CHAPTER 4

COMPUTATIONAL INVESTIGATIONS

5.1 INTRODUCTION

From the vast literature review, it was understood that the solidification rate has a strong influence on the metallurgical and mechanical properties of the cast Al-Si alloys. According to Jose (2012) these properties of castings are largely depending on thermal behaviour of metal/mold system during solidification. The thermal behaviour of the metal / mold system is the heat transfer from the cast to the mold by partial convection / conduction within the mold and the convective heat loss from the mold to the ambient. As discussed in Chapter 3, the ambient for the mold can either be air or water, based on the cooling media used. The mechanisms of heat transfer during solidification at metal-mold and mold-ambient are complex and much effort has been taken to compute the same at the interfaces. The complexity in the interface lies in the formation of micron to mm level air gaps in the metal-to-mold interface, which acts as a thermal barrier. These air gaps effectively reduce the heat transfer, which in turn reduces the solidification rate. Higher the heat transfer rate across the mold, higher will be the solidification rate and finer will be the grain formation. It is essential to know the interfacial heat transfer coefficient (IHTC) fluctuations with time during the solidification of metals, since its value at the metal-mold and mold-ambient interfaces have a predominant effect on the rate of heat transfer.

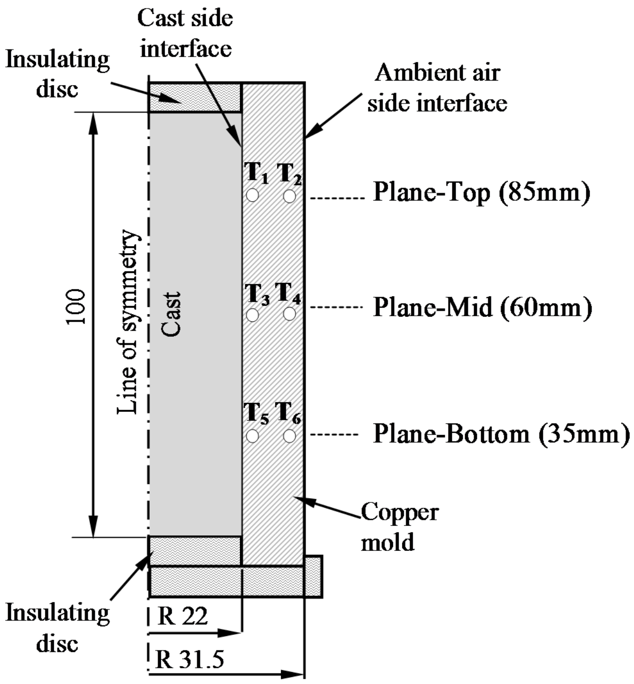
Estimating the IHTC using experiments is complex and not feasible in most of the situations. This is due to the fact that IHTC is a function of several variables like air gap between cast and mold, mold surface roughness, mold coatings, oxide growth on the surface, mold material and its thickness etc. Hence numerical methods of estimating the Interfacial Heat Flux (IHF) was preferred by many researchers in-lieu of direct estimation of IHTC. Estimating the IHF in a casting process will help in quantifying the heat transfer rate and thus the solidification rate. The IHF is a surface condition that needs to be estimated from the known values such as wall temperatures measured with thermocouples at specific points. This method of estimating a surface condition from the measured wall temperature is referred as '*Inverse Heat Conduction Problem – IHCP*'. The numerical techniques of this class of problems are well documented and reported by Prasanna Kumar (2004). The IHCP theory was first developed with single known temperature history which limits the estimation of heat flux to a given single region. The principle was then extended to multiple temperature history locations ie., thermal sensors, which led to the simultaneous estimation of heat fluxes at multiple regions in the domain under study. The computation of heat flux using IHCP, for multiple boundary components of both air-cooled and water-cooled gravity copper die, while casting Al-Si alloys considered for this study is discussed in this chapter.

