MI meeting

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Session 2 - Ammonia-Salt Research at Warwick

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STET

Modelling adsorption reactors in Matlab

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MISSION INNOVATION

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Modelling adsorption reactors in Matlab

Aims:

- Simulate heat pump designs
- Model LTJ and cycling rig tests

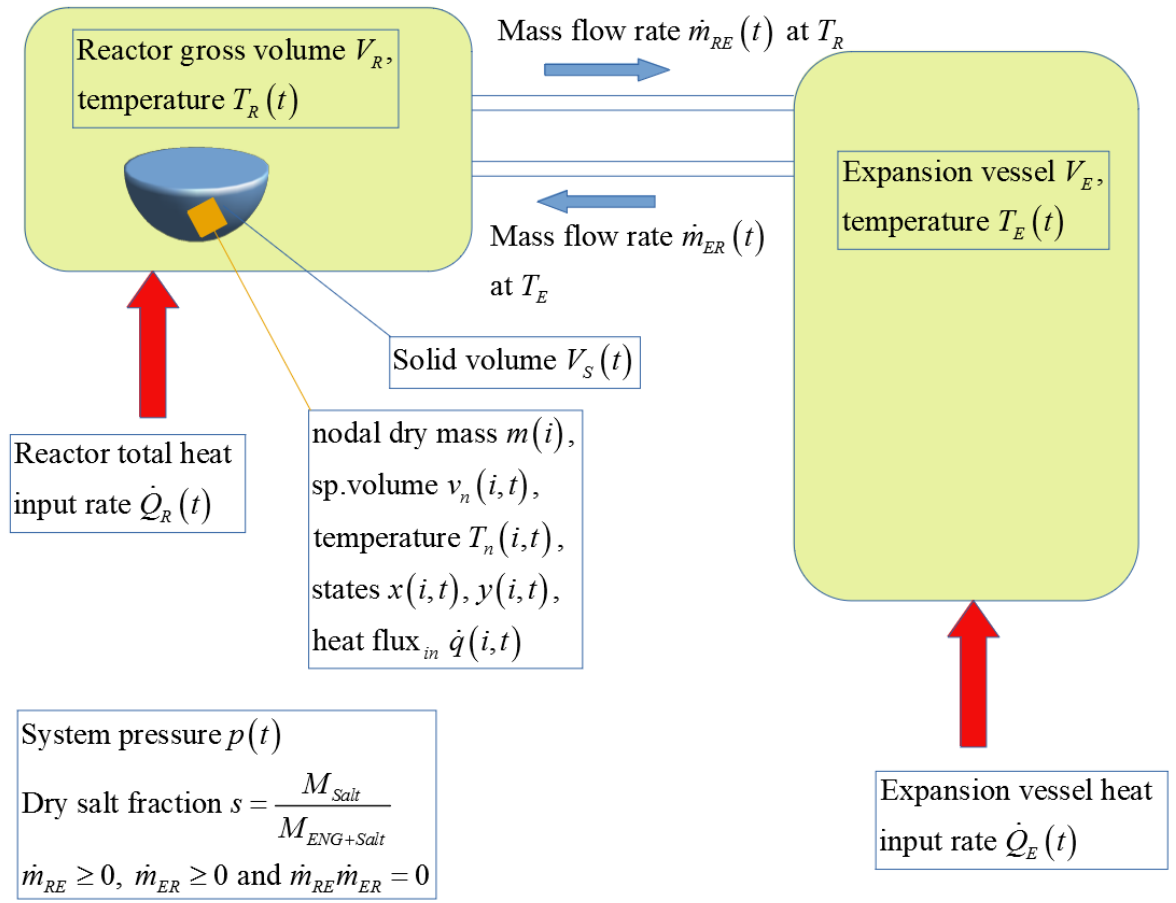
Inputs:

- 1, 2 or more reactors
- Driven by temperature versus time water flows (heat transfer coefficient).

