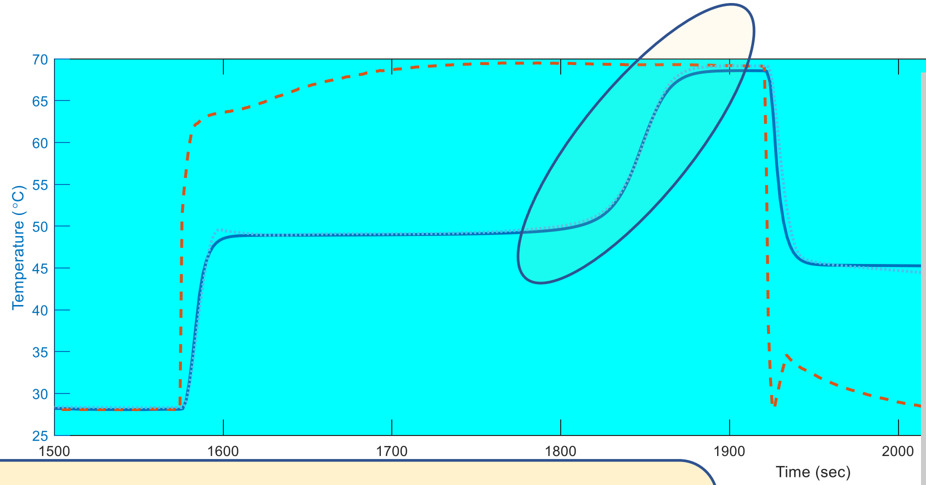
Gaps	0.09 mm
y_{des}	1.5
A_{des}	1

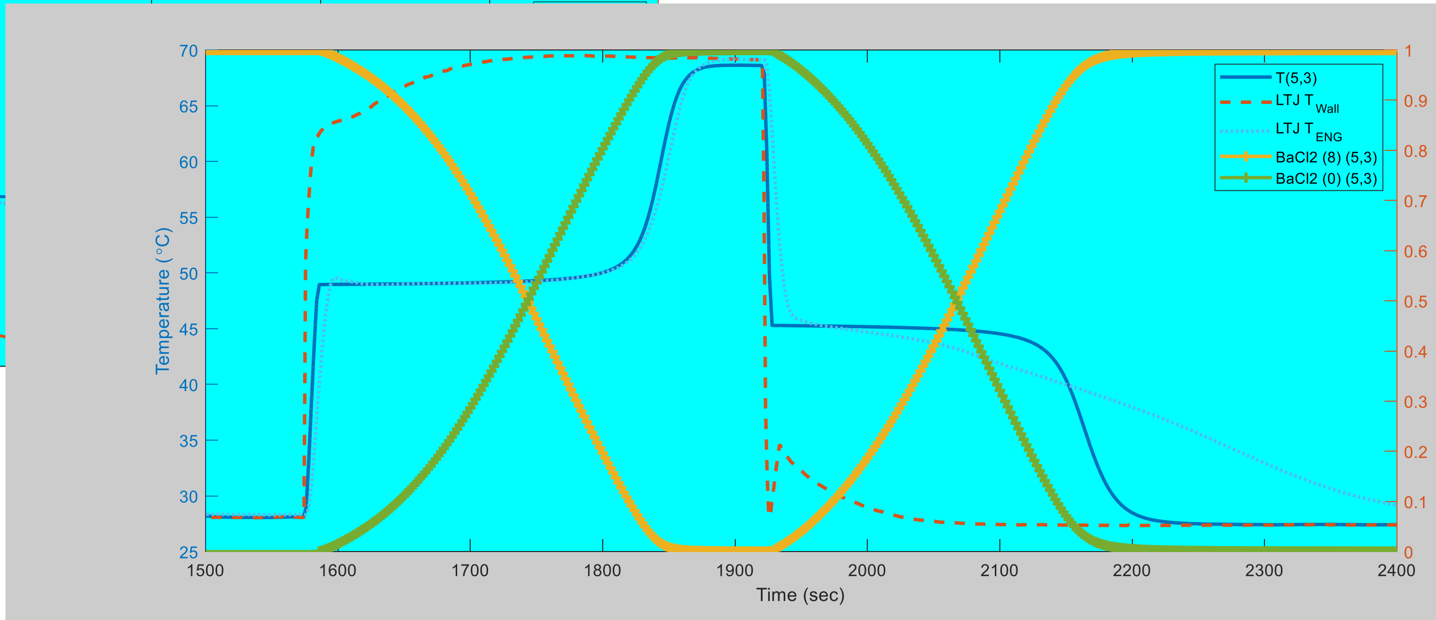
$$\frac{1}{f_A + f_B}\frac{\mathrm{d}f_A}{\mathrm{d}t} = A_{AB}\left(\frac{f_A}{f_A + f_B}\right)^{y_{AB}}\left(1 - \frac{p_{Clap}}{p}\right)$$