5.2 PHYSICAL DOMAIN

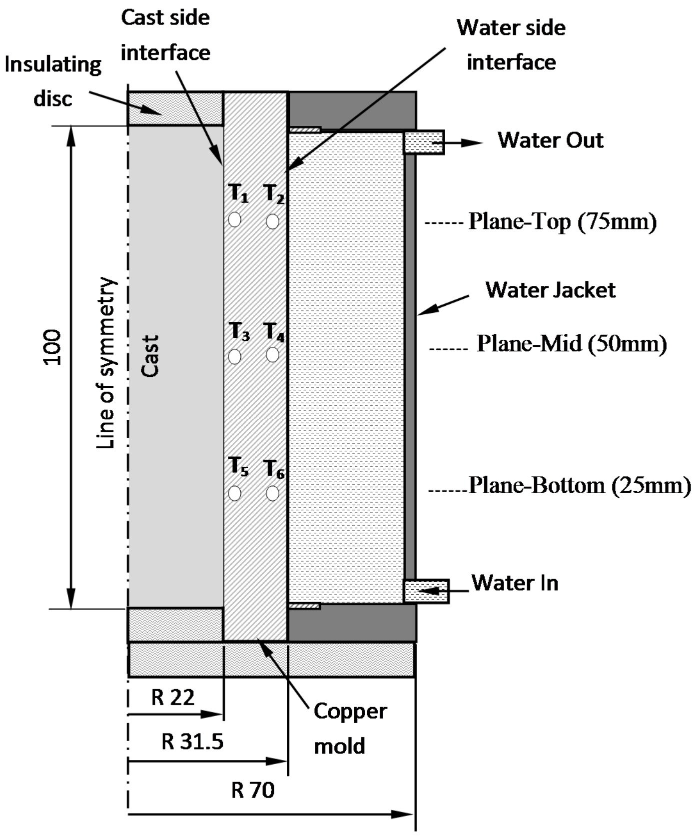
The physical geometry chosen for the present study is a cylinder, which is cast in a gravity die made of copper. Considering the axisymmetric nature of the three dimensional physical domains of the casting setups, the computational tool offer a flexibility to carry out the simulation in a simplified two dimensional domain. Sectional axisymmetric view of the mold and the cast assembly, for both the air-cooled and water-cooled setups used for the present study are shown in Figures 4.1 (a) and (b) respectively.

The thermocouples were shown on same vertical plane as in Figures 4.1 (a) and (b) for clarity. In actual measurements, these thermocouples are located in three different radial directions, as discussed earlier in Chapter 3. A total of six K-type thermocouples were used to measure the mold temperatures.

A gist of the experimental procedure is detailed here for immediate reference. An insulating disc was placed at the bottom of the mold before the molten metal was poured. Once the molten metal of chosen quantity was poured into the mold, another insulating disc was placed at the top. These two insulating discs are used to prevent axial heat loss through the top and bottom of the die. This helps in confining the thermal loss from the cast only in the radial direction through the mold wall to the ambient. Since the computational analysis takes the boundary condition from the experiments, this way of unidirectional confinement of heat loss in the radial direction will help in estimating the interfacial heat flux in a more straight forward way. In the water cooled experiments, any small loss of heat to the ambient outside the water jacket outer wall can be ignored as the water jacket is made of acrylic, which is an insulating material.