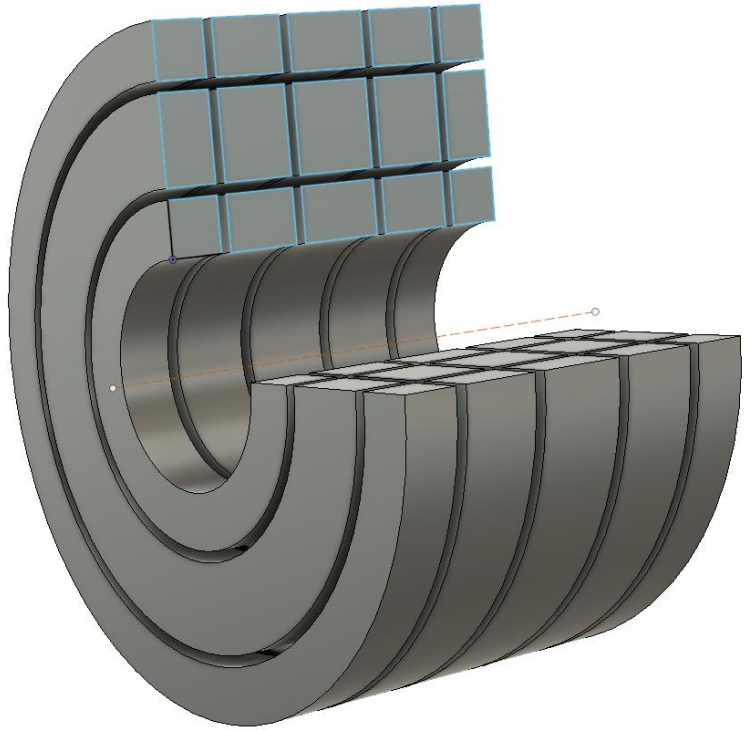
Uses Matlab's ODE23s solver (linked system of ODEs, "Method of Lines").

Code builds a time-derivatives vector for:

- Pressure vessel temperatures
- Temperature of each cell
- Salt ammoniation state in each ENG cell



1D or 2D structured grids
Cuboid (*x*,*y*) or cylindrical (*r*,*z*)

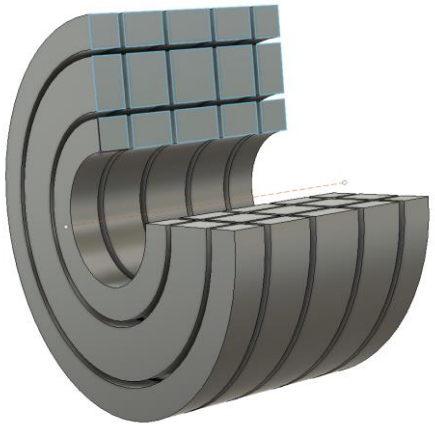


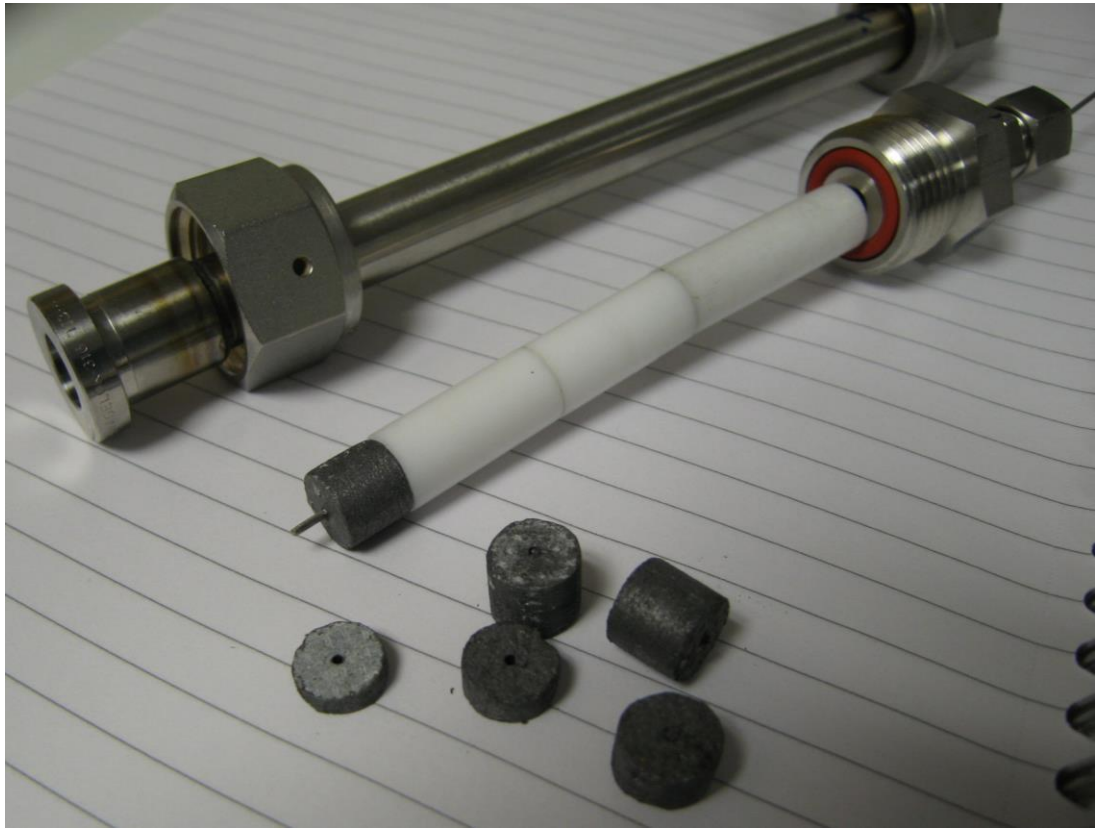
No heat flux in the third direction.

