A 2D heat transfer and reaction model for ammonia-salt reactions: Applications for LTJ and resorption heat pumping.

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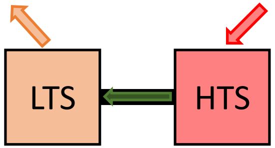
Monday 14th December 2020 | Mission Innovation | Online

Principle of operation

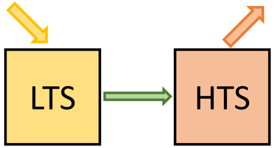
Heat output Q_M at temperature T_M ( ) as useful heat.



Heat input Q_H at temperature T_H ( ) from high temperature source.

Ammonia flow from HTS bed to LTS bed ( ).

Heat input Q_L at temperature T_L ( ) from low temperature source.



Heat output Q_M at temperature T_M ( ) as useful heat

Ammonia flow from LTS bed to HTS bed ( ).

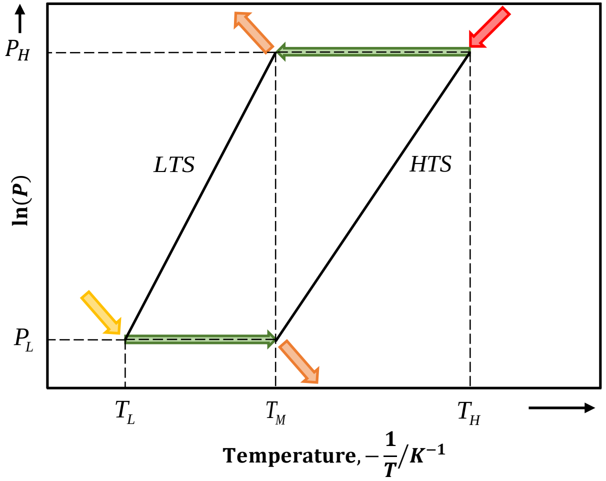
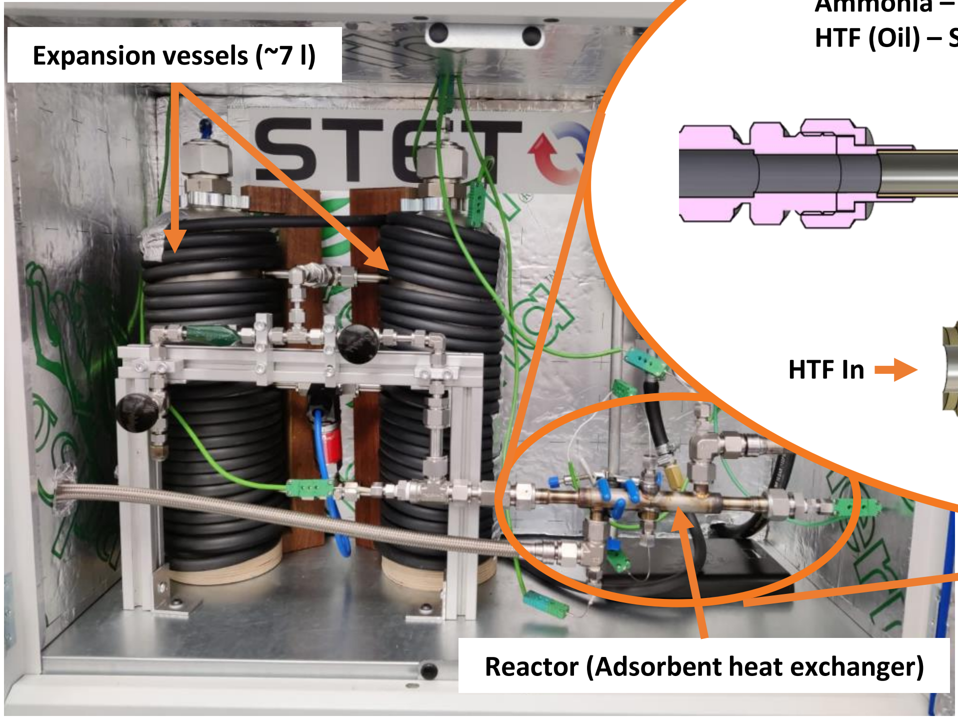
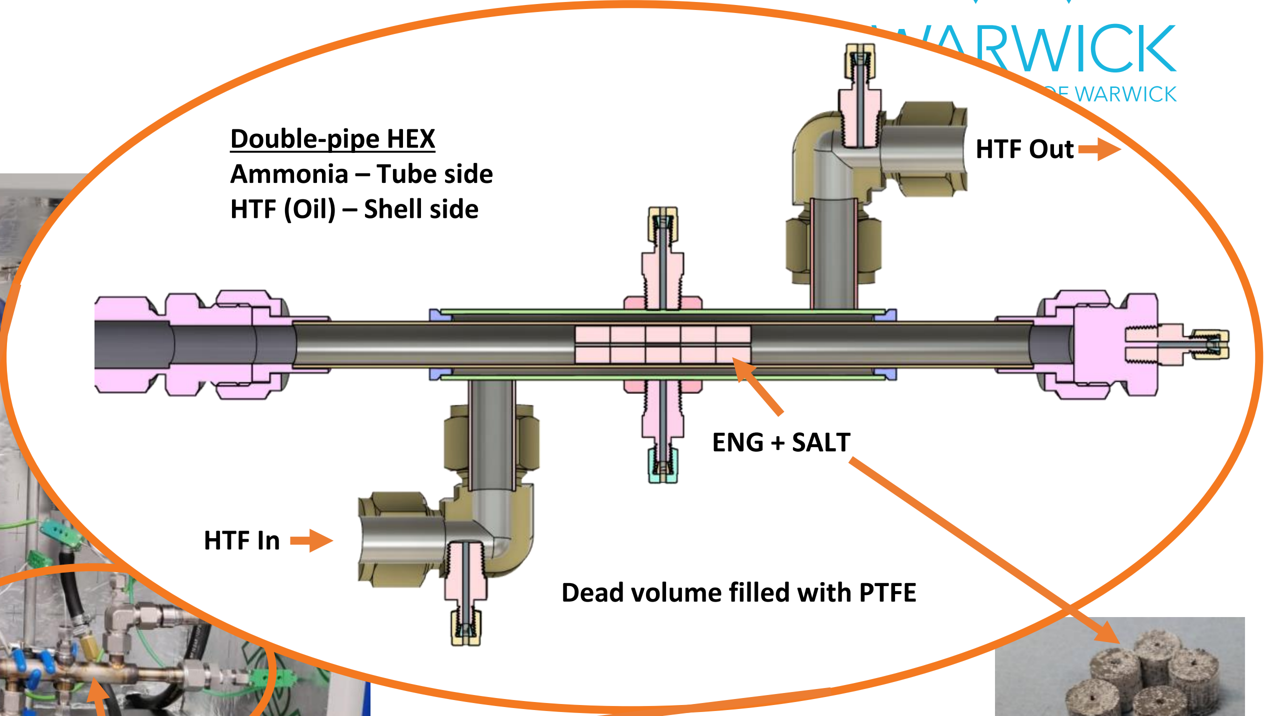