LTJ comparisons (2) – desorption, matching internal thermocouple



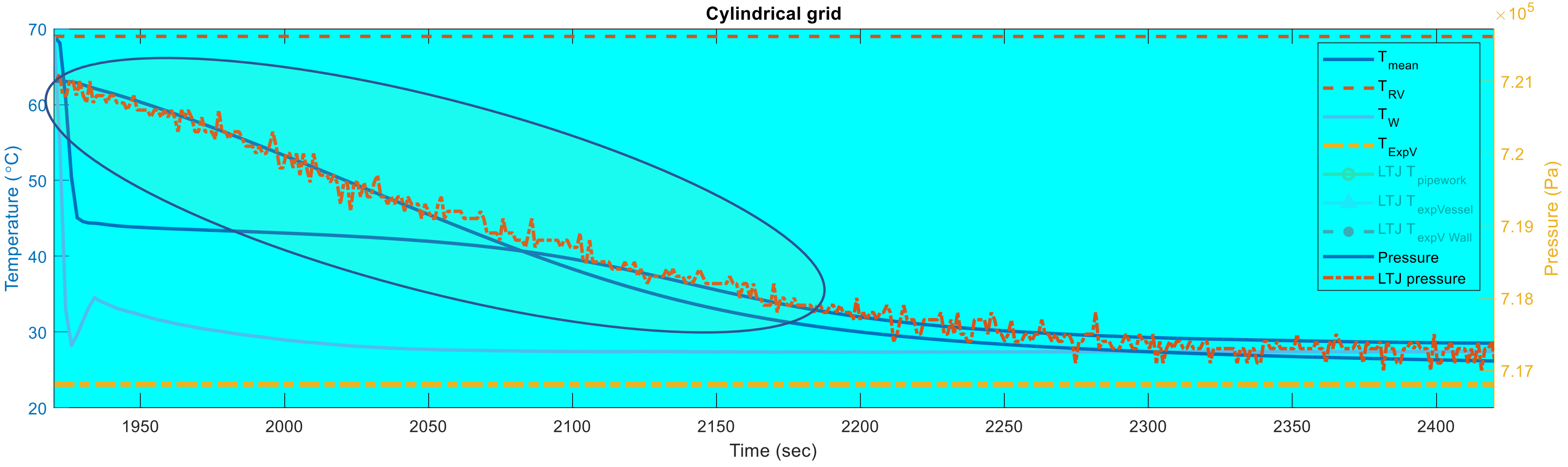
Gaps	0.115 mm
y_{des}	1.5
A_{des}	1

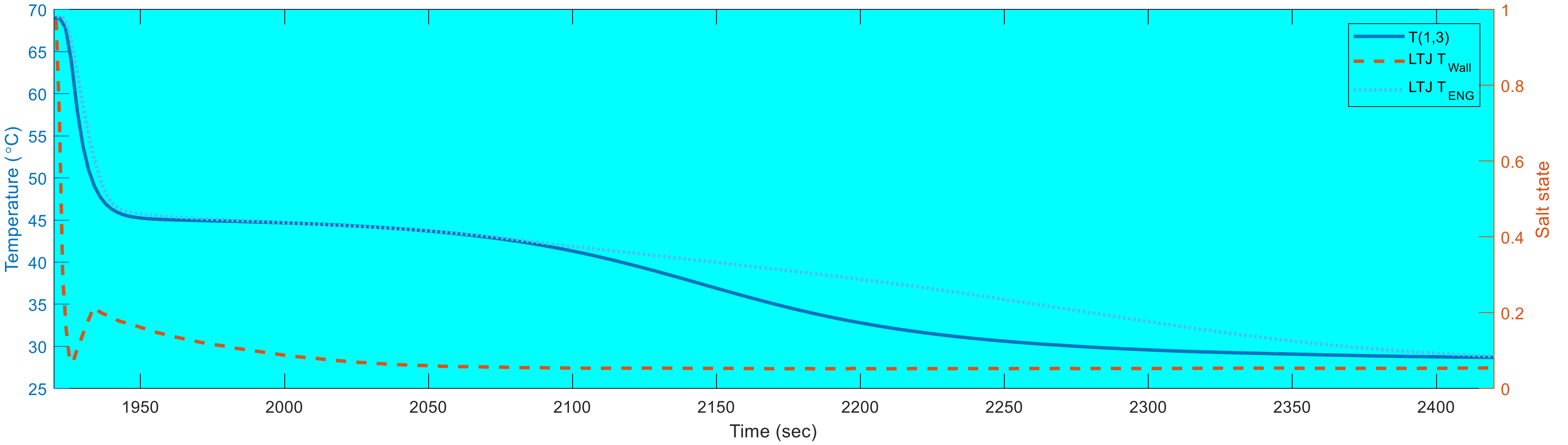




- Very sensitive to the thermal resistance of the “gap”.
- Heat transfer drives reaction rate.