- 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.

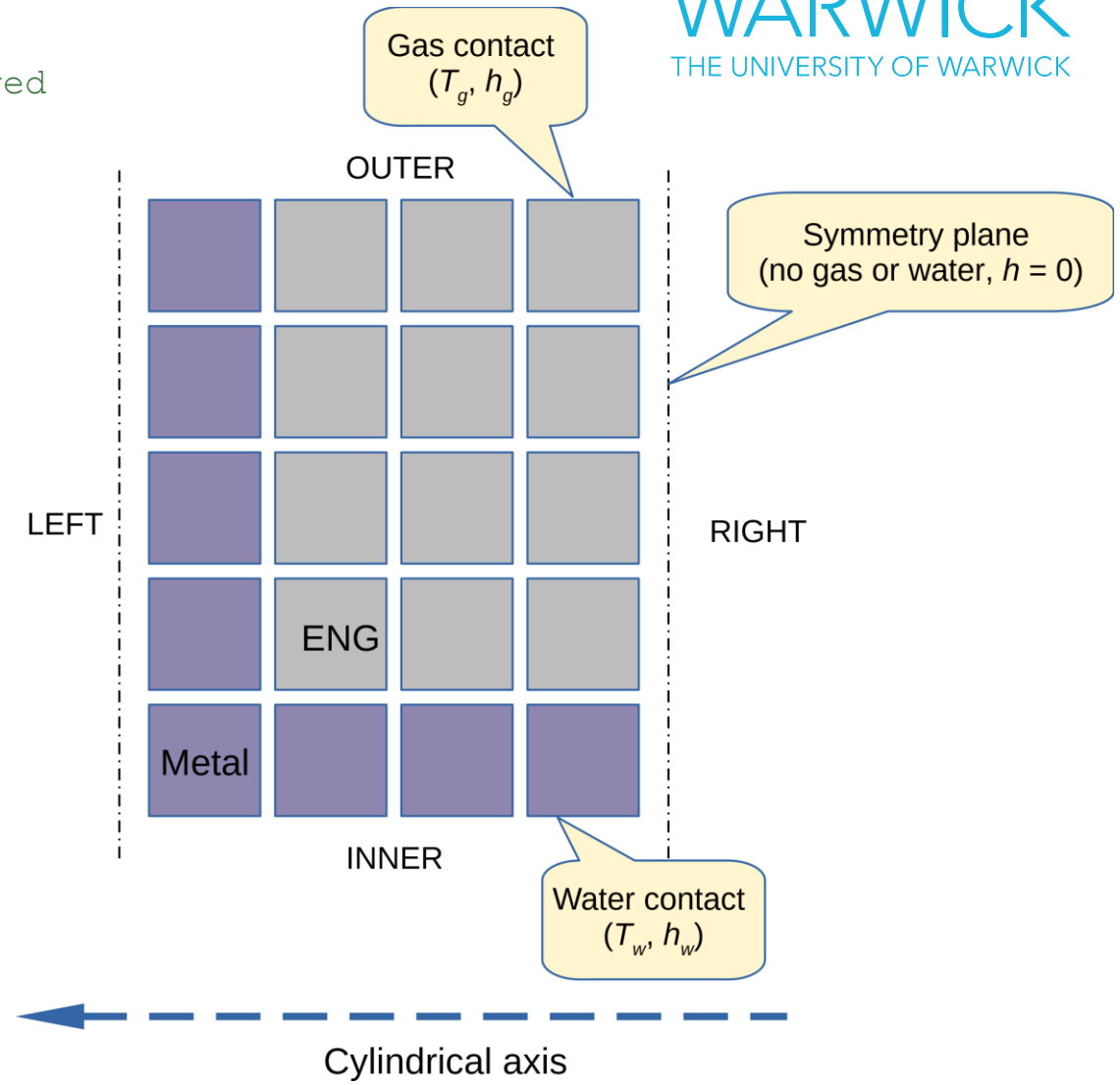




Grid definition

```
iR = 1;
rig.Reactor(iR).gVol = 0.5E-3;  % volume with grids removed
rig.Reactor(iR).IOLR.gas = logical([0 1 0 0]);
rig.Reactor(iR).IOLR.metal = logical([1 0 1 0]);
rig.Reactor(iR).IOLR.water = logical([1 0 0 0]);
rig.Reactor(iR).m = 0;  % linear
rig.Reactor(iR).zlen = 0.3;  % width for m=0 cases
rig.Reactor(iR).mcs = 20e3;  % shell m*c
rig.Reactor(iR).mdotc_fluid = 20;
rig.Reactor(iR).repeats = 10;
rig.Reactor(iR).dim(1).gridx = linspace(0.01, 0.02, 8)';
rig.Reactor(iR).dim(2).gridx = linspace(0, 0.04, 6);
rig.Reactor(iR).gap = 0.2E-3; % metal-ENG gap
rig.Reactor(iR).h_fluid = 20;  % W/m2K
rig.Reactor(iR).h_gas = 5;  % W/m2K

rig.Reactor(iR).Salt = salt_reaction_props('BaCl2');
rig.Reactor(iR).Salt(1).saltFrac = 0.4;
```



Grid cells are either ENG+salt or metal (plate, tube or fin), with contact resistance between metal and ENG.

