Ammonia-Salt Updates

George Atkinson | STET | The University of Warwick

Mission Innovation Workshop | Online | Thursday 3rd June 2021

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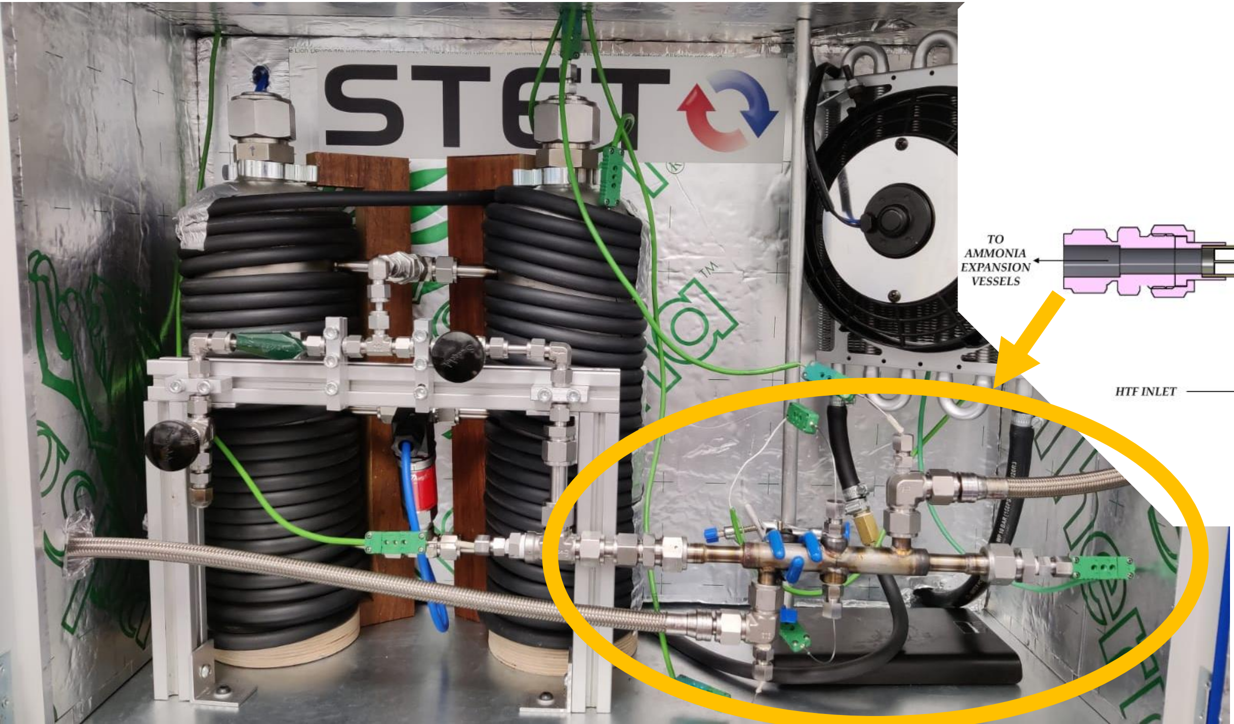
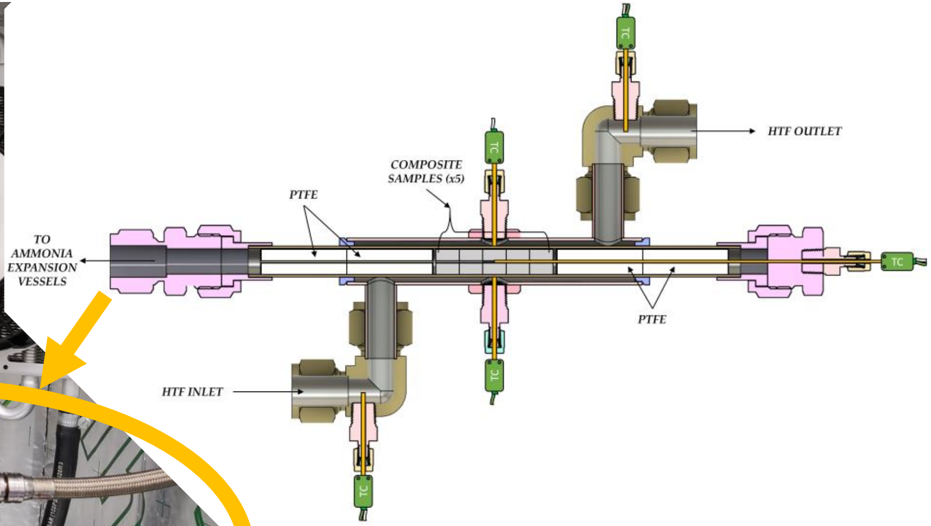
Two Experimental Methods, Two Reactor Configurations

- Large Temperature Jump (LTJ) – reactor with expansion volume





1. Tube side ENG-salt samples (x 5)

Two Experimental Methods, Two Reactor Configurations

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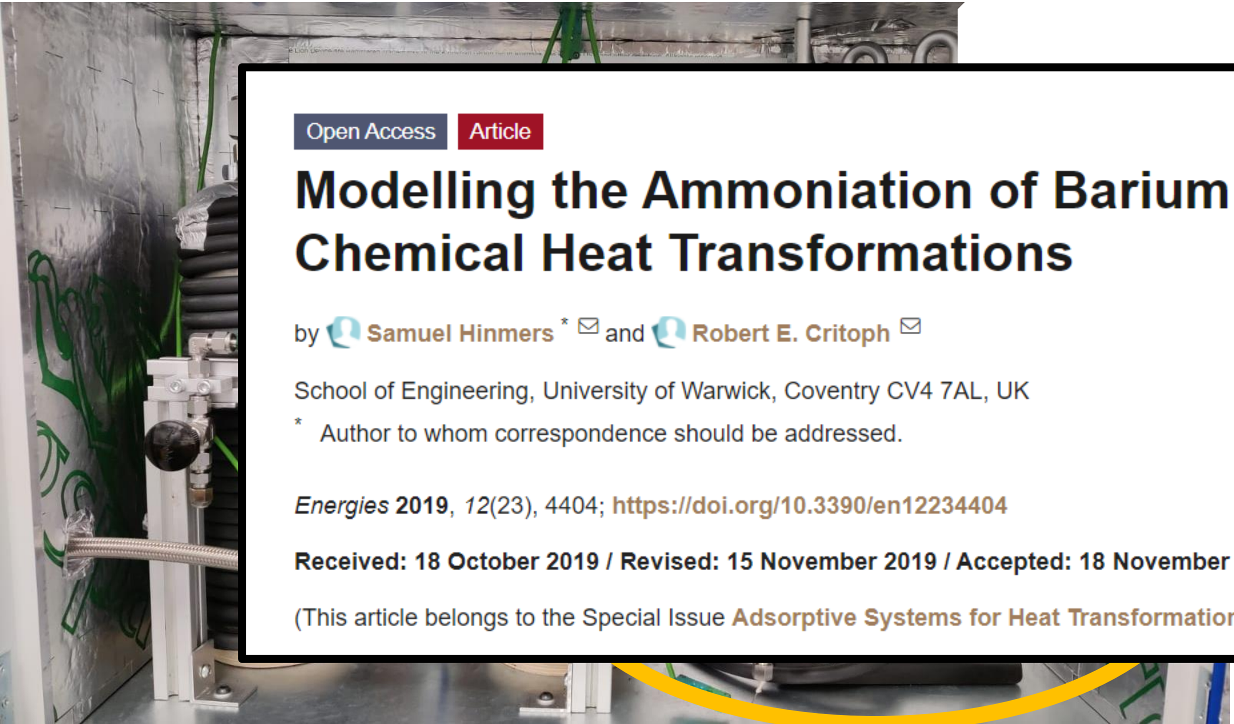
- Large Temperature Jump (LTJ) – reactor with expansion volume