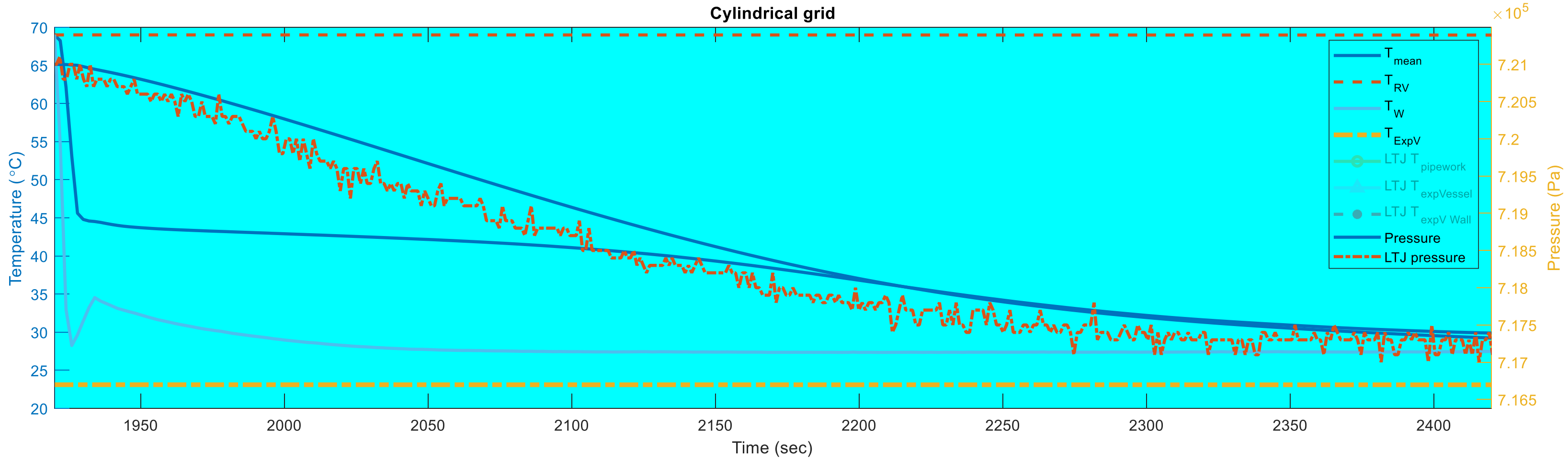
LTJ comparisons (3) – adsorption, matching pressure change