(a) Air cooled setup



(b) Water cooled setup

Figure 4.1 Details of the axisymmetric physical domain

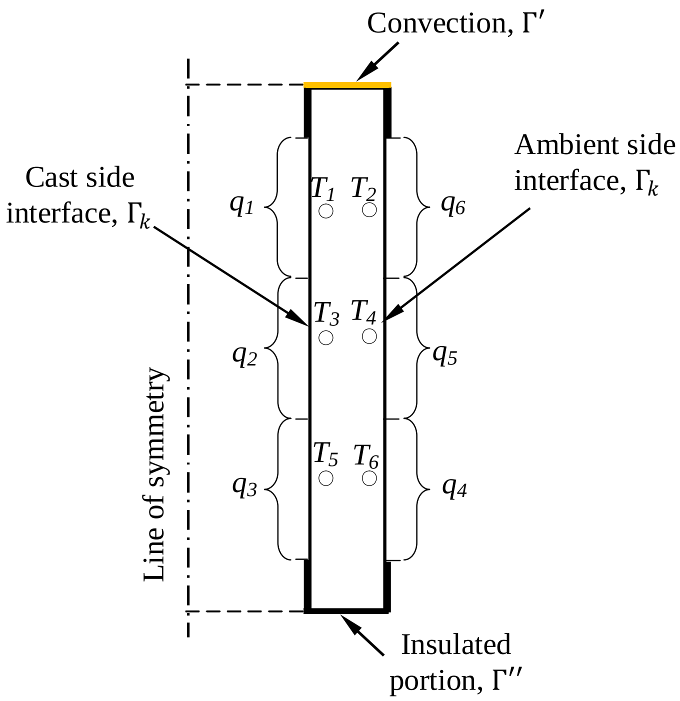
5.3 SOLVER DETAILS

The numerical computations were carried out for estimating the multiple boundary IHF during the casting solidification of both the Al-Si alloys (A413 & A380) using a serial solution based IHCP solver Thermal-mechanical-metallurgical Finite Elements (TmmFE). The computational technique adopted in the solver TmmFE is briefly discussed here in this section. This includes the numerical procedure adopted in using the TmmFE solver for the estimation of unknown heat fluxes from the known (measured) values of temperatures. It is based on the IHCP to reliably describe the nature and amount of the interface heat transfer in metallic molds. The computational tool does not limit the maximum number of flux components estimated to the number of observations available. More details of the IHCP solver TmmFE was reported by Prasanna Kumar (2004)

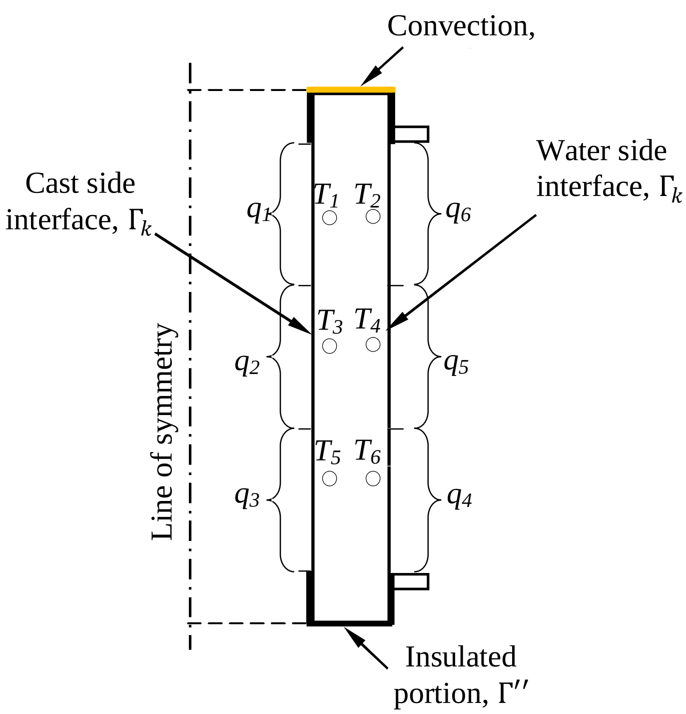
5.4 COMPUTATIONAL METHODOLOGY

The physical domain considered for the present study was symmetric about its axis and hence two dimensional axisymmetric computational domains were conceived as shown in Figure 4.2(a) and (b) for air-cooled and water-cooled casting setups respectively. The assumption of heat loss from the cast only in the radial direction is also valid with the chosen computational domain. The present approach is to predict the IHF at the cast-to-mold wall interface and the mold wall-to-ambient interface, using the temperatures measured from the experiments.

To estimate the interfacial heat flux at the mold boundary, the axisymmetric computational domain of the mold was sufficient for the TmmFE solver. This indicates that the domain of the cast or the domain of the ambient need not be modelled.



(a) Air-cooled setup



(b) Water-cooled setup

Figure 4.2 Computational domain used for the numerical analysis

The mold wall regions which are not in direct contact with either the cast or ambient are declared as insulating boundaries (Γ''), since there was no heat transfer between these segments to the surroundings. The top surface of the mold is considered to lose heat to the ambient air by convection and an appropriate heat transfer coefficient value (Γ') was specified for this edge. The cast side and ambient side interfaces of the mold are divided into three regions of equal length, totalling six regions.

It was assumed that there are no variations along the length in the corresponding values of cast side and ambient side heat fluxes (Γ_k). This heat flux boundary was divided into three regions on each side and thus the assumption was extended that there are no variations in heat fluxes within these regions considered. These heat flux values will be estimated from the temperature values measured in the corresponding regions. For example, the heat flux values q_1 and q_6 were estimated from the measured temperatures T_1 and T_2 respectively. The transient heat flux values, as obtained from the solver, can be used as an input boundary condition for a subsequent numerical thermal analysis. Further details on the solution algorithm, the estimation of sensitivity coefficients for multiple heat fluxes and the objective functions are discussed by Prasanna Kumar (2004) and Arunkumar et al. (2008).