Open Access Article

Modelling the Ammoniation of Barium Chloride for Chemical Heat Transformations

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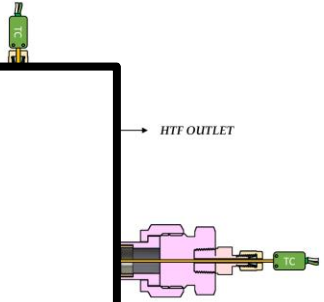
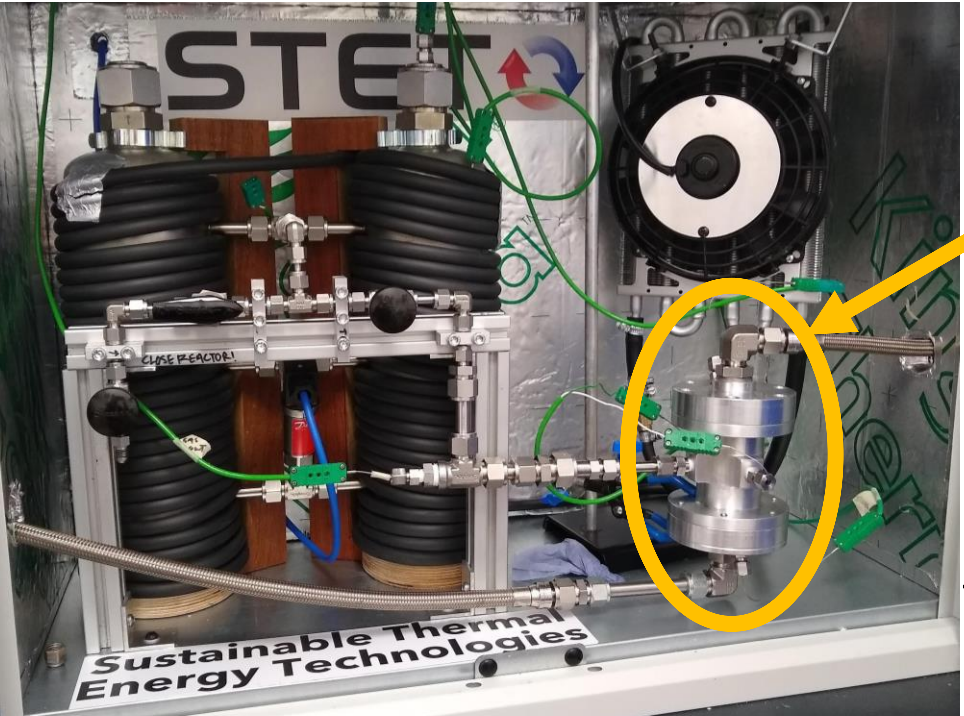
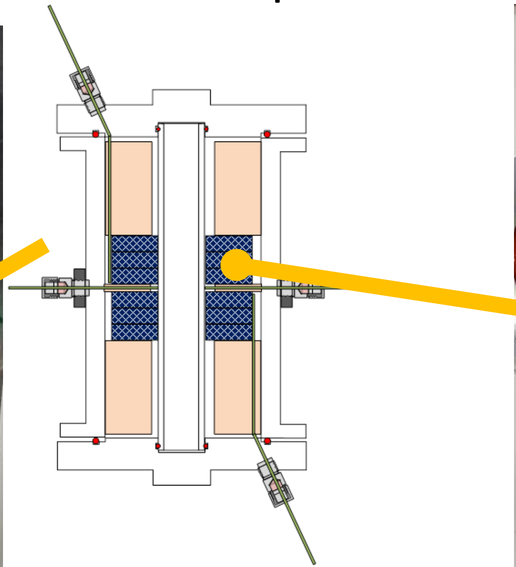


Two Experimental Methods, Two Reactor Configurations

- Large Temperature Jump (LTJ) – reactor with expansion volume

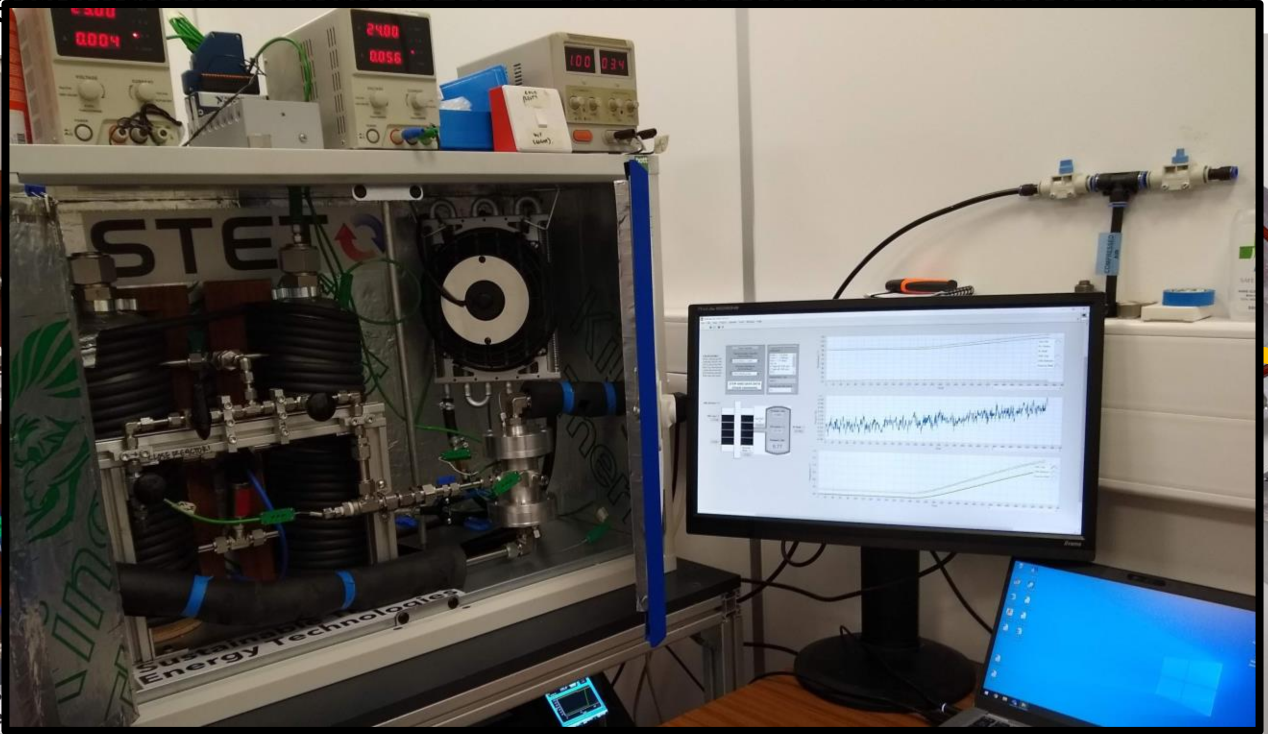




2. Shell side ENG-salt samples (x 2-8)

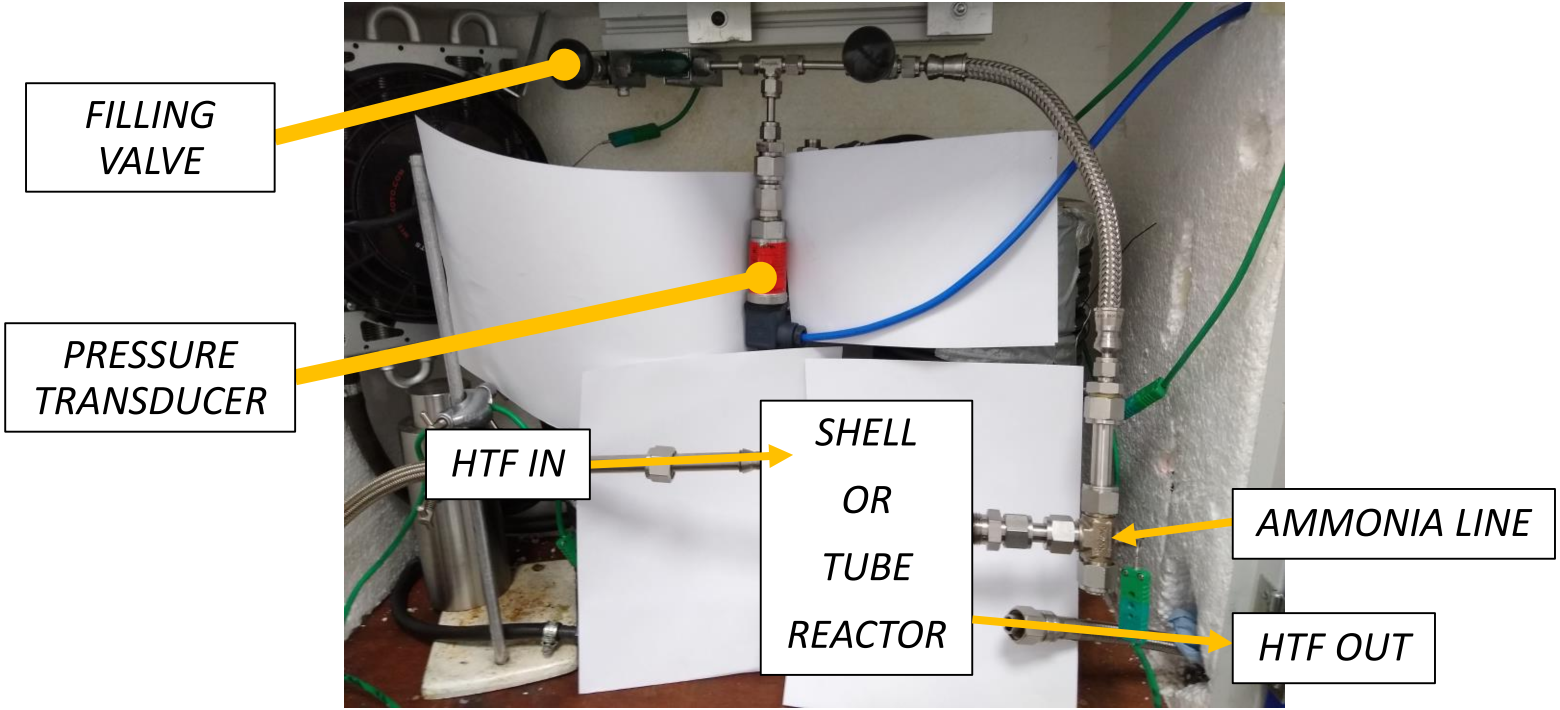
Two Experimental Methods, Two Reactor Configurations