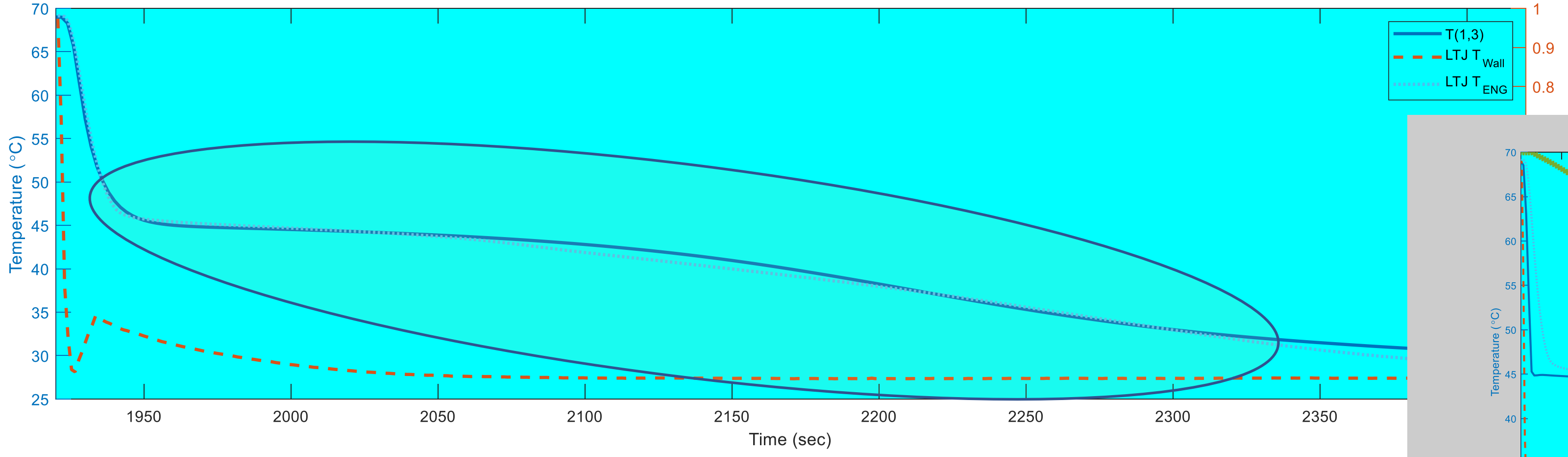


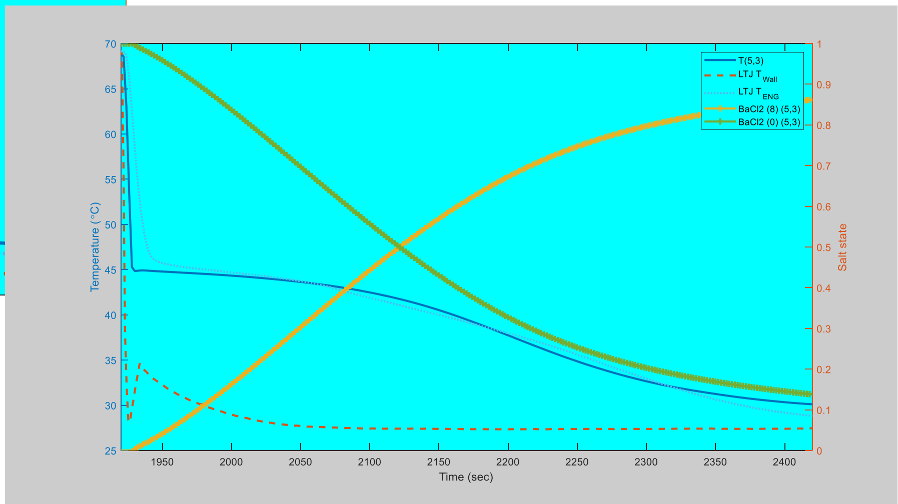
Gaps	0.12 mm
y_{ads}	2.5
A_{ads}	0.2

LTJ comparisons (4) – adsorption, matching