4.4.1 Governing Equations

The fundamental governing equation of the TmmFE solver is the two dimensional steady state heat transfer equation as shown in Equation (4.1).

$$\frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) = \rho c \frac{\partial T}{\partial t} \qquad (4.1)$$

Further to Prasanna Kumar (2004), the IHCP is to find $(q_p)_m$; assuming $(q_k)_i$, where k=1,..,l; i =1,...,m-1 and k =1,..,p_1;i=1,2..m are known (already determined). More explicitly, the flux values for all the unknown boundaries till the previous time step and up to the present boundary till the present time step are assumed to have been determined. The m^{th} time step is the current time step and the p^{th} flux boundary is the current unknown boundary. The material properties may be treated as functions of temperatures, in which case the problem becomes non-linear. The solution technique is based on finite element method for the direct solution part, which makes this IHCP formulation applicable for non-linear cases also. However, in the following discussion, the material properties are taken as independent of temperature and hence, the problem can be treated linear.

4.4.2 Boundary Conditions

The two dimensional domain used for the numerical computations, as given in Figure 4.2, was discretized into four node iso-parametric elements. The total number of elements used in this case was 1320 and the convergence limit for the Gauss-Siedel iterations was set to be 1e-6. The thermo physical properties of the mold made of copper are given in Table 4.1.

Table 4.1 Thermo physical properties of mold material

Temperature	**Density**	**Specific heat**	**Thermal Conductivity**
[^{o}C]	[kg/m^{3}]	[J/kg-K]	[W/m-K]
35	8978	385	401
100		389	394
200		402	389
500		427	341
800		473	339

The boundary nodes at the interface regions were specified with a boundary type '*unknown heat flux boundary*' available within the solver TmmFE. The unknown boundaries are marked Γ_k; k=1, 2… and it was assumed that the other boundaries as well as the material properties are known and specifiable. The initial conditions for the presently considered case will be $T(x, y) = T'$ at t=0 and the boundary conditions are given by Equation (4.2):

$$\left.\begin{aligned} -\lambda\frac{\partial T}{\partial x}n_x - \lambda\frac{\partial T}{\partial y}n_y &= q_k(x,y,t) \text{ on } \Gamma_k;\ k=1, 2, \ldots p, \ldots l \\ -\lambda\frac{\partial T}{\partial x}n_x - \lambda\frac{\partial T}{\partial y}n_y &= h(T - T_\infty) \text{ on } \Gamma' \\ -\lambda\frac{\partial T}{\partial x}n_x - \lambda\frac{\partial T}{\partial y}n_y &= 0 \text{ on } \Gamma'' \end{aligned}\right\} \quad (4.2)$$

In general, only the metal–mold interface was considered as unknown boundary and the outer surfaces of the mold walls were assigned with a nominal heat transfer coefficient. However, in the present study, the outer surface of the mold wall was also considered as an unknown boundary similar to Arunkumar et al. (2008). This helps in avoiding the error caused by the assumption of a constant heat transfer coefficient Γ' at the outer boundary. A constant Γ' will not be logical as the temperature along the boundary length (top to bottom) was different and the corresponding heat loss to its ambient will be different with spatial location.

4.4.3 Estimation of Heat Flux

The q_k is the unknown independent flux at the boundaries. This section discusses the procedure adopted in the numerical solver TmmFE to estimate the heat flux values on the boundary surfaces $q_1 - q_6$ identified earlier. To estimate the heat flux the experimentally measured temperature values at the thermocouple locations $T_1 - T_6$ were fed as a notepad file in a format suitable to the solver. The transient simulations were performed by the solver with a time step size of 0.1s till 500s, with the inputs and boundary conditions specified. Figure 4.3 shows the snapshot of the TmmFE solver graphics window with the computational domain modelled for the air cooled mold. The domain was created within the solver with points *P1 – P13* as shown. The points were connected using edges and a two dimensional face was created using the edges. The geometry created was meshed with quadrilateral elements as shown in Figure 4.3. The corresponding unknown heat flux regimes q_1 – q_6 identified earlier was also marked for immediate reference.