- Large Temperature Jump (LTJ) – reactor with expansion volume

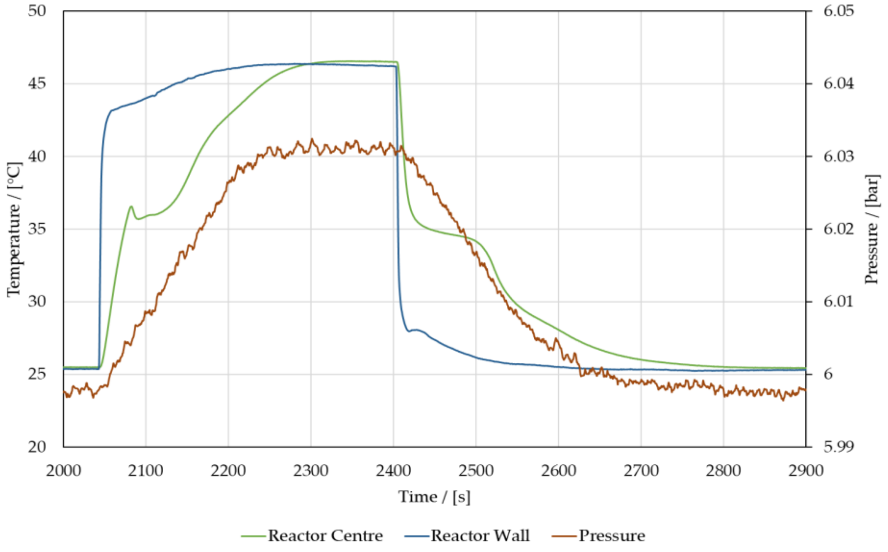


Two Experimental Methods, Two Reactor Configurations

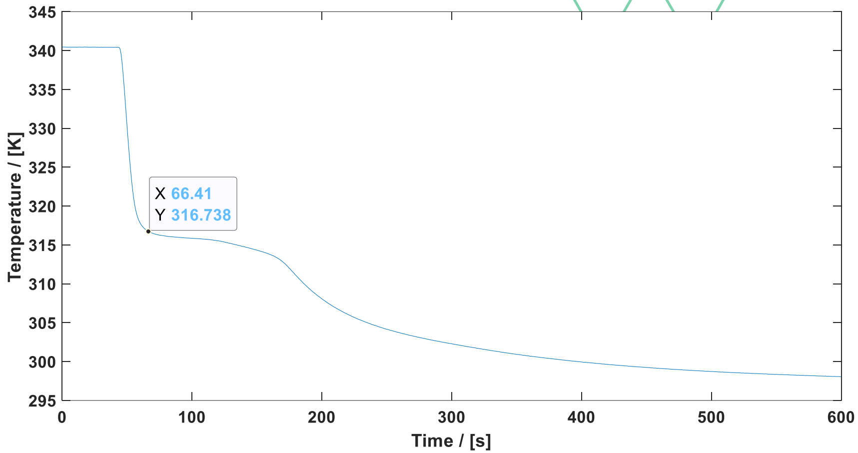
- Isosteric Temperature Change (ITC) – reactor **without** expansion volume