internal thermocouple

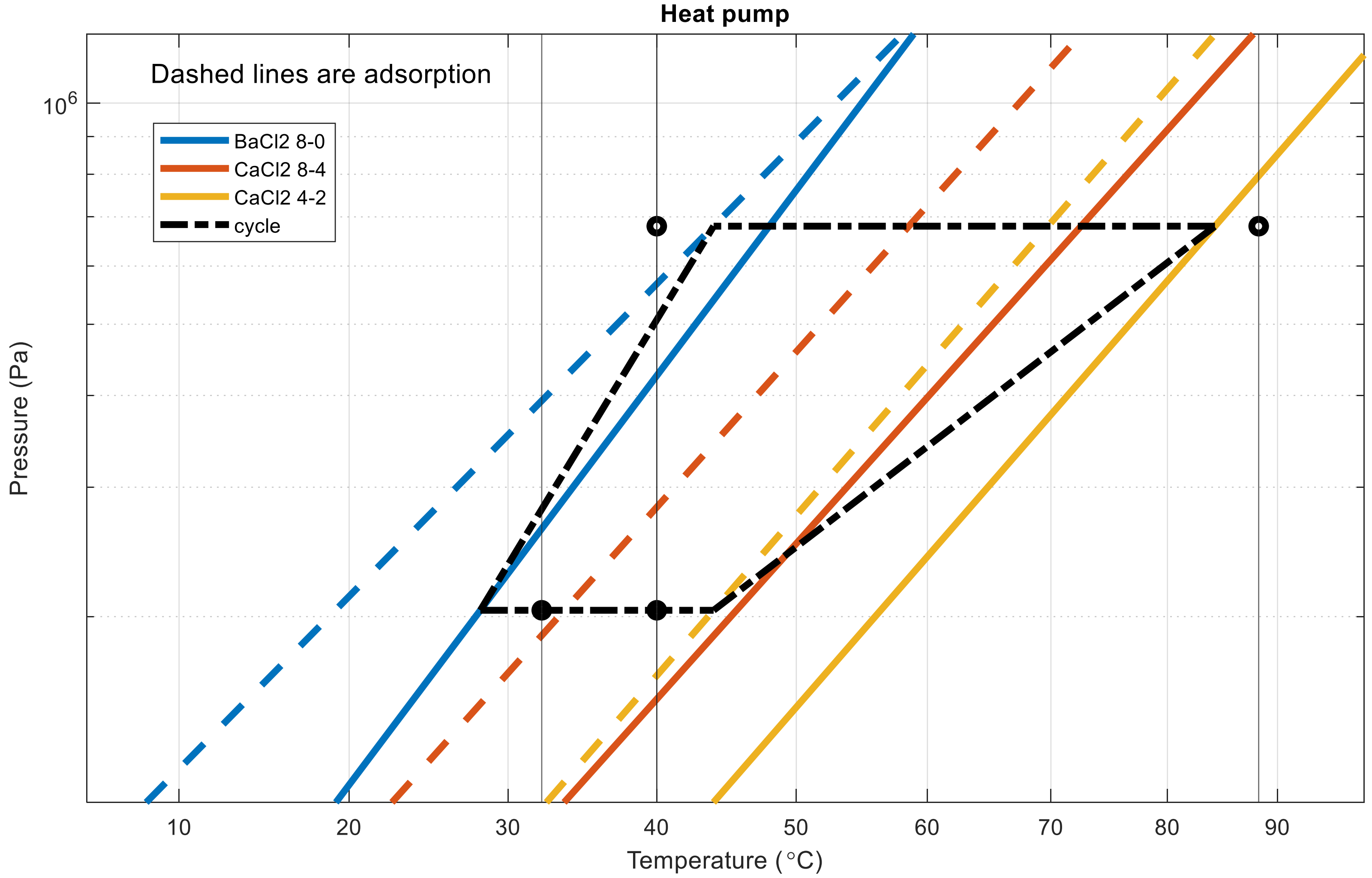


Gaps	0.17 mm
y_{ads}	2.5
A_{ads}	0.1



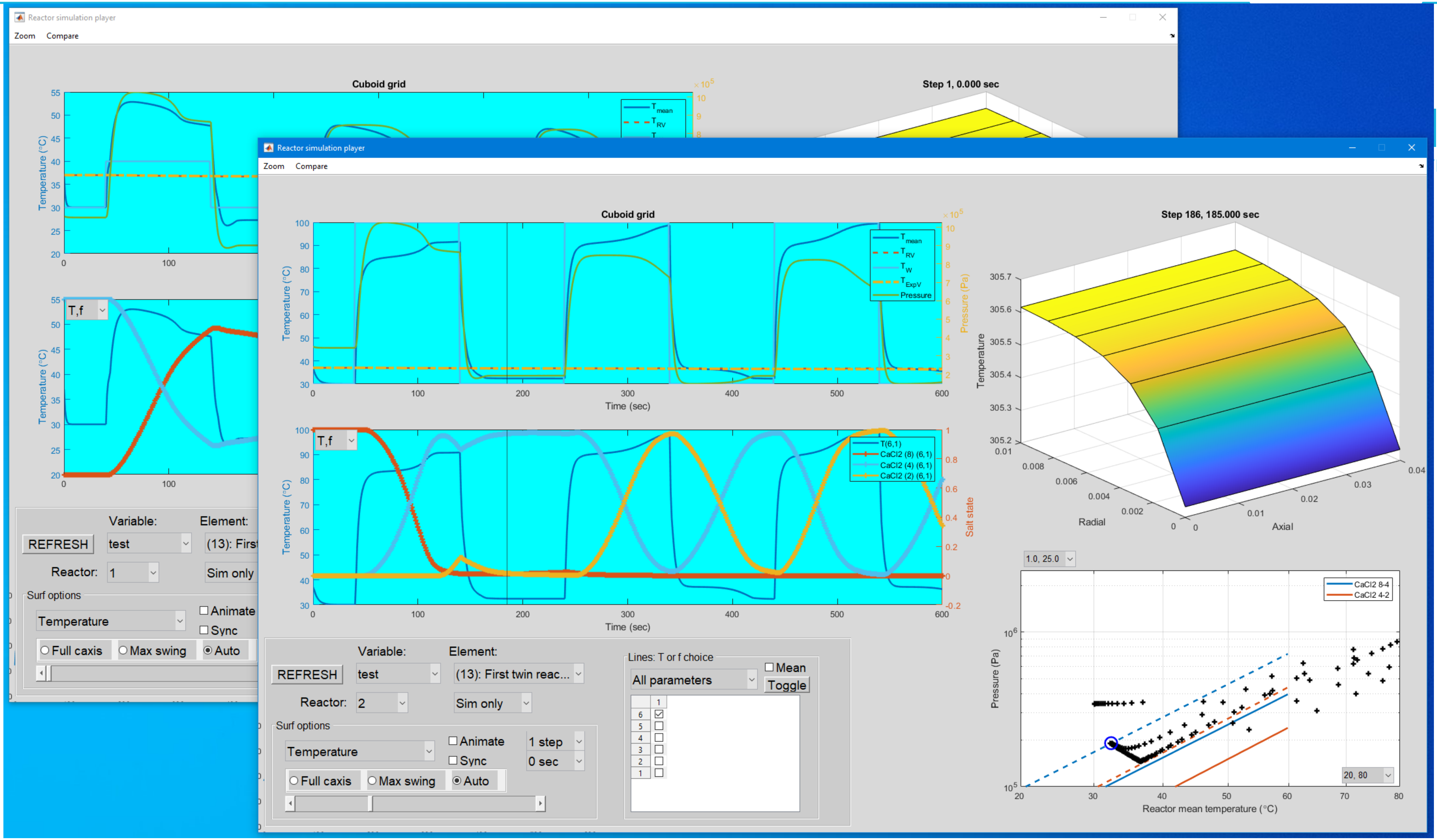


