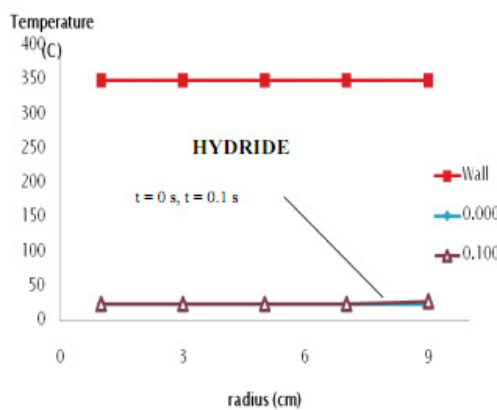


To gauge the thermal performance of the store, a 3-D heat transfer model was constructed using Microsoft Excel spreadsheet. The simple model was built based on explicit numerical method (lumped-capacity analysis) incorporating heat convection from the exhaust gas to the reactor and conduction within the reactor. The computation model was not aimed at giving in-depth analysis of the whole reaction process but merely justifying the viability of using exhaust gas as a heating source. Temperature distribution across the radius of the reactor (including copper fins) was observed until thermal equilibrium was reached.

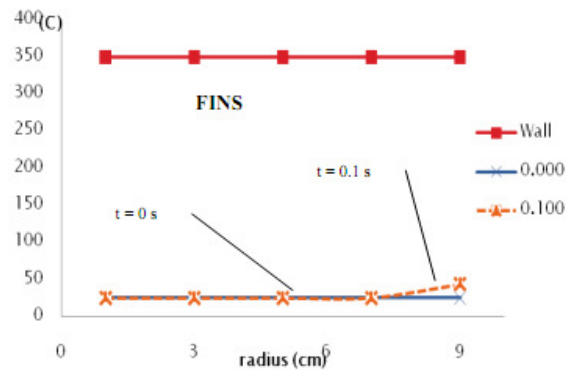
The assumption(s) taken in constructing the model are as follow:

- (i) The initial temperature of the system (reactor bed and shell) is taken at 20°C.
- (ii) The exhaust gas is supplied at a constant flow rate at 67.83 g/s and 350°C.
- (iii) The model corresponds to the cross-section of the store (i.e. x, y-direction) while the length in the z-direction is taken as 1 m.
- (iv) Conduction equation assumes 100% surface contact of the hydride element.
- (v) Heat resistant network is built based on 2-D symmetry of the cross section (see Appendix 2.3, Figure 1).
- (vi) No heat is lost to ambient during discharge (perfect insulation).
- (vii) Energy transferred into the the hydride bed does not take into account the additional 74 kJ/mol enthalpy required to liberate the hydrogen gas from the adsorption bond.

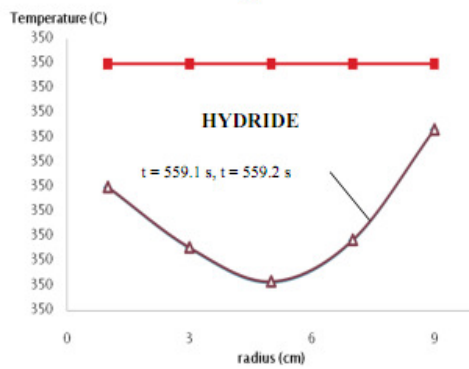
With these assumptions and applying energy balance into the equations (refer Appendix 2.3.2) yields the following results in Figure 29.



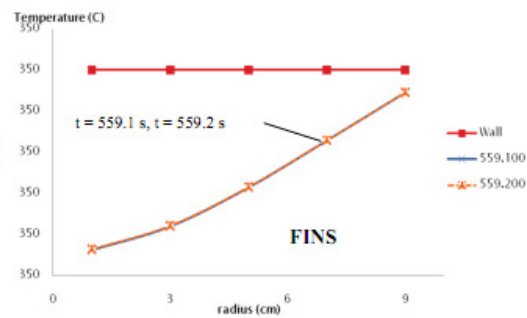
(i)



(ii)



(iii)



(iv)

Figure 29: Simulation results showing the temperature distribution across the radius of the reactor based on the hydride bed (i) & (iii); and copper fins (ii) & (iv). Wall temperature (red line) is maintained at 350°C for each computation. ( $t = 0.05$  s, temperature distribution was computed along the radial length of 100 mm).