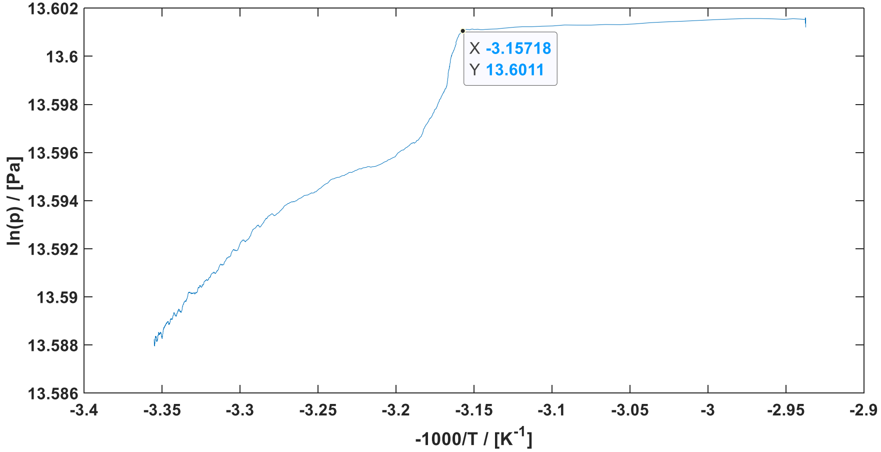


Large Temperature Jump Outputs

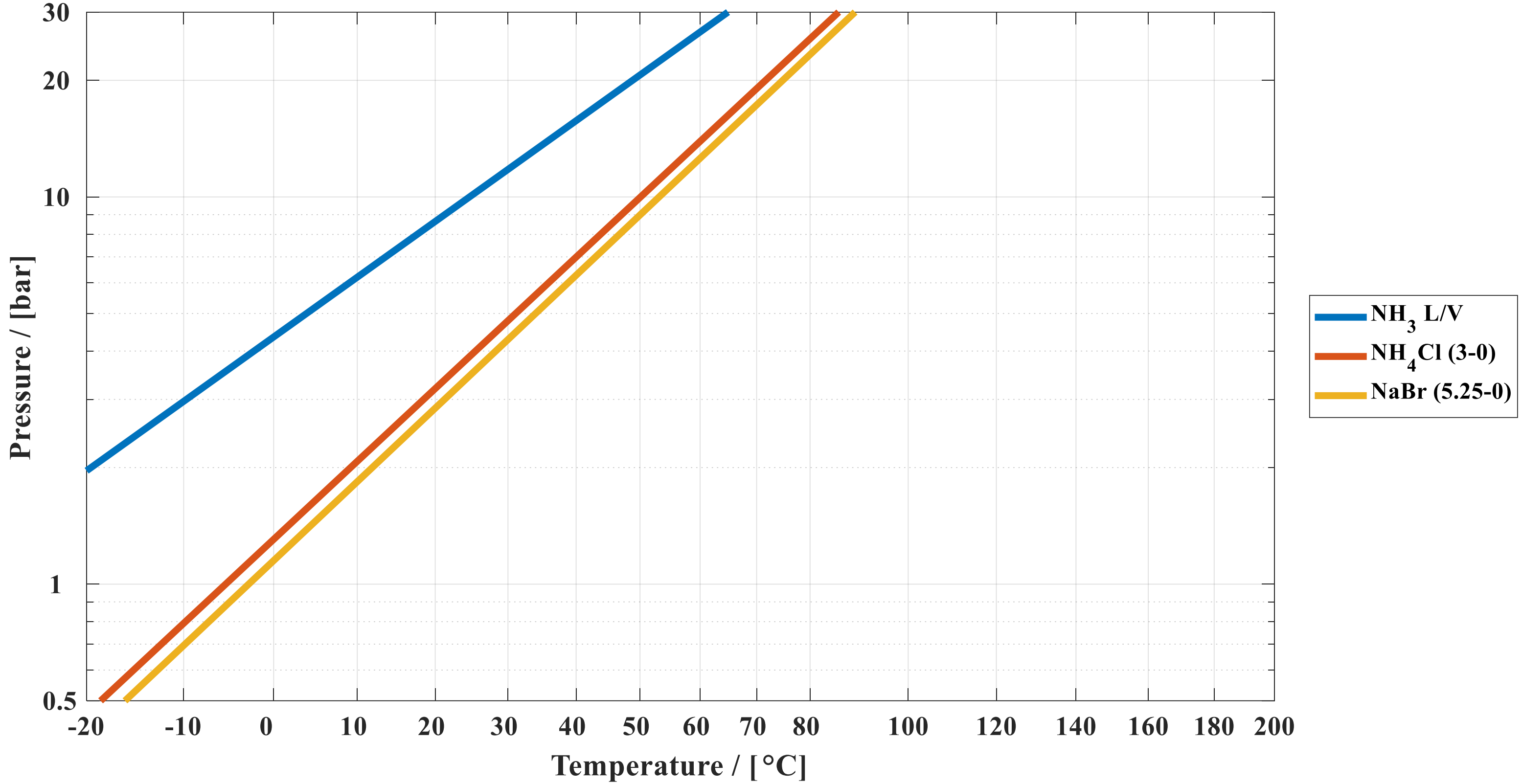


- NH_4Cl, NaBr, $BaCl_2$, $CaCl_2$ & $MnCl_2$

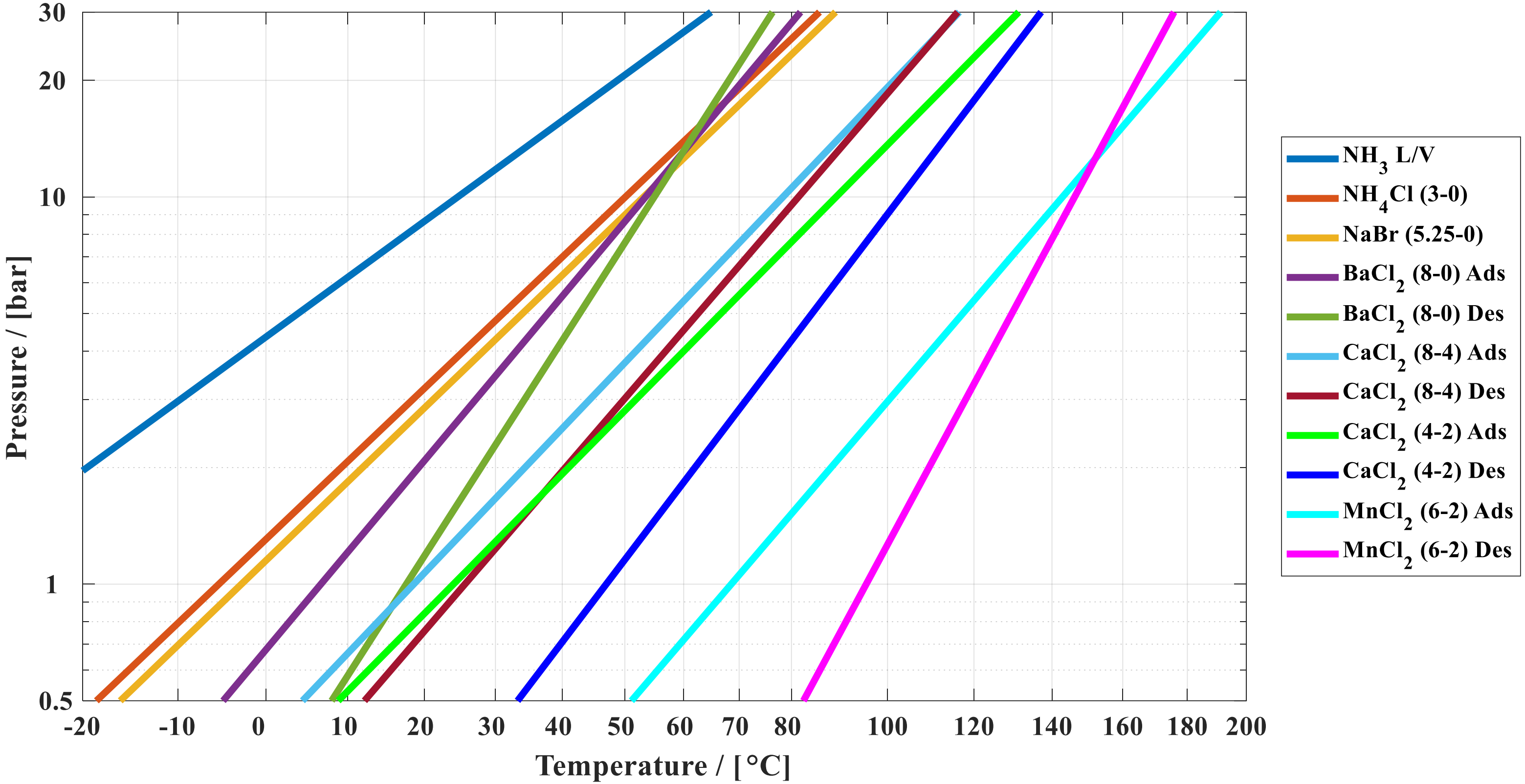




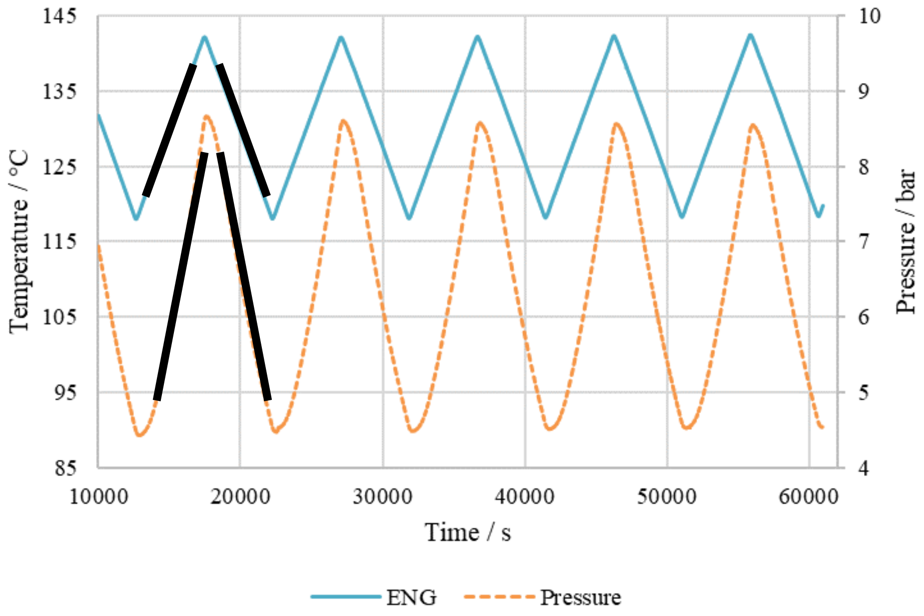
Experimental Equilibrium Lines



Experimental Equilibrium Lines

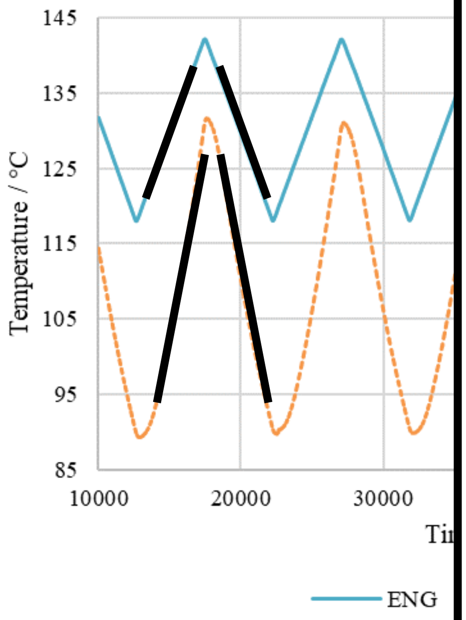


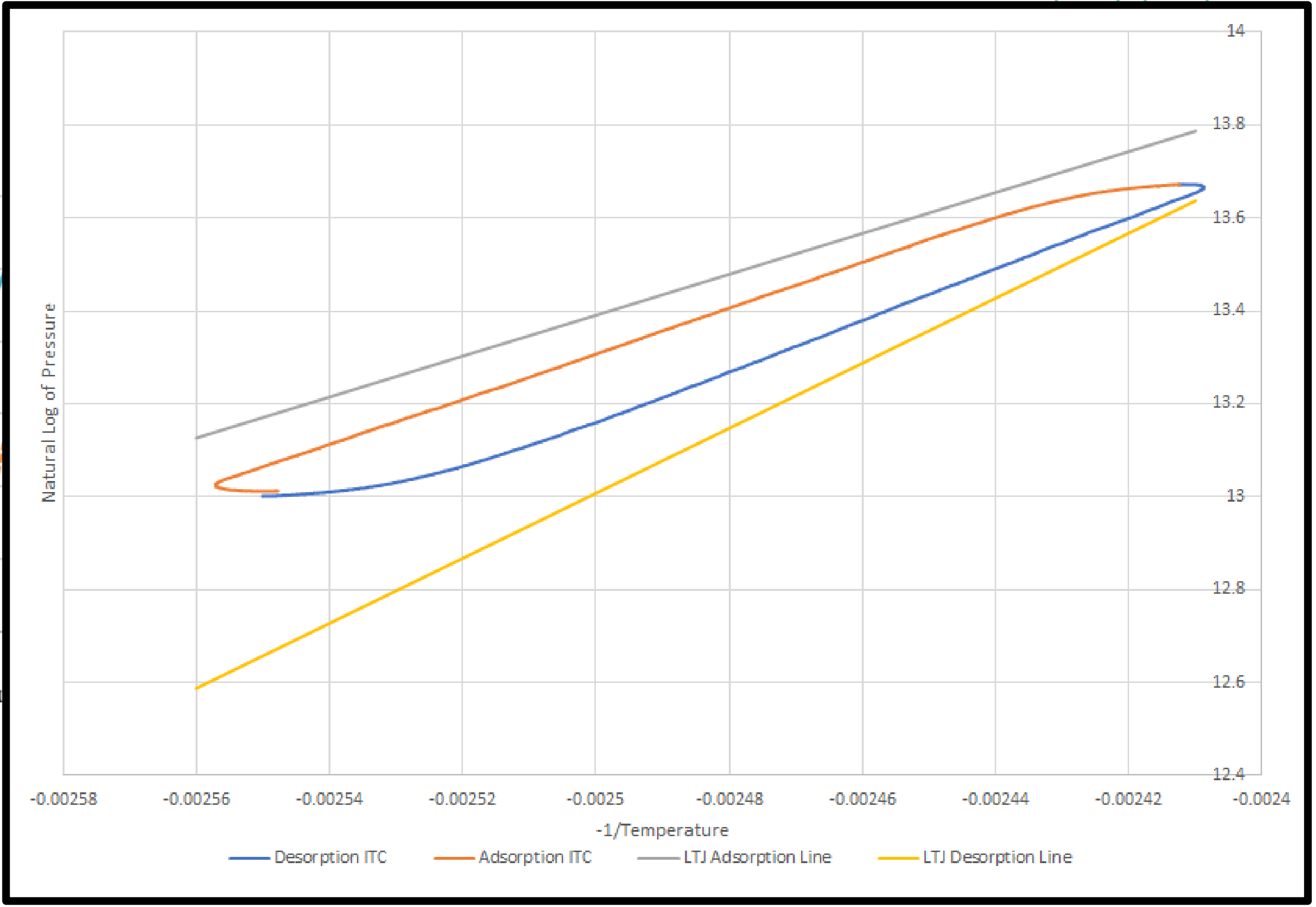
ITC Outputs



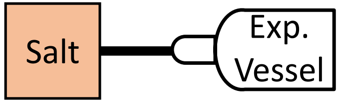
Temperature / °C
Pressure / bar
145
135
125
115
105
95
85
10
9
8
7
6
5
4
10000
20000
30000
40000
50000
60000
Time / s
ENG
Pressure

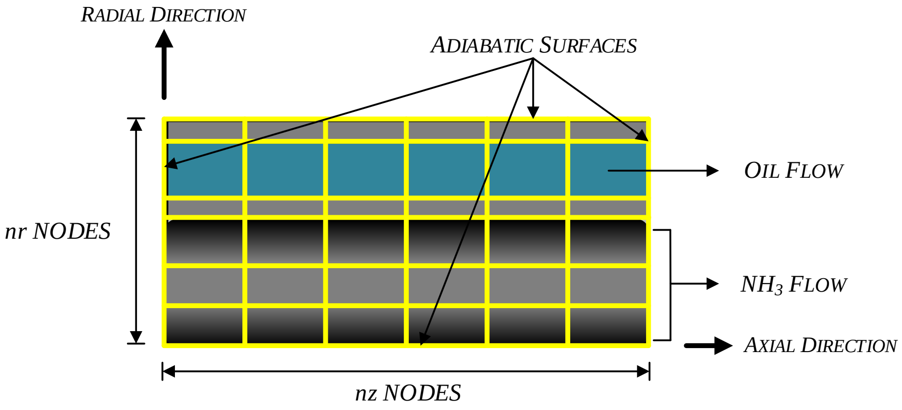
ITC Outputs

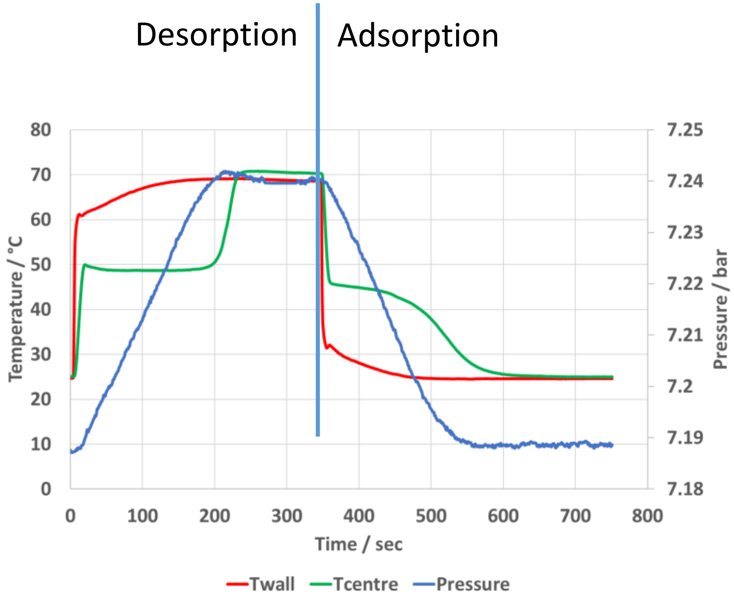

145
135
125
115
105
95
85
Temperature / °C
10000
20000
30000
Ti
ENG


Natural Log of Pressure
14
13.8
13.6
13.4
13.2
13
12.8
12.6
12.4