Test definition example

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```
test.control_tTW{1} = @(t) squarewave(t, [400 200], [10 90], 100);
test.duration = 300; % secs
test.fdOrder = 1;  % 1 or 2, first or second order conduction model
test.ExpVessel.Tinit = 310;  % expansion vessel
test.Pinit = 5E5;  % Sets mass of ammonia (Pa).
test.Reactor(1).Tinit = 310; % repeat for each reactor
```

Reaction rate equations

State J to state K (desorption) or K to J (absorption).
Salt mole fraction in each ammoniated state f_J, f_K such that $\sum_{i=1:N} f_i = 1$

Desorption rate equation:

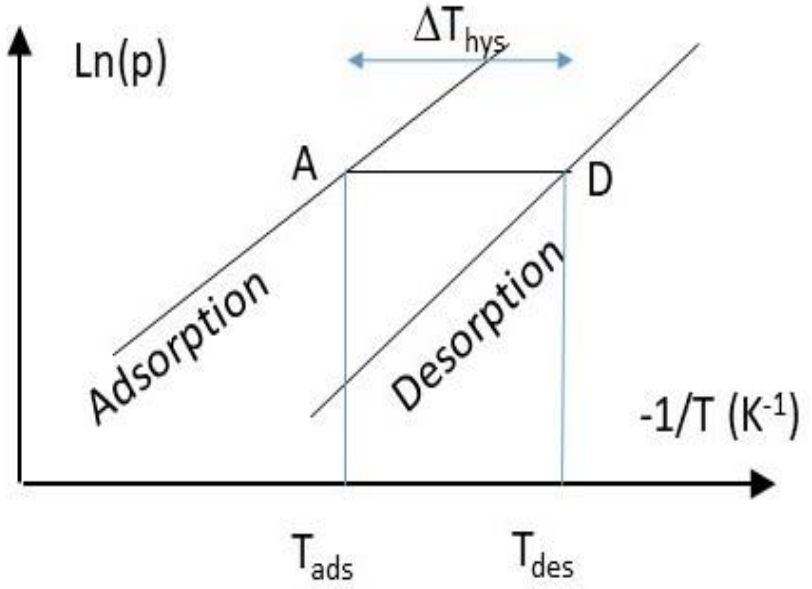
$$\frac{df_K}{dt} = -\frac{df_J}{dt} = A_d \left(f_J + f_K \right) \left(\frac{f_J}{f_J + f_K} \right)^{y_d} \left(\frac{p_{eq,d} - p}{p} \right)$$

$p < p_{EQ}$ causes desorption i.e. positive $\frac{df_K}{dt}$

Adsorption similarly using A_a, y_a, $p_{eq,a}$

$p > p_{EQ}$ causes adsorption i.e. negative $\frac{df_K}{dt}$