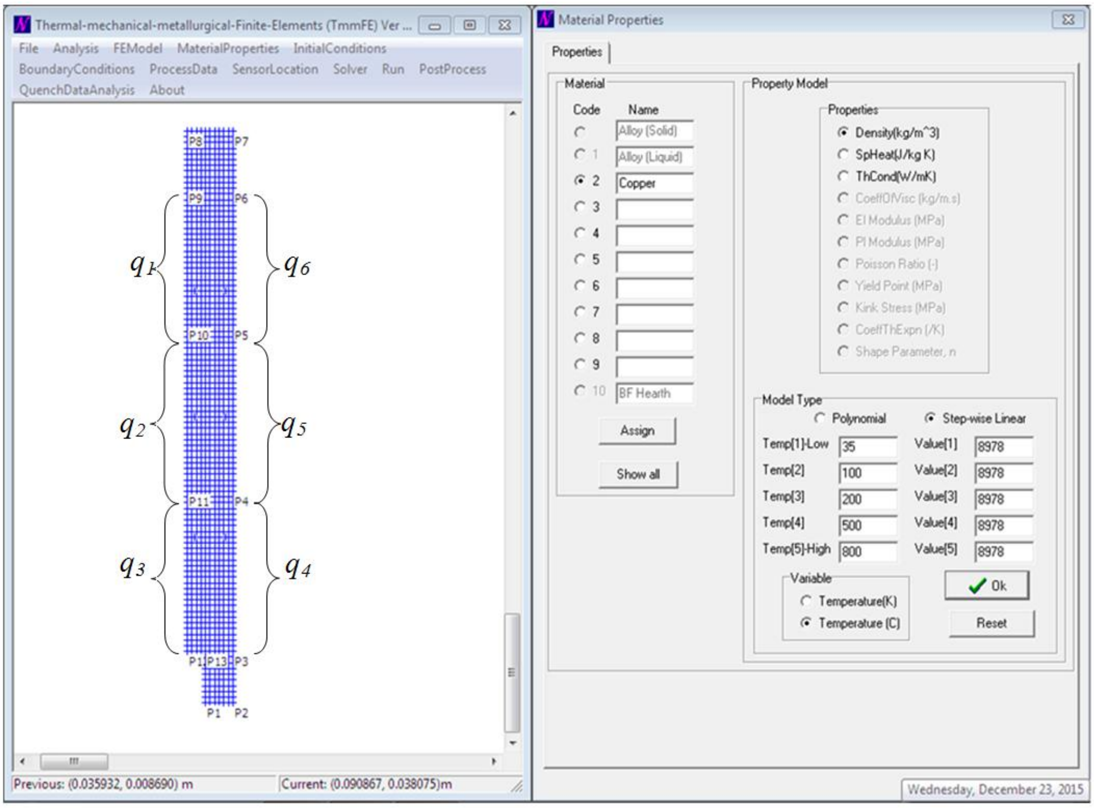


Figure 4.3 Snapshot of the TmmFE solver graphics window – Air-cooled mold

The right side of Figure 4.3 shows the material properties definition window where the Copper material is defined in the solver. The step-wise linear variation of density (it is assumed constant for the present computational study) with temperature was specified in this window. Similarly, the step-wise linear variation of other thermo-physical properties of copper such as specific heat and thermal conductivity were fed into the solver before starting the computation.

The edges between the points *P9-P10, P10-P11*, *P11-P12, P3-P4, P4-P5*, and *P5-P6* were declared as unknown heat flux boundaries in the solver. Once the assignment is done, the solver will highlight the corresponding boundaries in the GUI with the type of the boundary displayed as Flux?1, Flux?2, Flux?3 Flux?4, Flux?5 and Flux?6, as shown in Figure 4.4. The rights side of the figure shows the boundary declaration panel for the unknown heat flux.