Heat pump salt and temperature options (1)
$BaCl_2$ & $CaCl_2$

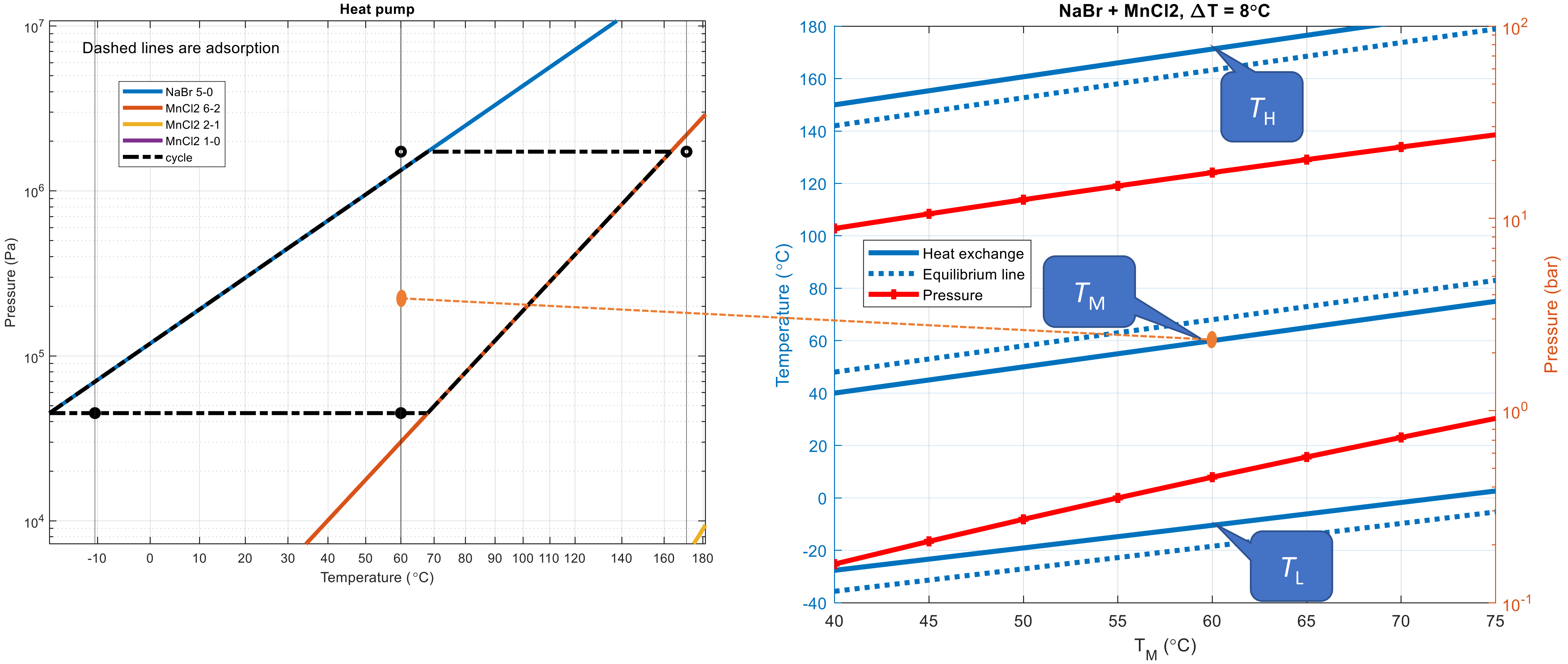


- Not useful – low temperature “not low enough”.