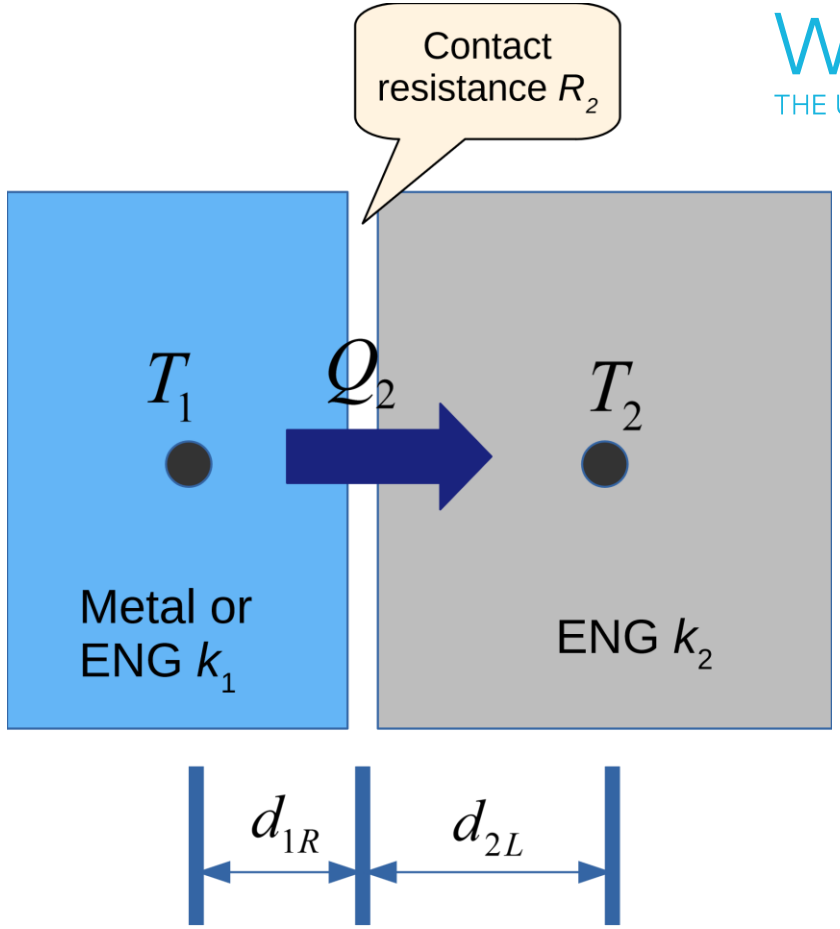
$p_{eq} = e^{\frac{\Delta S}{R} - \frac{\Delta H}{RT}}$ using different $\Delta S, \Delta H$ for each line.



- Pressure assumed uniform (no porosity pressure drop)
- Temperature from conduction and heat generation calculation
- No reaction between the adsorption and desorption lines.
- Calculation repeats over all reactions (e.g. 8-4, 4-2, 2-1).
- If using a salt mixture, repeats for each salt.
- Gas heat transfer during diffusion modelled at its source/sink cell only.

Choice of heat flux calculations (1): Simple model

Assume constant 1D heat flux (linear W/m^2, radial W/m) between a pair of cell centres

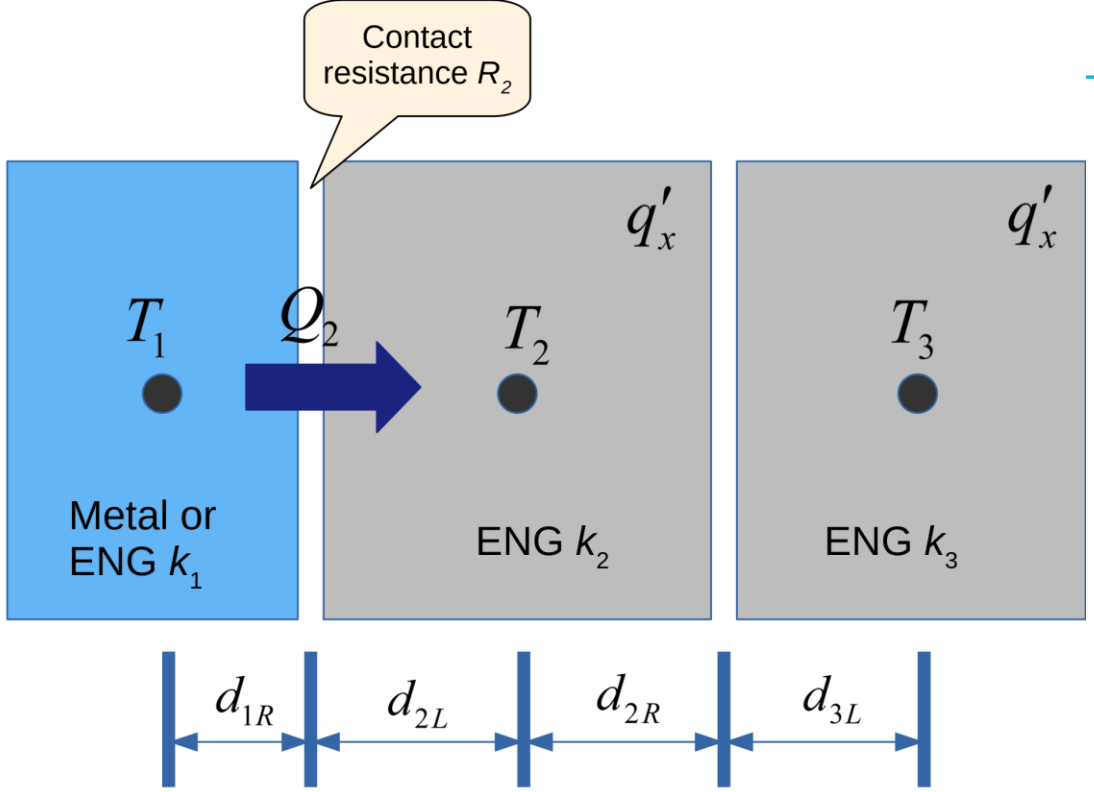


When post-processing, the same finite difference coefficients give “left” and “right” temperatures for each gap, T_{w2L} and T_{w2R}

$$\left(R_2 + \frac{d_{1R}}{k_1} + \frac{d_{2L}}{k_2}\right) Q_2 = T_1 - T_2$$