Fig. 2 (Approx.) Clausius-Clapeyron diagram for a 2-salt heat pump operation.

Current work





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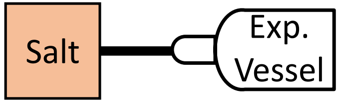
Published modelling approach!



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Modelling the Ammoniation of Barium Chloride for Chemical Heat Transformations

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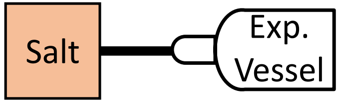
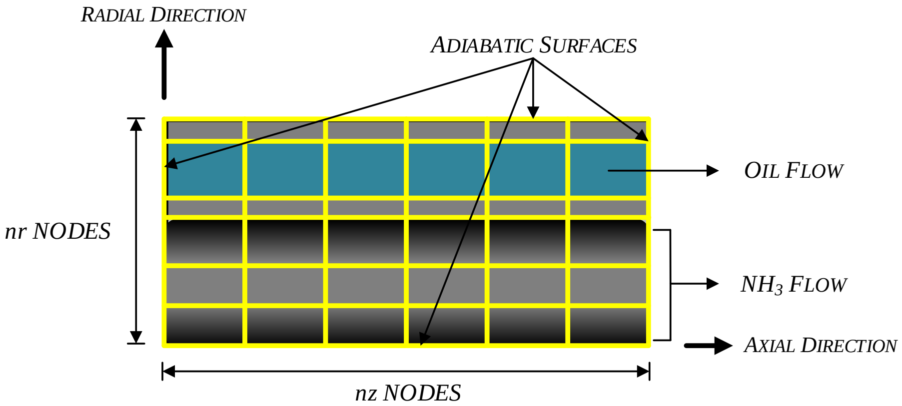
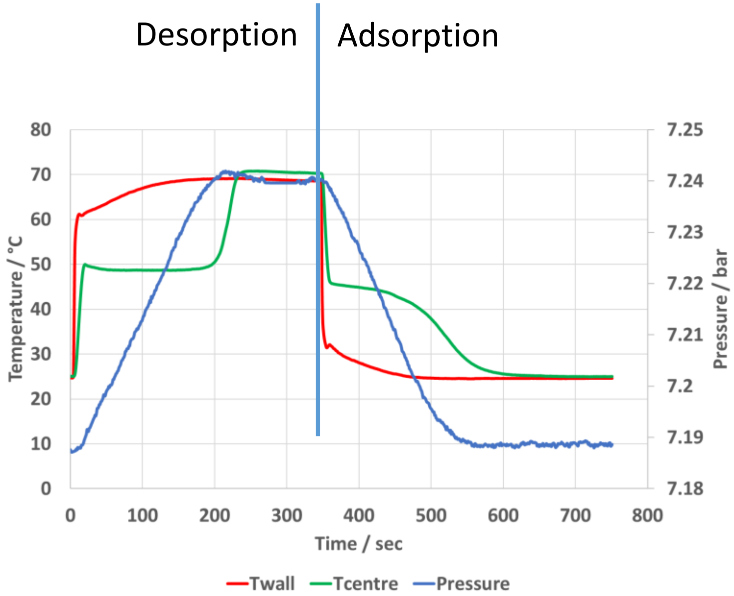
1D to 2D


Salt
Exp.
Vessel


RADIAL DIRECTION
ADIABATIC SURFACES
OIL FLOW
nr NODES
NH3 FLOW
AXIAL DIRECTION
nz NODES


Desorption
Adsorption
Temperature / °C
Pressure / bar
Time / sec
0
10
20
30
40
50
60
70
80
100
200
300
400
500
600
700
800
7.18
7.19
7.2
7.21
7.22
7.23
7.24
7.25
Twall
Tcentre
Pressure

Governing Eqns. – Reaction (dm)

Reaction **AB** e.g $BaCl_2$ A = 8 & B = 0, $MnCl_2$ A = 6 & B = 2 or $CaCl_2$ A = 8 & B = 4

$$dm_{SALT_{AB}} = \left(m_{SALT_A} + m_{SALT_B}\right) dt \left(\frac{m_{SALT_A}}{m_{SALT_A} + m_{SALT_B}}\right)^{y_{AB}} A_{AB} \left(\frac{p_{EQ_{AB}} - p}{p}\right)$$

Reaction **BC** e.g $MnCl_2$ B = 2 & C = 1 or $CaCl_2$ B = 4 & C = 2

$$dm_{SALT_{BC}} = \left(m_{SALT_B} + m_{SALT_C}\right) dt \left(\frac{m_{SALT_B}}{m_{SALT_B} + m_{SALT_C}}\right)^{y_{BC}} A_{BC} \left(\frac{p_{EQ_{BC}} - p}{p}\right)$$

Derived & based on Lebrun and Spinner[1] and Mazet, Amouroux and Spinner[2]. X = Advancement

$$\frac{dX}{dt} = (1 - X)^n \cdot Ar \cdot \left(\frac{P - P_e(T)}{P}\right)$$

1 M. Lebrun and B. Spinner, "Models of heat and mass transfers in solid-gas reactors used as chemical heat pumps," Chemical Engineering Science, vol. 45, no. 7, pp. 1743-1753, 1990.
2 N. Mazet, M. Amouroux, and B. Spinner, "Analysis and experimental study of the transformation of a nonisothermal solid/gas reacting medium," Chemical Engineering Communications, vol. 99, no. 1, pp. 155-174, 1991, doi: 10.1080/00986449108911585.