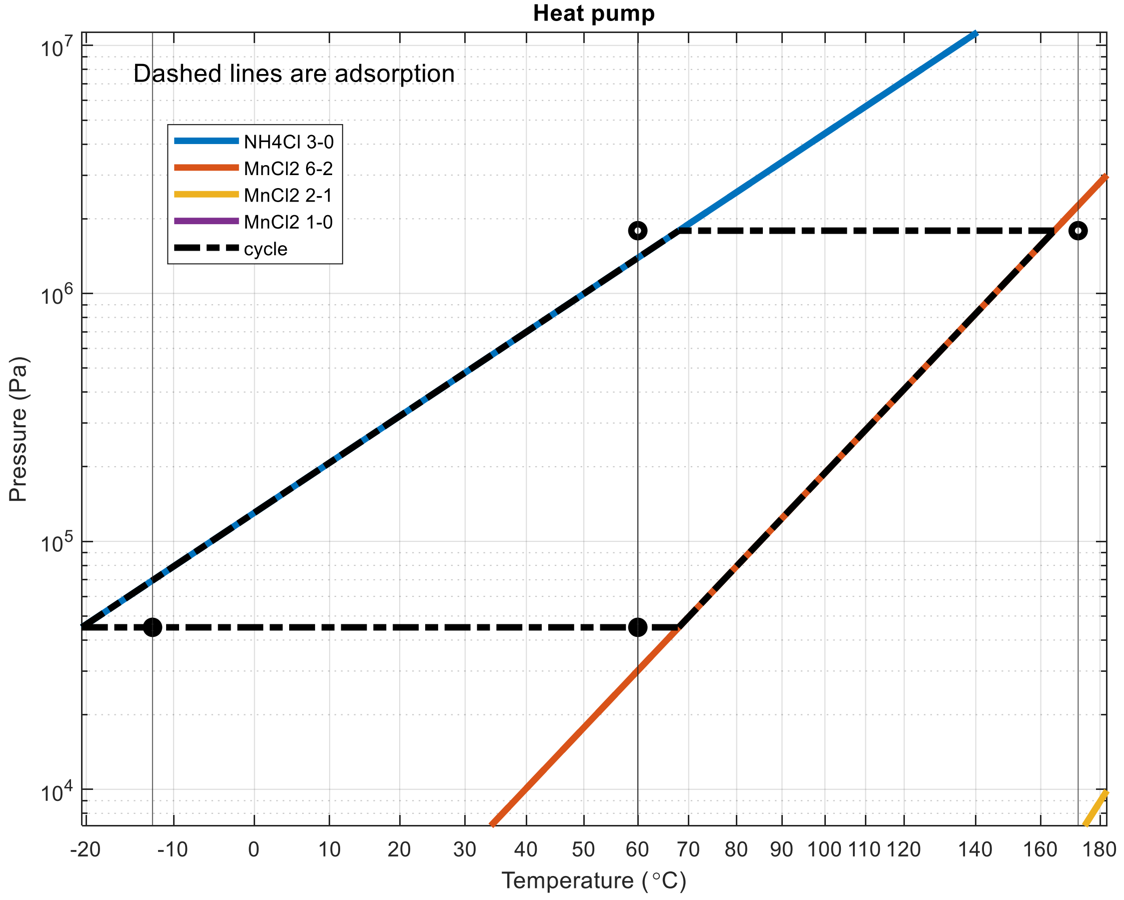
Initial simulation of two reactors

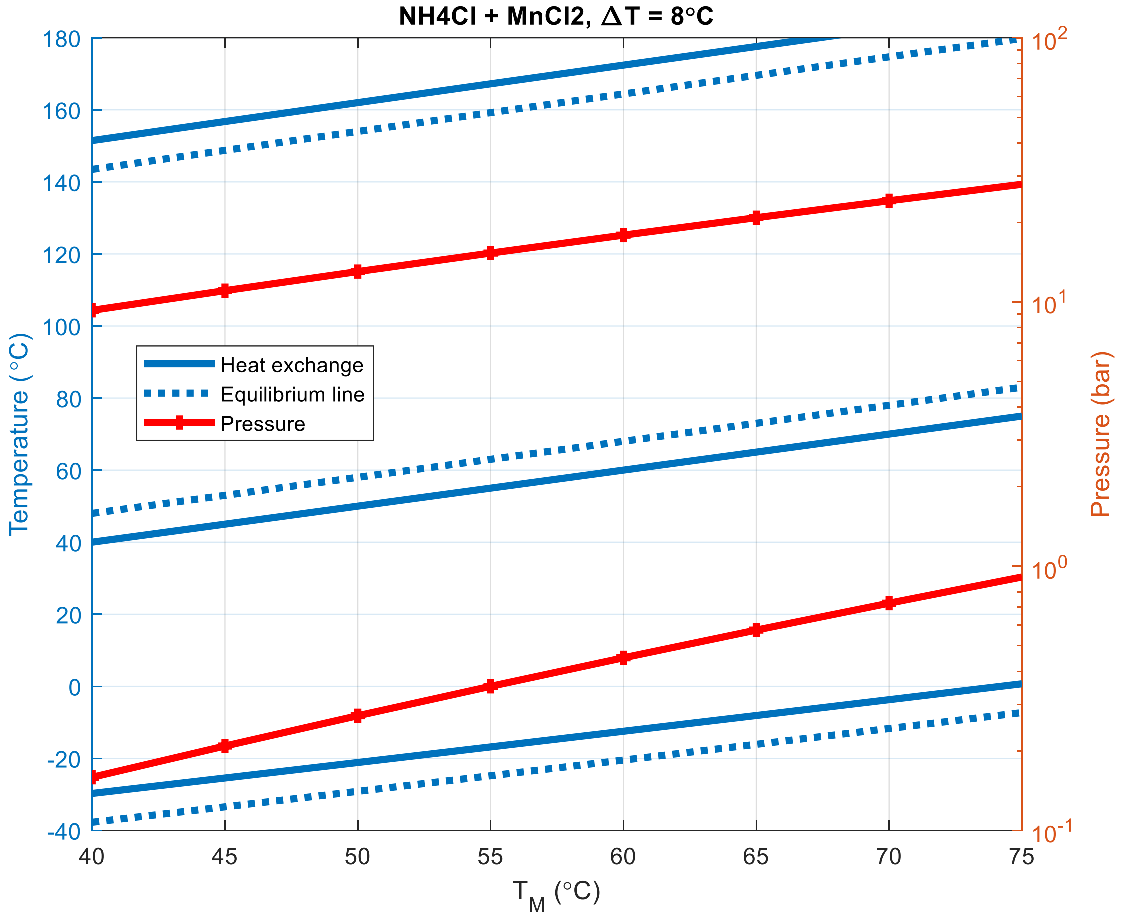


Heat pump salt and temperature options (2)
NaBr & $MnCl_2$

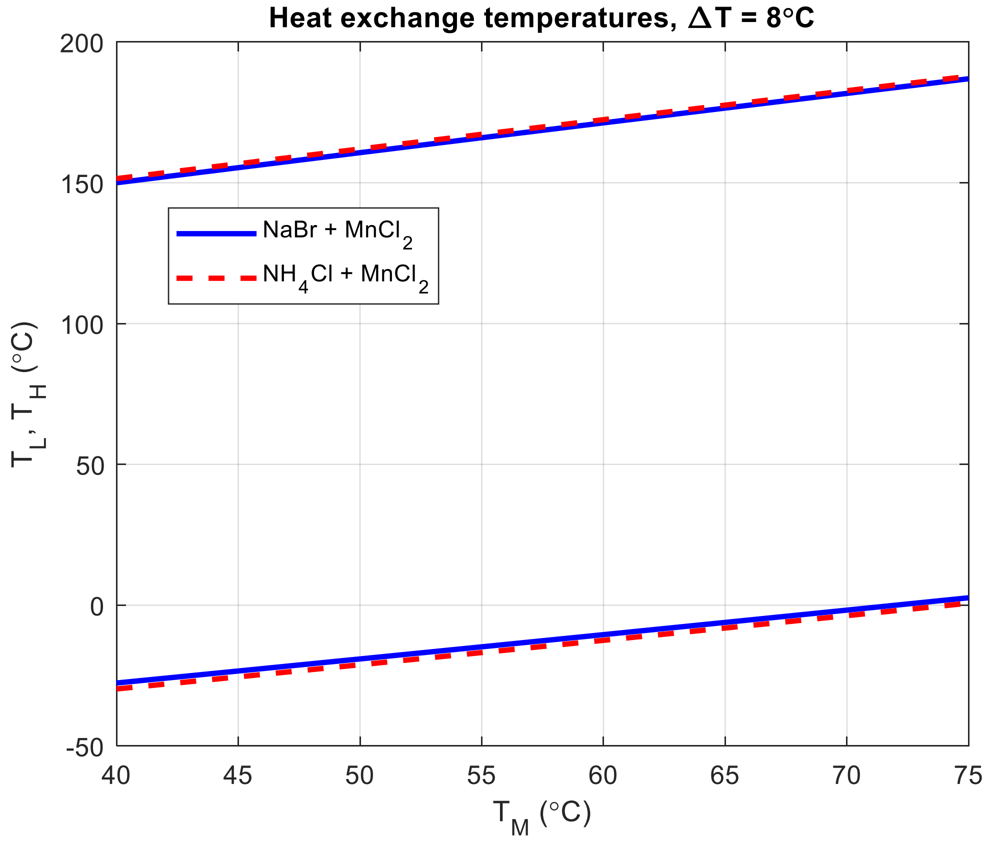