Heat flux calculations (2): Second-order model

Assume heat generation *q*' causes linear increase of heat flux in each grid direction.



Linear grid; radial expression is more complicated.

$\delta_i = \{0,1\}$ for metal and ENG cells

$$\left(R_2 + \frac{d_{1R}}{k_1} + \frac{d_{2L}}{k_2}\right)Q_2 + \left(\frac{\delta_1 d_{1R}^2}{2k_1} - \frac{\delta_2 d_{2L}^2}{2k_2}\right)q' = T_1 - T_2$$

$$\left(\begin{array}{l}\left(R_2 + R_3 + \frac{d_{1R}}{k_1} + \frac{d_2}{k_2} + \frac{d_{3L}}{k_3}\right)Q_2 + \ldots \\ \left(R_3\delta_2 d_2 - \frac{\delta_1 d_{1R}^2}{2k_1} + \frac{\delta_2 d_2^2}{2k_2} + \frac{\delta_2 d_2 d_{3L}}{k_3} + \frac{\delta_3 d_{3L}^2}{2k_3}\right)q'\end{array}\right) = T_1 - T_3$$

All the finite difference coefficients are calculated prior to iteration.

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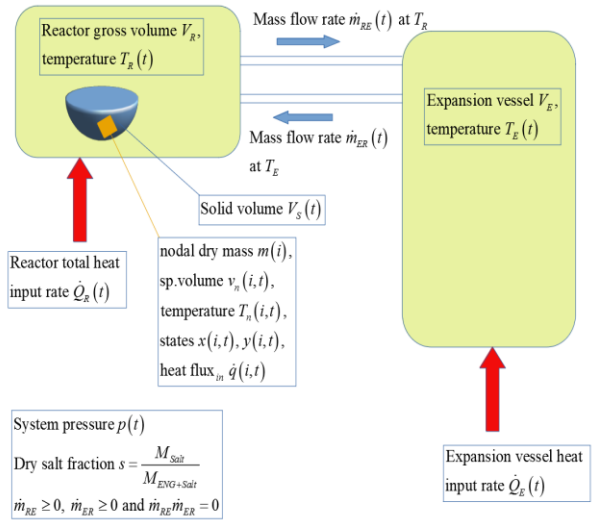
Calculating the cell wall heat fluxes in dimensions 1 & 2 takes just 2 lines of code:

```
for i = 1:ra(2), Q1(:,i) = interps(1).W(:,:,i) * uR(iR).Taug(:, i+1); end
for i = 1:ra(1), Q2(i,:) = uR(iR).Taug(i+1,:) * interps(2).W(:,:,i); end
```

(The augmented temperature matrix `Taug` includes the gas or water temperatures as well as the cell-centre temperatures).

Heat transfer to reactor shell and expansion vessel.



➢ Absorption, desorption and temperature changes lead to gas flow between vessels.

At each time step:

i. Use mass of non-absorbed ammonia to calculate the system pressure.

ii. Calculate the rate of pressure change: $$\frac{\dot{P}}{P}\sum_{0:N}\left(\frac{\gamma-1}{\gamma}c_v m_i T_{R,i}\right) = P\sum\left(\dot{m}_i v_{io,i}\right)$$

iii. Calculate adiabatic mass flow rate between vessels $$\dot{m}_{RE,i} = \dot{m}_{D,i}\left(\frac{T_{io}}{T_R}\right) - \frac{V_{R,i}}{\gamma R T_R}\dot{P}$$

iv. Unsteady energy equation for each vessel - find rate of change of mixed-out temperature.

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \dot{Q}_{in} + \dot{W}_{in} + \sum \dot{m}_{in,j} h_j \qquad \therefore \quad \left(m_w c_w + m_g c_v\right)\frac{\mathrm{d}T_{R,i}}{\mathrm{d}t} = P\left(\dot{m}_{D,i} v_{Dio} - \dot{m}_{RE,i} v_{Eio}\right) + \dot{Q}_{in}$$

$$\left(m_w c_w + m_g c_v\right)\frac{\mathrm{d}T_E}{\mathrm{d}t} = P\sum_{1:N}\left(\dot{m}_{RE,i} v_{Eio}\right)$$

Ammonia properties from superheat tables

Saturated Properties							Superheated Properties ($t - t_s$)			
Temperature - t_s - (°C)	Pressure - p_s - (bar)	Specific Volume - v_f - (m^3/kg)	Specific Enthalpy		Specific Entropy		Abs. Temperature (50 K)		Abs. Temperature (100 K)	