### 9.3.1. HEAT TRANSFER CALCULATION & MODELLING

The following figures explain the 2-D symmetry on the cross section of the reaction, taking the length in z-direction as 1 m and hence the geometry of the problem:

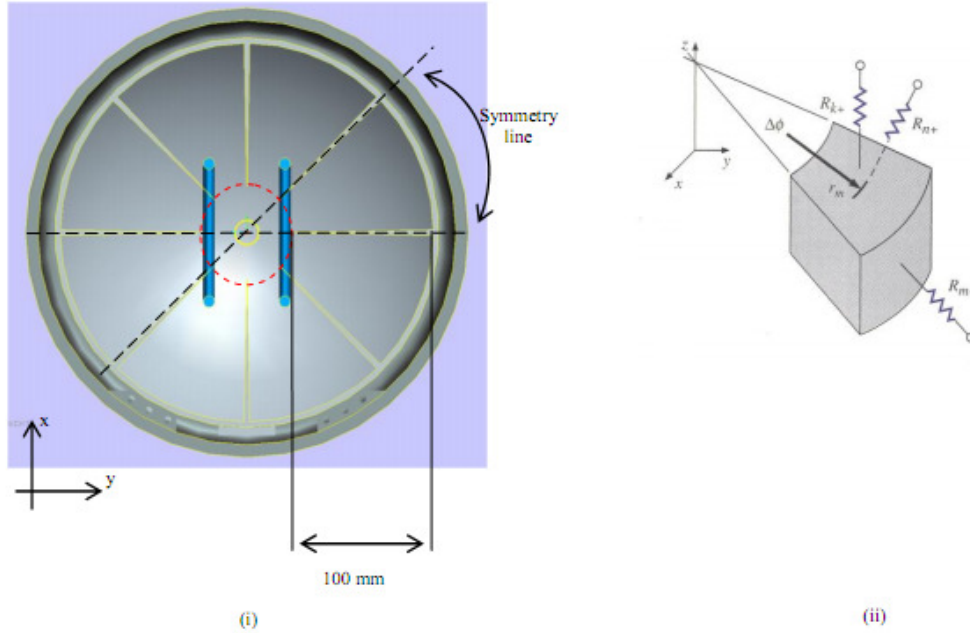


Figure 2: (i) Cross-section of the reactor showing symmetry lines; (ii) Internal Nodal Resistance of the heat transfer model.

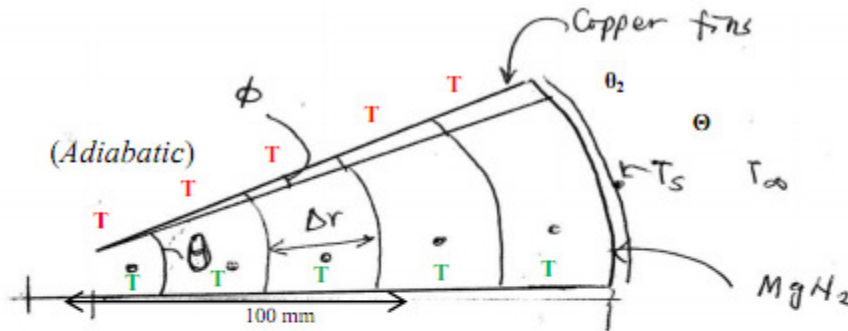


Figure 3: 2-D representation of the heat transfer geometry

#### Resistance Values

$$R_{m+} = \frac{\Delta r}{\left(r_m + \frac{\Delta r}{2}\right) \Delta \theta k}$$

$$R_{n+} = \frac{r_m \Delta \theta}{\Delta r \Delta z k}$$

$$R_{k+} = \frac{\Delta z}{\Delta r \Delta \theta r_m k}$$

### 9.3.2. ENERGY BALANCE EXPRESSION

The following energy balance equation is applied for each node:

$$\left[ \begin{array}{c} \text{Sum of heat transfer} \\ \text{in and out of the node} \end{array} \right] + \left[ \begin{array}{c} \text{Internal heat Generation} \\ \text{of node} \end{array} \right] = \left[ \begin{array}{c} \text{Rate of energy change} \\ \text{of node} \end{array} \right]$$

$$[q_{i-1,i} + q_{i+1,i}] + [q_i'''] = m_i c \frac{T_i' - T_i^0}{\Delta t}$$

Internal heat generation

Internal heat generation of node  $i^{th}$ ,  $q_i'''$ , is confined to node 1-5 (hydride) only. During  $H_2$  discharge, the process is endothermic therefore 74 kJ/mol  $H_2$  energy is required from the heat transfer. This is complicated to be expressed algebraically as the energy generated per 1 m<sup>3</sup> of element needs to be quantified first. The number of moles of  $H_2$  which reacts at the instant when enough energy is supplied per volume of element must also be determined. For the sake of simplicity, this was neglected as it was not the main focus of the project and elaborated modelling would have seriously prolonged the project duration. Hence  $q_i''' = 0$  in this case.

Equation (1-5) are derived to solve for  $i^{th}$  -node while equation (A- E) are for  $j^{th}$  -node where  $i = 1, 2, \dots, 5$  and  $j = A, B, \dots, E$ .

$$\text{Eqn 1: } T_1' = T_1 + \frac{\Delta t}{c_1} \left[ (T_2 - T_1)\theta_1 k_1 + (T_A - T_1) \frac{\Delta z k_{avg}}{(0.5 \times 0.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 2: } T_2' = T_2 + \frac{\Delta t}{c_2} \left[ (T_1 - T_2)\theta_1 k_1 + 2(T_3 - T_2)\theta_1 k_1 + (T_B - T_2) \frac{\Delta z k_{avg}}{(0.5 \times 1.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 3: } T_3' = T_3 + \frac{\Delta t}{c_3} \left[ 2(T_2 - T_3)\theta_1 k_1 + 3(T_4 - T_3)\theta_1 k_1 + (T_C - T_3) \frac{\Delta z k_{avg}}{(0.5 \times 2.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 4: } T_4' = T_4 + \frac{\Delta t}{c_4} \left[ 3(T_3 - T_4)\theta_1 k_1 + 4(T_5 - T_4)\theta_1 k_1 + (T_D - T_4) \frac{\Delta z k_{avg}}{(0.5 \times 3.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 5: } T_5' = T_5 + \frac{\Delta t}{c_5} \left[ 4(T_4 - T_5)\theta_1 k_1 + 9.5(T_s - T_5)\theta_1 k_1 + (T_E - T_5) \frac{\Delta z k_{avg}}{(0.5 \times 4.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 6: } T_A' = T_A + \frac{\Delta t}{c_A} \left[ (T_B - T_A)\theta_2 k_2 + (T_1 - T_A) \frac{\Delta z k_{avg}}{(0.5 \times 0.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 7: } T_B' = T_B + \frac{\Delta t}{c_B} \left[ (T_A - T_B)\theta_2 k_2 + 2(T_C - T_B)\theta_2 k_2 + (T_2 - T_B) \frac{\Delta z k_{avg}}{(0.5 \times 1.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 8: } T_C' = T_C + \frac{\Delta t}{c_C} \left[ 2(T_B - T_C)\theta_2 k_2 + 3(T_D - T_C)\theta_2 k_2 + (T_3 - T_C) \frac{\Delta z k_{avg}}{(0.5 \times 2.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 9: } T_D' = T_D + \frac{\Delta t}{c_D} \left[ 3(T_C - T_D)\theta_2 k_2 + 4(T_E - T_D)\theta_2 k_2 + (T_4 - T_D) \frac{\Delta z k_{avg}}{(0.5 \times 3.5)\theta_1 + \theta_2} \right]$$

$$\text{Eqn 10: } T_E' = T_E + \frac{\Delta t}{c_E} \left[ 4(T_D - T_E)\theta_2 k_2 + 9.5(T_s - T_E)\theta_2 k_2 + (T_5 - T_E) \frac{\Delta z k_{avg}}{(0.5 \times 4.5)\theta_1 + \theta_2} \right]$$