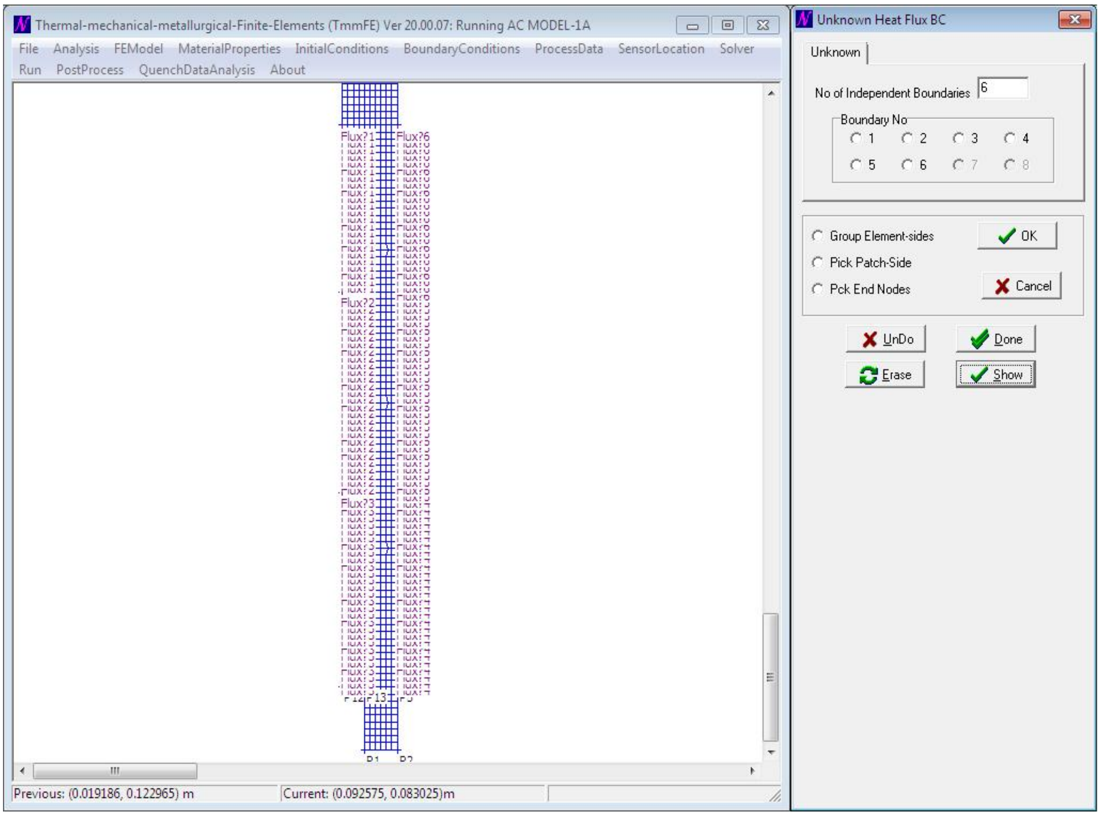


Figure 4.4 Declaration of *unknown heat flux* boundary in the solver

Figure 4.5 shows the location of the thermocouples specified in the solver – *TC(1) to TC(6).* These locations are the same as that of the thermocouples used in the experiments to measure the mold temperature, for both the air cooled and water cooled die experiments. These thermocouple locations were declared by specifying the appropriate geometrical coordinates in the solver. The identity number of the node (of the meshed domain) at the corresponding coordinate was identified from the solver and specified at the TC positions panel as shown in Figure 4.5. The inverse heat transfer coefficient IHTC parameters were set as shown, with a time step ratio of 1 and the total number of thermocouples as 6. The convergence limit for the solution residuals was set as 1e-8. The solver selected was direct solver with constant properties since the problem was treated as linear.