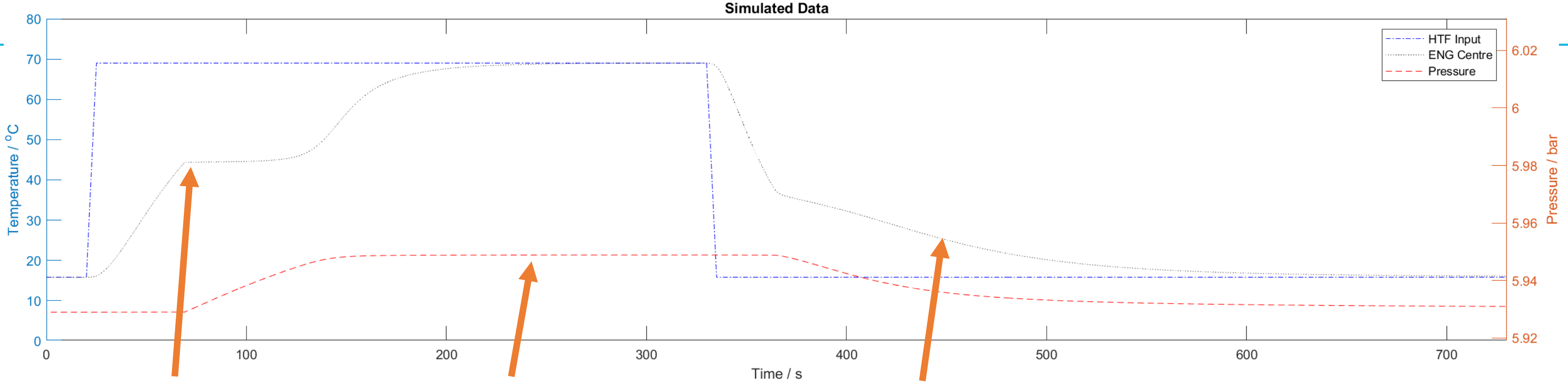
Governing Eqns. – Heat Transfer

Desorption[3]

$$dT=\frac{dQ-dm_{GAS_{AB}}\Delta h_{AB}-dm_{ADS_{AB}}pv_{ADS}\left(1-\frac{B}{A}\right)-dm_{GAS_{BC}}\Delta h_{BC}-dm_{ADS_{BC}}pv_{ADS}\left(1-\frac{C}{B}\right)+\frac{dpV_V}{1+\frac{dp}{p}}}{\left(MC_p+\sum_{A}^{C}m_{NR-ADS}c_{V_{ADS}}+m_{GAS_V}c_{V_{GAS}}-\frac{\frac{pV_V}{T}}{1+\frac{dp}{p}}\right)}$$

Adsorption[3] – similar but with additional gas void terms.

[3] *R.E.Critoph, email 08/07/2020.*



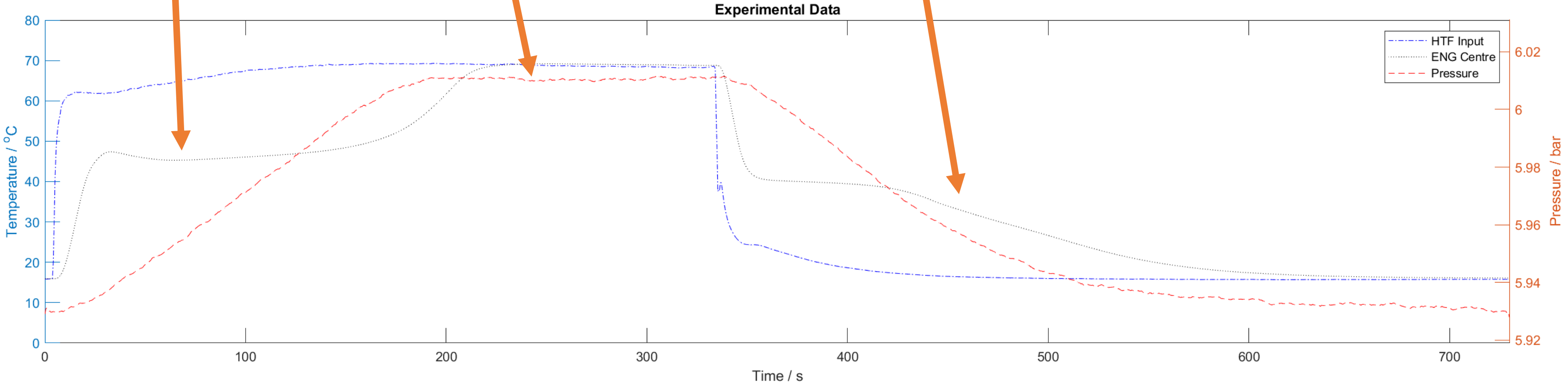
Good prediction of equilibrium temperature + overall good reaction shape (but no superheat!)