-0.00258
-0.00256
-0.00254
-0.00252
-0.0025
-0.00248
-0.00246
-0.00244
-0.00242
-0.0024
-1/Temperature
Desorption ITC
Adsorption ITC
LTJ Adsorption Line
LTJ Desorption Line

Modelling


Salt
Exp.
Vessel


RADIAL DIRECTION
ADIABATIC SURFACES
OIL FLOW
nr NODES
NH_3 FLOW
AXIAL DIRECTION
nz NODES


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

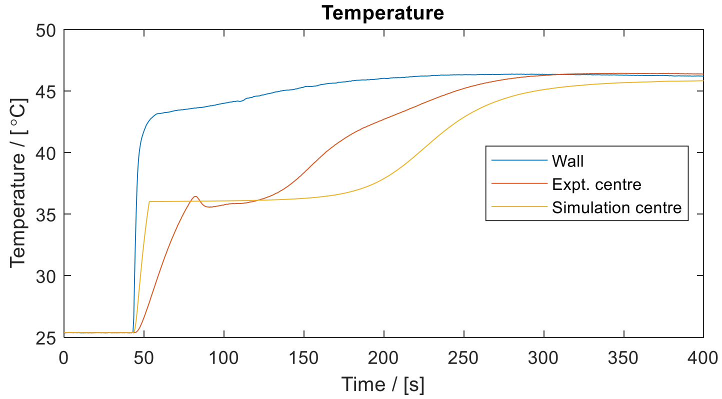
$$dT = \frac{dQ - dm_{GAS_{AB}}\Delta h_{AB} - dm_{ADS_{AB}} pv_{ADS}\left(1-\frac{B}{A}\right) - dm_{GAS_{BC}}\Delta h_{BC} - dm_{ADS_{BC}} pv_{ADS}\left(1-\frac{C}{B}\right) + \frac{dpV_V}{1+\frac{dp}{p}}}{\left(MC_p + \sum_A^C m_{NR-ADS} c_{V_{ADS}} + m_{GAS_V} c_{V_{GAS}} - \frac{\frac{pV_V}{T}}{1+\frac{dp}{p}}\right)}$$

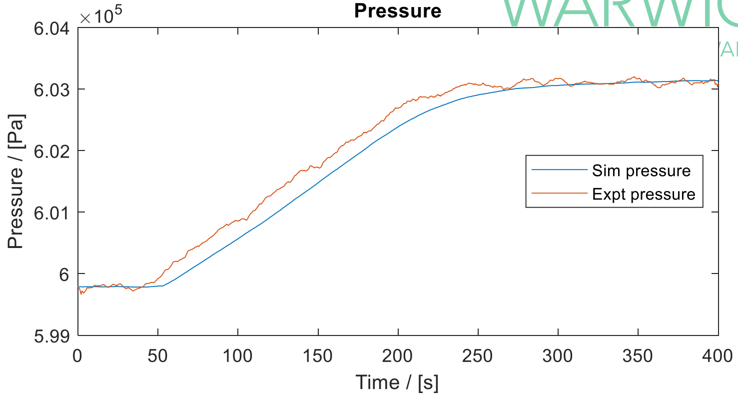
Adsorption[3] – similar but with additional gas void terms.