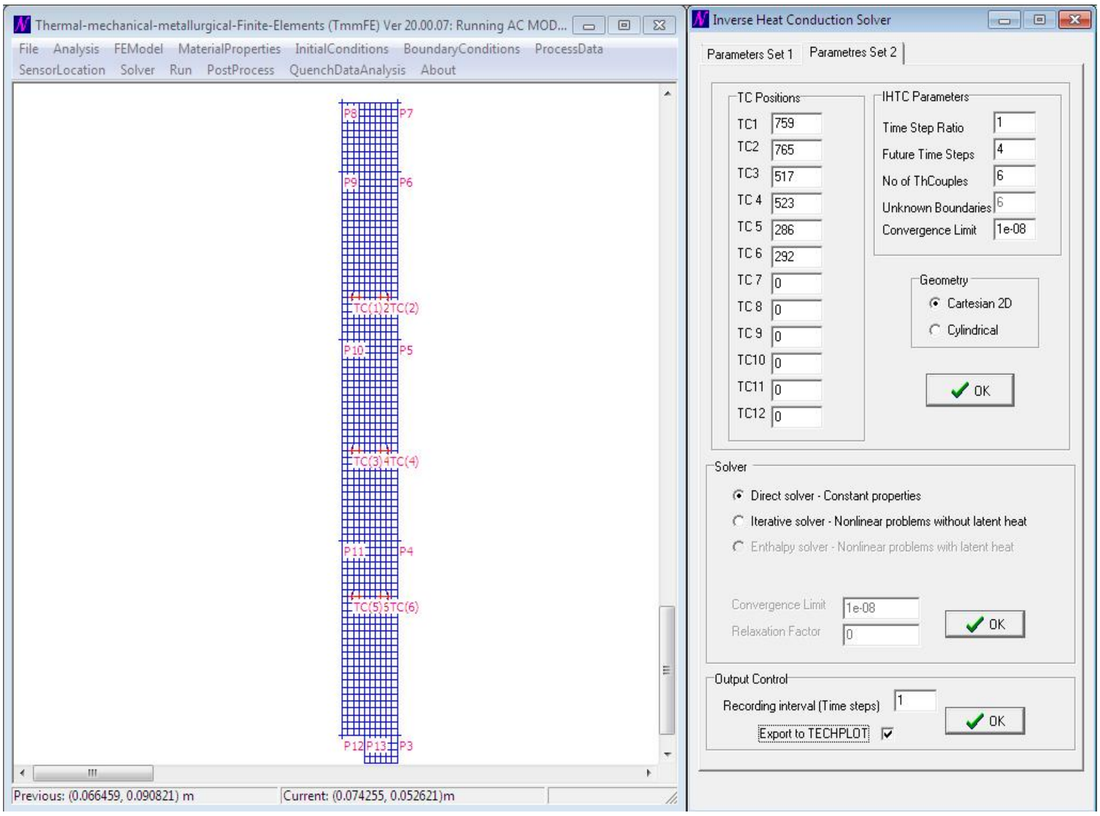


Figure 4.5 Specification of thermocouple location in the domain

Figure 4.6 shows the snapshot of the solver GUI, where the experimentally measured temperature data (from the thermocouples) were fed as input to the numerical solver. The time step was chosen as 0.1s and the input data was also arranged such that the data is available for 0.1s time steps. This ensures that when the solver computes the governing equations at a particular time step, the input data updates the temperatures in the thermocouple locations with the corresponding data from the experiments.