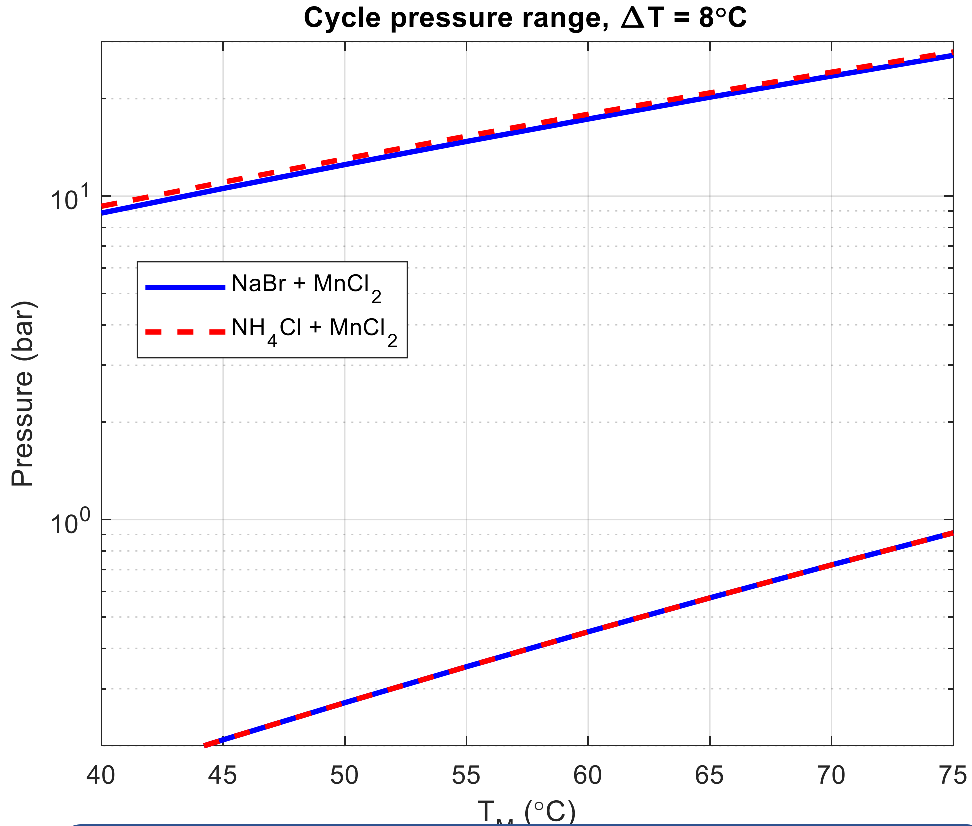
Heat pump salt and temperature options (2)
NH_4Cl & $MnCl_2$





$NaBr + MnCl_2$ versus $NH_4Cl + MnCl_2$





- NaBr and NH_4Cl almost identical in terms of operating pressure and temperature.