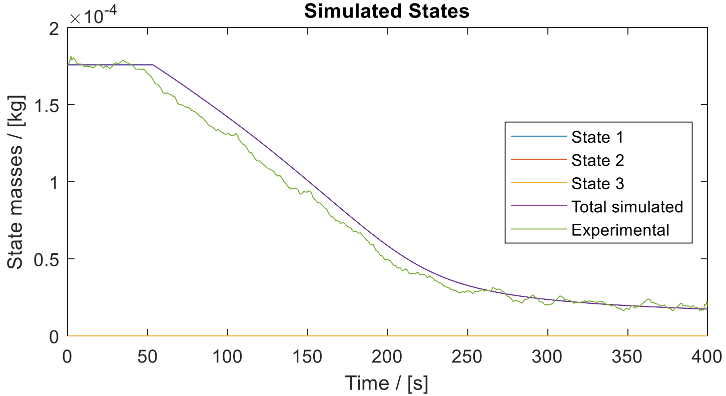
[3] *R.E.Critoph, email 08/07/2020.*

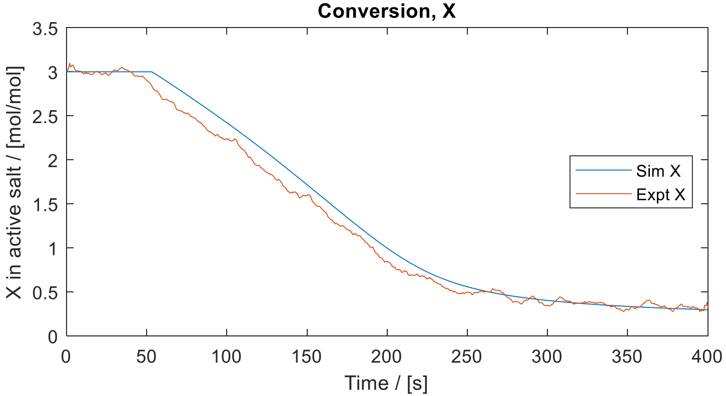
Proof is in the plotting…

Ammonium Chloride, NH_4Cl – 6 bar DES

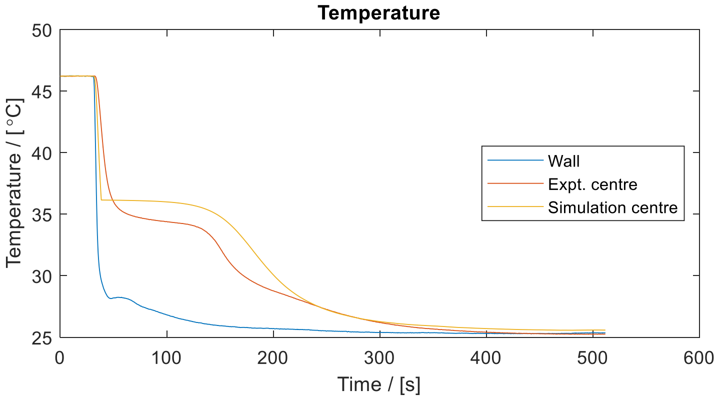


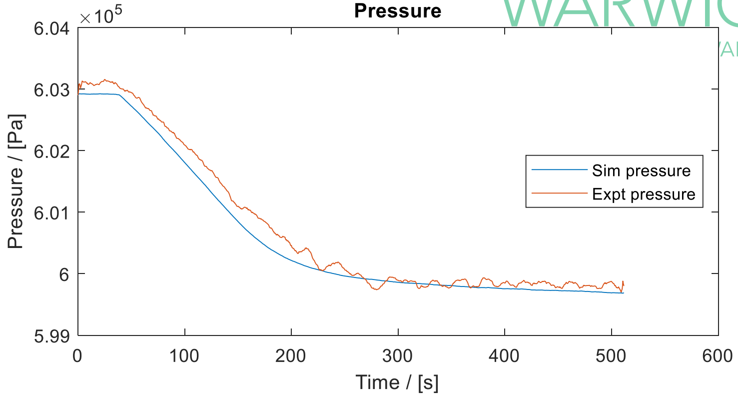


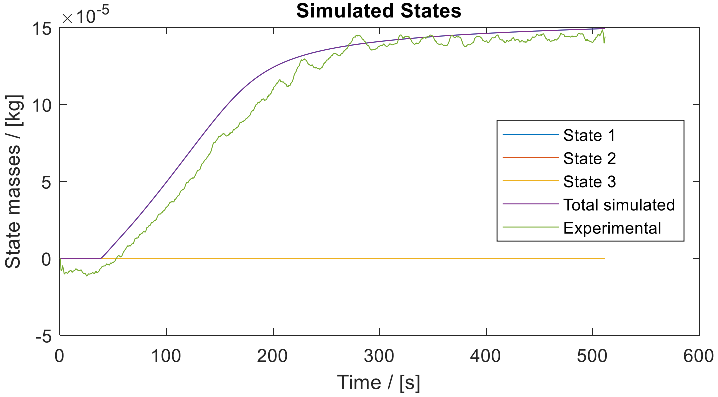


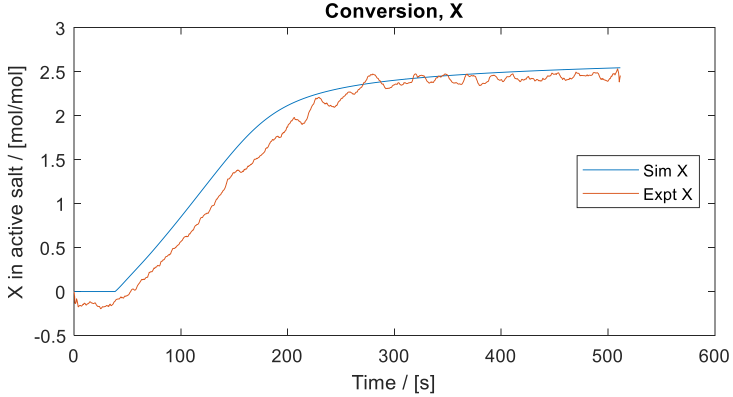


Ammonium Chloride, NH_4Cl – 6 bar ADS

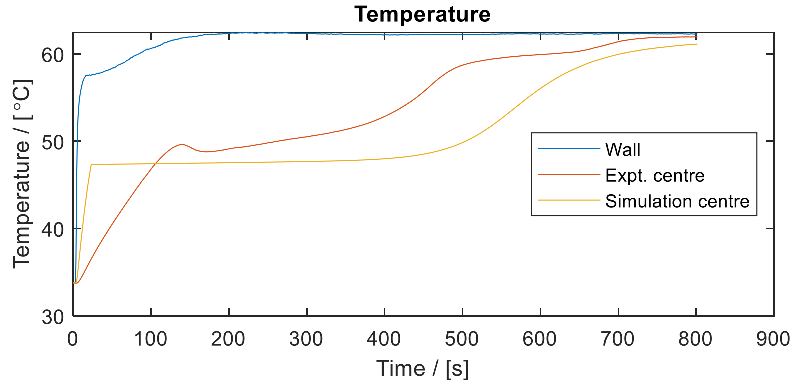