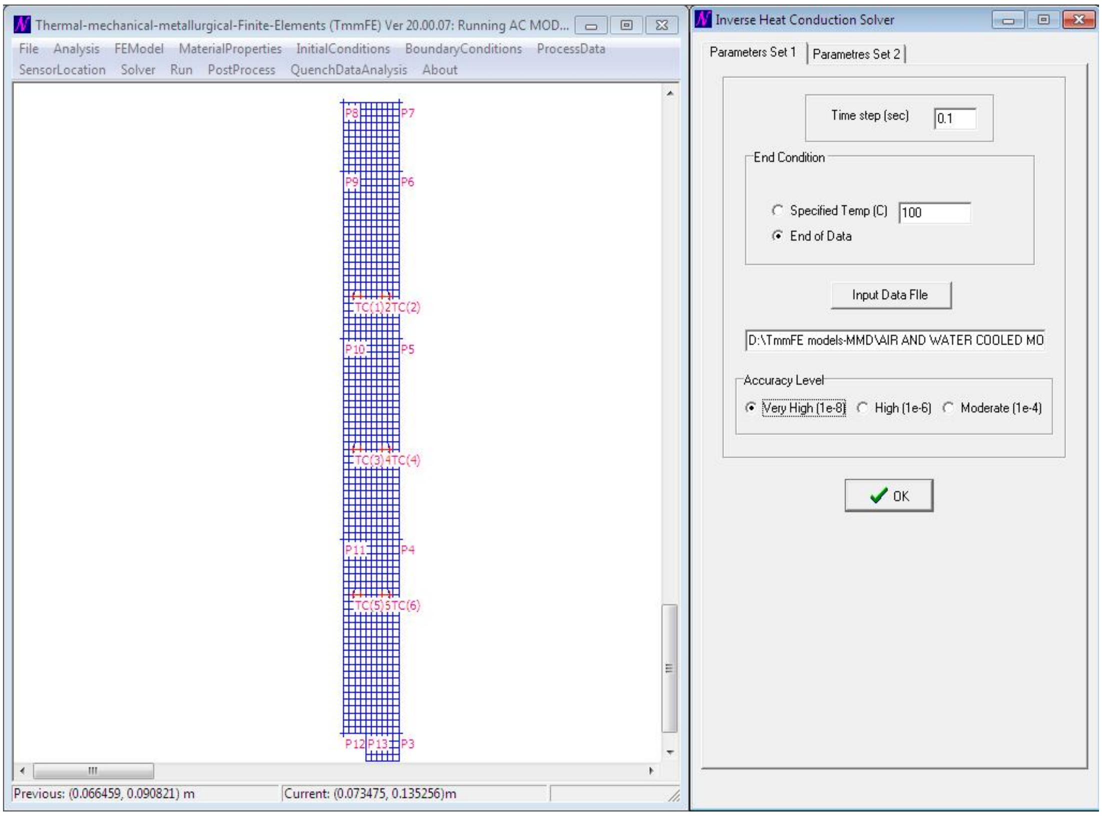


Figure 4.6 Coupling experimental data with the numerical solver

Figure 4.7 shows the GUI snapshot showing the solution in progress after 8 hours. Typically each case took around 48 hrs to 72 hrs wall clock times to arrive at the convergence specified in the solver. The computations were carried out in a desktop computer with Intel i5 Processor having 8GB RAM.

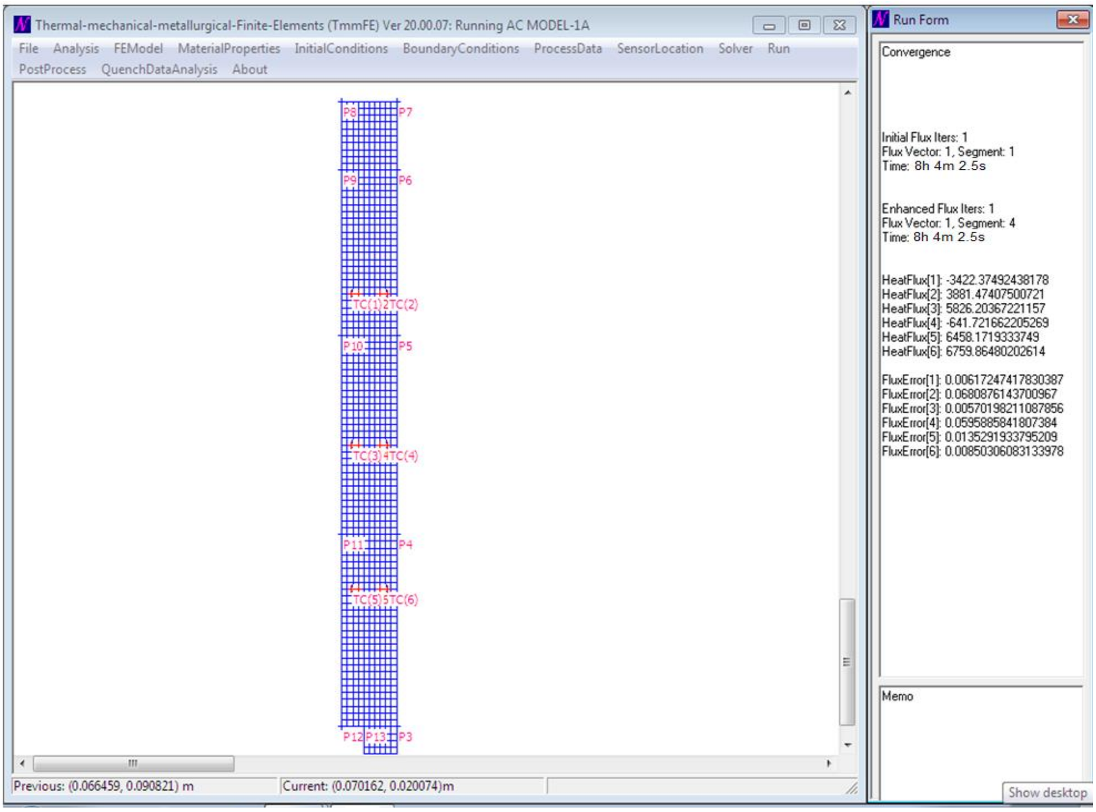


Figure 4.7 GUI snapshot showing solution in progress

The output from the computations was stored in a separate folder in the user specified directory. The data from the computations will be used for analysing the experiments and to interpret meaningful insights, which will be discussed in detail in the next chapter.