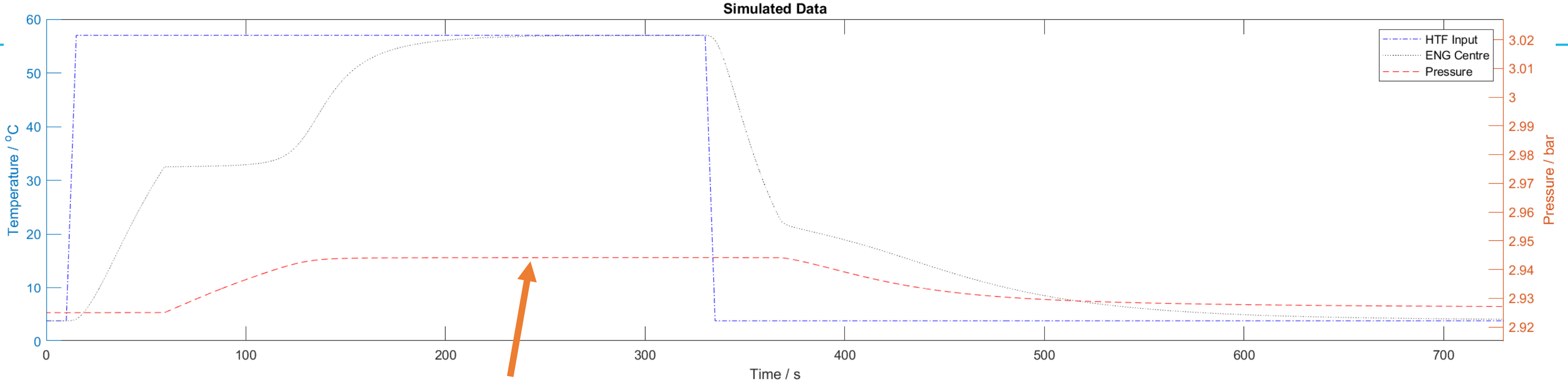
Major sticking point with the pressure rise at present – needs more digging into!

Currently fast on the desorption reaction but for adsorption reaction time is comparable

6 BAR EXAMPLE

(nr = 3, nz = 2)

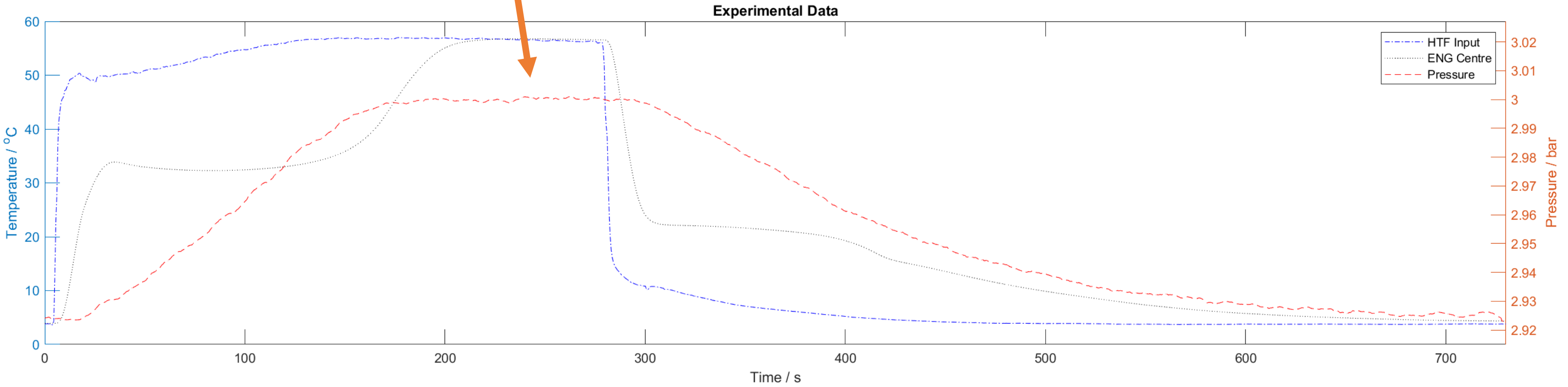




Pressure rise still an issue but changes in temperature look good.

3 BAR EXAMPLE

(nr = 3, nz = 2)



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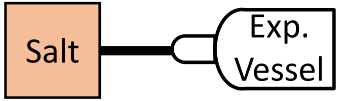
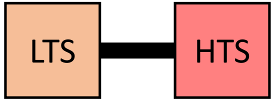
Up next…



Understand the pressure swing issues.
Check heat transfer model



Design for two reactors

Reactor design – Design for shell side or tubeside

Cycle simulations

Performance analysis

Thank you for listening

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