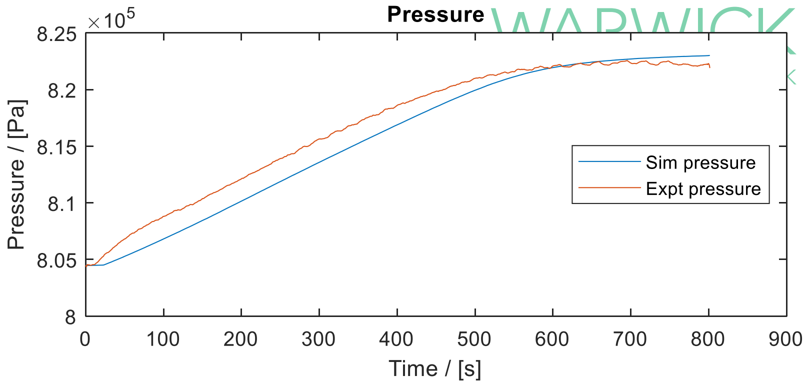


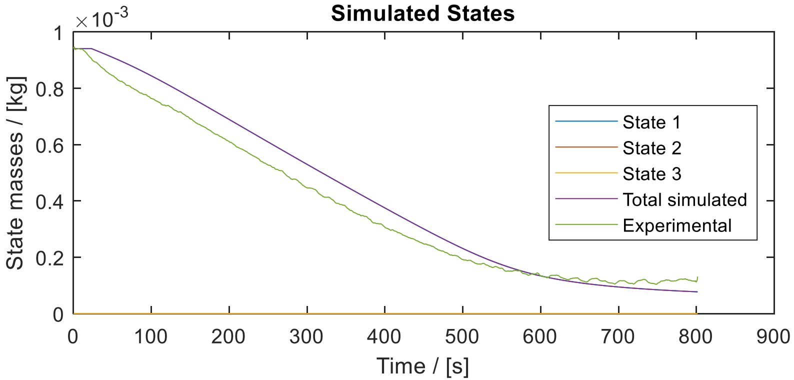


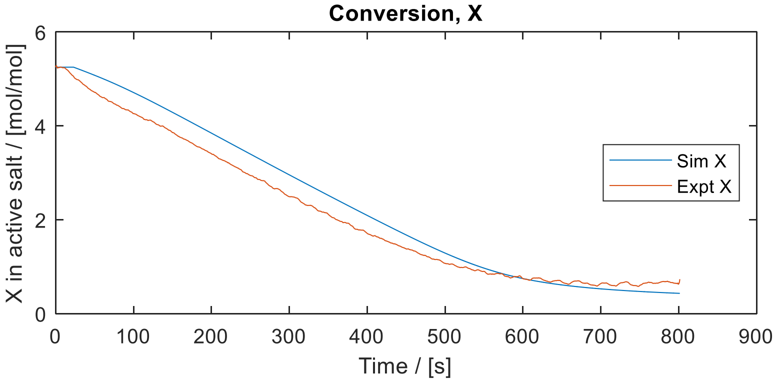


Sodium Bromide, NaBr – 8 bar DES

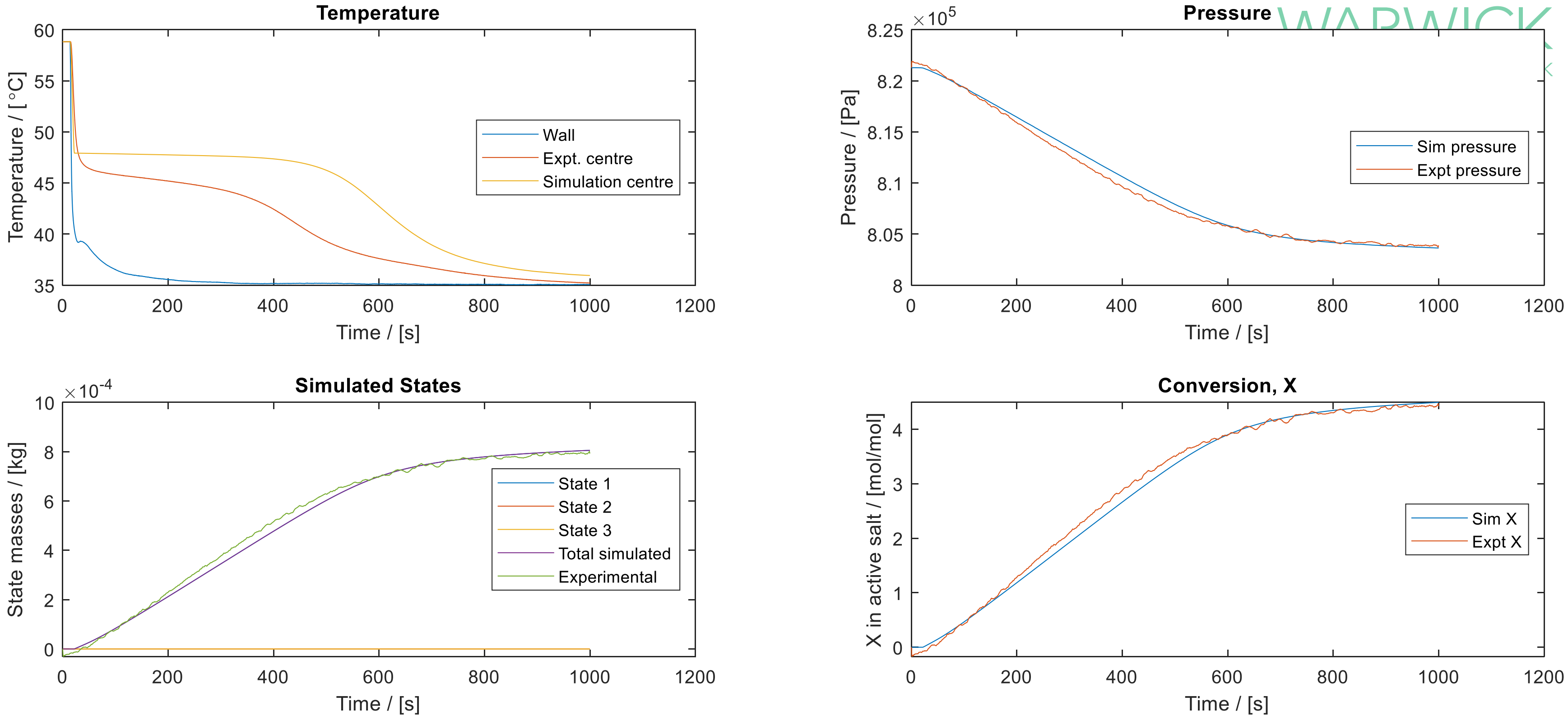




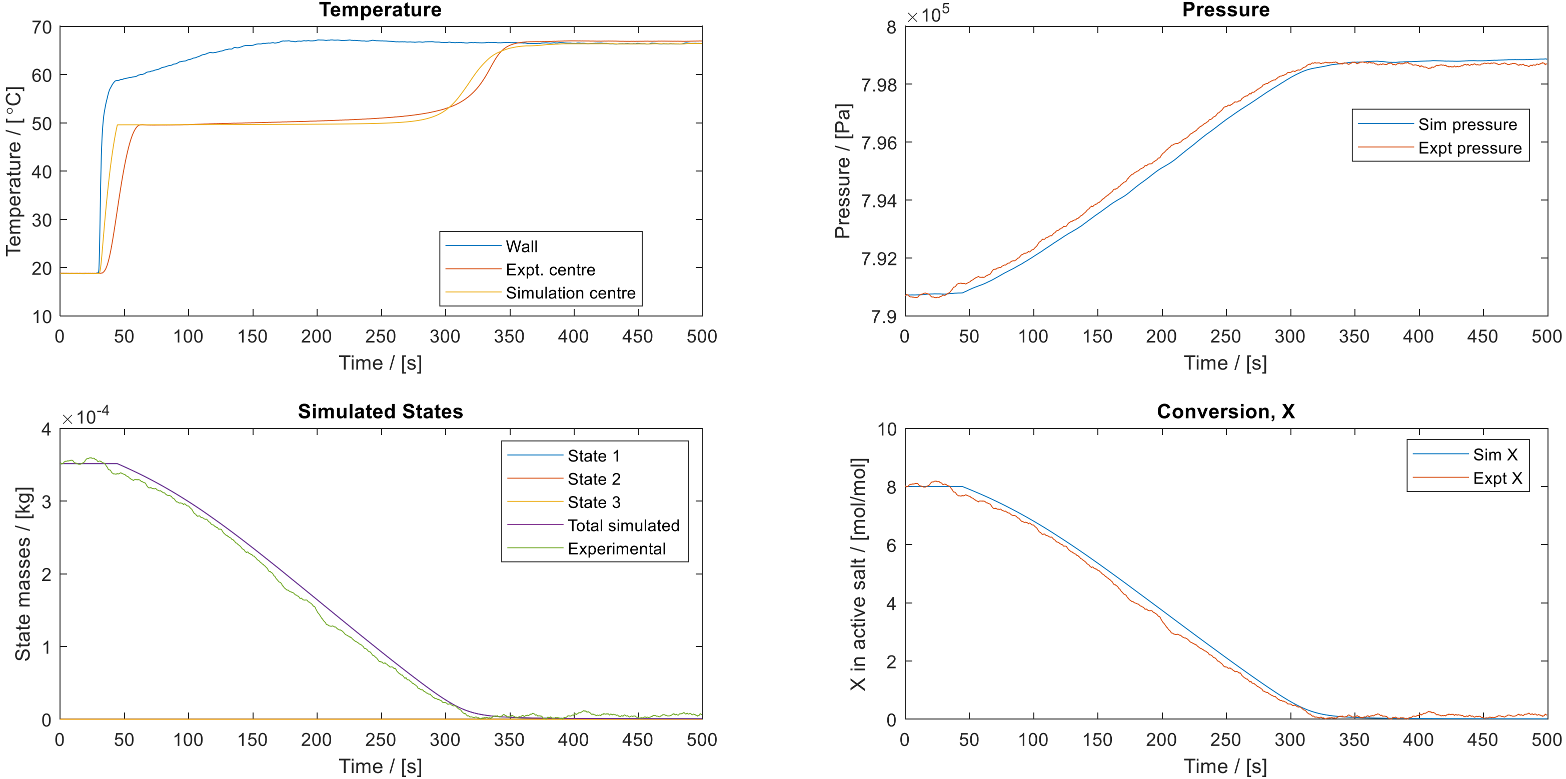




Sodium Bromide, NaBr – 8 bar ADS



Barium Chloride, $BaCl_2$ – 8 bar DES



Barium Chloride, $BaCl_2$ – 8 bar ADS

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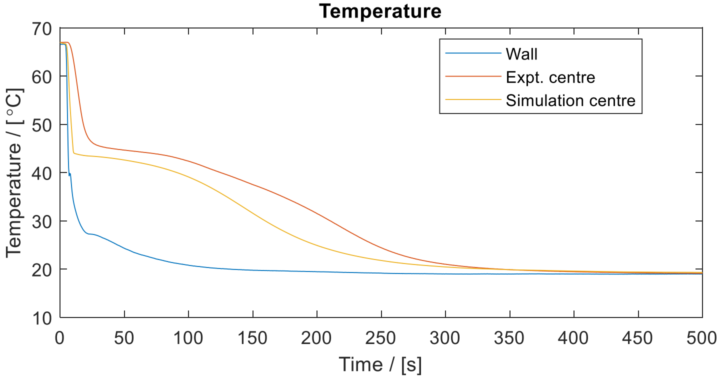