			saturated liquid - h_f - (kJ/kg)	saturated vapor - h_g - (kJ/kg)	saturated liquid - s_f - (kJ/kgK)	saturated vapor - s_g - (kJ/kgK)	Specific Enthalpy - h - (kJ/kg)	Specific Entropy - s - (kJ/kgK)	Specific Enthalpy - h - (kJ/kg)	Specific Entropy - s - (kJ/kgK)
-50	0.4089	2.625	-44.4	1373.3	-0.194	6.159	1479.8	6.592	1585.9	6.948
-45	0.5454	2.005	-22.3	1381.6	-0.096	6.057	1489.3	6.486	1596.1	6.839
-40	0.7177	1.552	0	1390.0	0	5.962	1498.6	6.387	1606.3	6.736
-35	0.9322	1.216	22.3	1397.9	0.095	5.872	1507.9	6.293	1616.3	6.639
-30	1.196	0.9633	44.7	1405.6	0.188	5.785	1517.0	6.203	1626.3	6.547
-28	1.317	0.8809	53.6	1408.5	0.224	5.751	1520.7	6.169	1630.3	6.512
-26	1.447	0.8058	62.6	1411.4	0.261	5.718	1524.3	6.135	1634.2	6.477
-24	1.588	0.7389	71.7	1414.3	0.297	5.686	1527.9	6.103	1638.2	6.444
-22	1.740	0.6783	80.8	1417.3	0.333	5.655	1531.4	6.071	1642.2	6.411

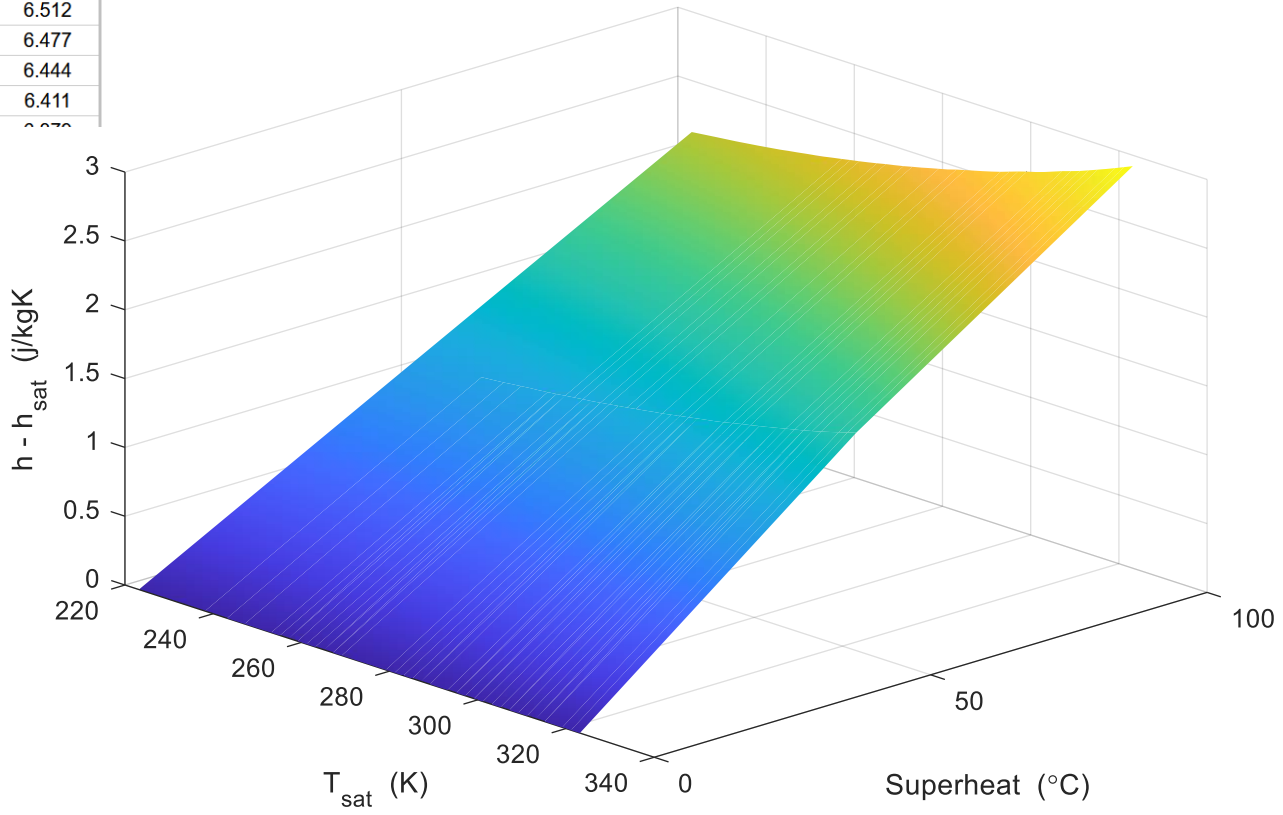
Quadratic fit at each tabulated T_{sat}

Then interpolate to:

- Convert P, T to T_{sat} and (T- T_{sat})
- Get coefficients for this T_{sat}
- Get h, s and v_g correction factor at this (T- T_{sat})

$$u = h - pv, \quad c_p = \left.\frac{\mathrm{d}h}{\mathrm{d}T}\right|_P, \quad c_v = c_p - \frac{\mathrm{d}(PV)}{\mathrm{d}T}$$

(Superheated specific volume estimated from van der Waals' equation.)



Status

- Simulation code is written.
- (x,y) conduction seems to work well
- (r,z) conduction nearly finished
- Reaction rate calculations need checking