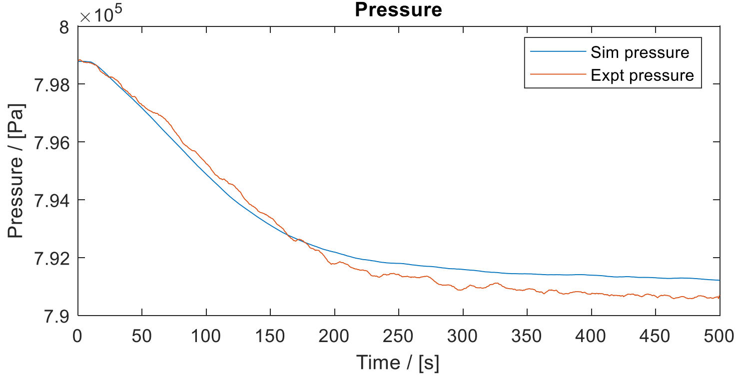

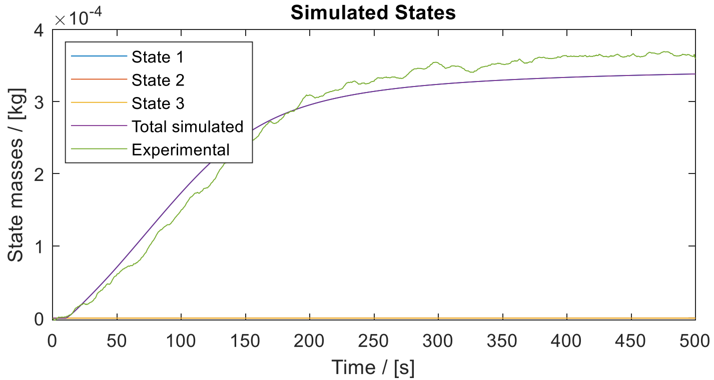

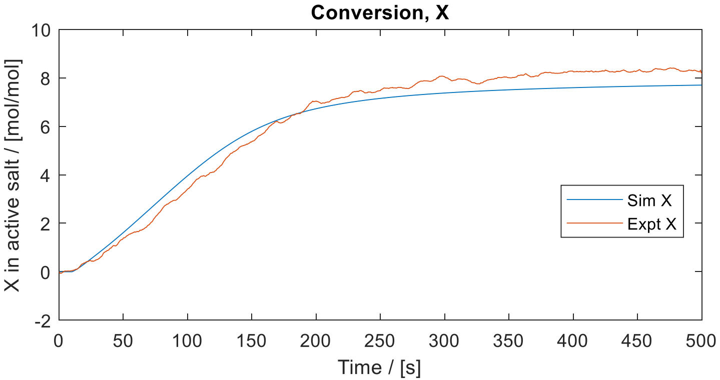

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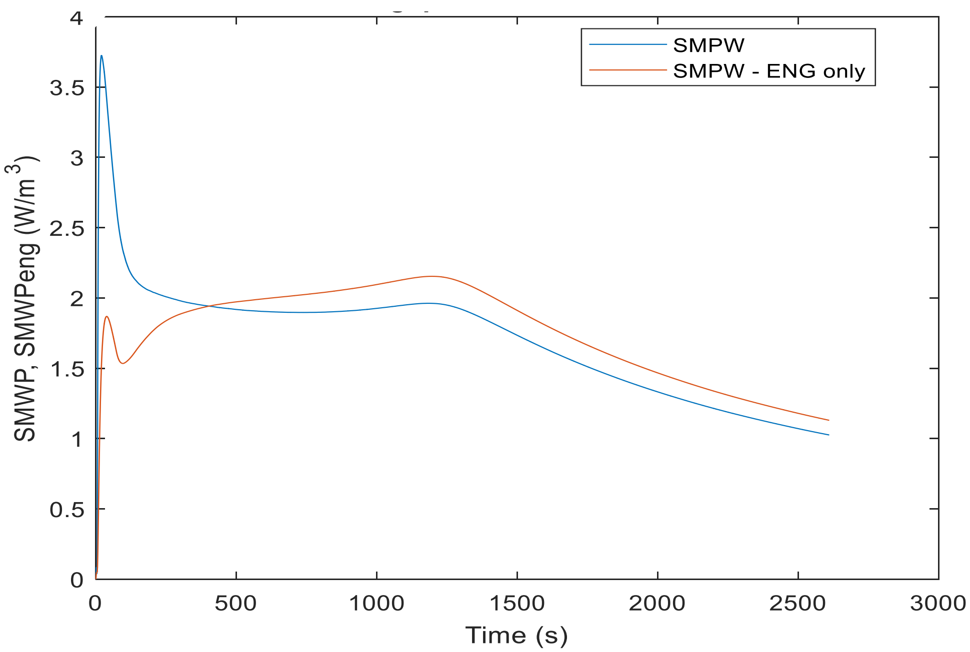
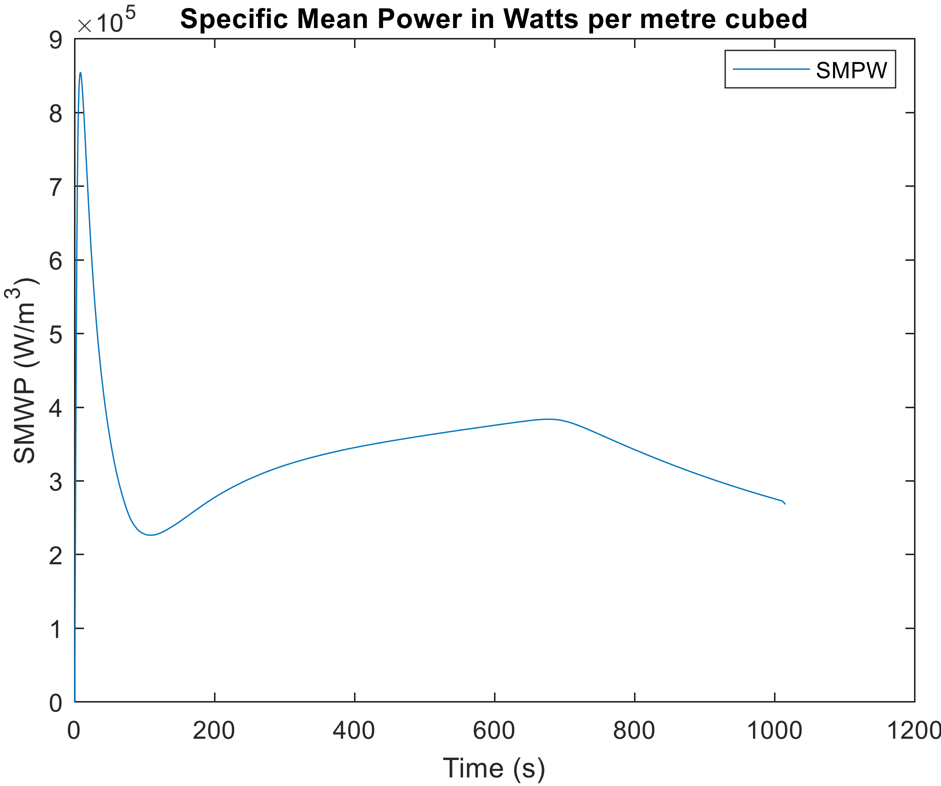
Model Refinement and Development

- The MATLAB model uses the experimental ΔH and ΔS values.
- + 5 modelling parameters:
  1. Conductivity of ENG
  2. Wall heat transfer coefficient (characterised by an ammonia gas gap between the tube side wall and composite sample);
  3. Fraction of salt accessible to gas (active fraction);
  4. and the two reaction rate constants, A
  5. and y, Slide 10, which are different for adsorption and desorption.
- The model has been developed to simulate output as well as determine specific mean power output from the reactions.

Specific Mean Power Output



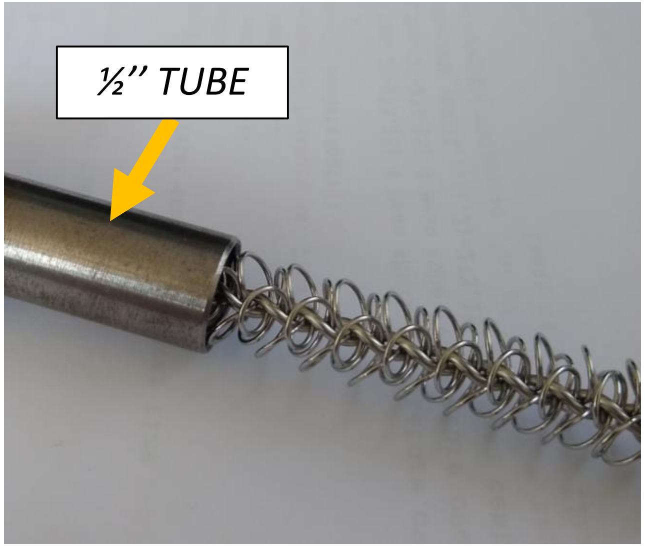


Target SMPW = 1 MW/m³ (= 1 kW/litre)

Heat Transfer Improvements

- Reduction of the gap

- Tube inserts



To Conclude

- Lots of salts tested: NH4Cl, NaBr, BaCl2, CaCl2 & MnCl2 for LTS and HTS thermal transformation and heat pump applications.
- Model outputs match well with experimental data through matching of five key modelling parameters – the **“gap”** identified as key to performance.
- SMPW output targeted for 1 kW/litre and work is ongoing to achieve this.
- Future plans are to produce working designs for proof-of-concept heat pump and thermal transformer resorption machines, with manufacture immanent.

Thank you for listening

Any questions?

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