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# INVERSE MODELING OF HEAT TRANSFER WITH APPLICATION TO SOLIDIFICATION AND QUENCHING

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## ABSTRACT

The inverse modeling of heat transfer involves the estimation of boundary conditions from the knowledge of thermal history inside a heat conducting body. Inverse analysis is extremely useful in modeling of contact heat transfer at interfaces of engineering surfaces during materials processing. In the present work, the one-dimensional transient heat conduction equation was inversely modeled in both cartesian as well as cylindrical coordinates. The model is capable of estimating heat flux transients, chill surface temperature, and total heat flow from the source to the sink for an input of thermal history inside the sink. The methodology was adopted to solve boundary heat transfer problems inversely during solidification and quenching. The response of the inverse solution to measured sensor data was studied by carrying out numerical experiments involving the use of varying grid size and time steps, future temperatures, and regularization techniques.

*Key Words*: Contact heat transfer; Data acquisition; Data noise; Future temperature; Heat conduction; Heat transfer; Interfacial heat flux; Interfacial heat transfer coefficient; Inverse modeling; Metal/mold interface; Regularization; Sensitivity coefficient; Solidification; Quenching; Quenchants

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## INTRODUCTION

Direct heat conduction problems are associated with the determination of temperature distribution inside a heat conducting body using appropriate boundary conditions. On the other hand, inverse problems are involved with the estimation of boundary conditions from knowledge of thermal history in the interior of the solid. A comparison of the direct and inverse heat conduction problem is shown in Fig. 1.

In many engineering problems, an accurate determination of the thermal boundary condition may not be feasible.[1,2] For example, the presence of a sensor may alter the thermal conditions in the boundary region affecting the true values of the temperatures to be measured.

Inverse problems find a wide variety of applications in the field of materials processing. During solidification processing, heat transfer across the casting/mold interface plays an important role in the heat removal from the molten metal and hence, the filling and solidification of a casting.[3–7] Especially, in the case of continuous casting, squeeze casting, and die casting, the metal/mold interface plays a dominant role in the removal of heat from the molten metal.[8,9] A reliable set of data on the casting/mold interfacial heat transfer coefficients are, therefore, required for an accurate simulation of the solidification process.

The direct determination of casting/mold interfacial heat transfer coefficients is difficult due to the nonconforming contact existing at the interface. In the interfacial region, the metal may contact the mold surface through a large number of microscopic contact points as shown in Fig. 2(A). The overall heat transfer coefficient at the interface is calculated as

$$h = \frac{q}{\Delta T}$$

where $q$ is the interfacial heat flux and $\Delta T$ is the temperature drop across the interface. The nature of the interface is, thus, very complex and it is not possible to determine the boundary temperatures directly. Instead, an inverse model could be adopted to estimate the interfacial heat flux and the surface temperatures utilizing the temperature distribution data inside the mold and the solidifying metal.

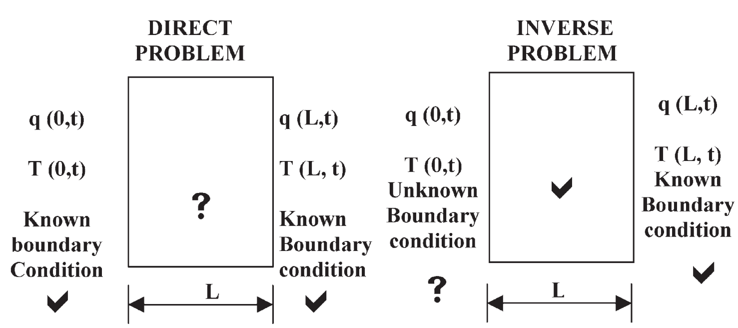


*Figure 1.* Comparison of direct and inverse problems.

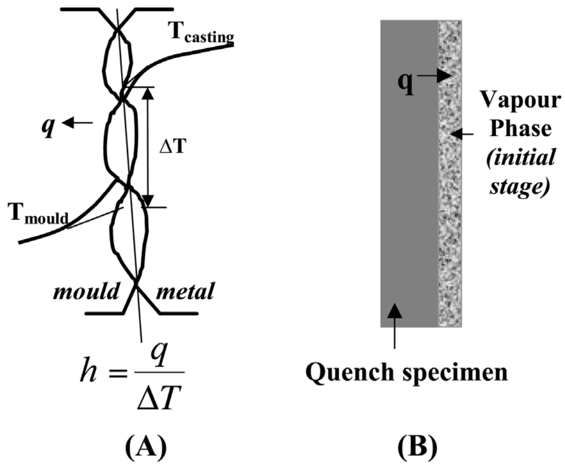


***Figure 2.*** Nature of casting/mold (A) and metal/quenchant (B) interfaces during solidification and quenching.

Recently, Tavares et al.[10] used an inverse model to determine the instantaneous heat fluxes between the roll and the solidifying metal in a twin-roll caster producing strips of low carbon steels.

A similar situation prevails during quenching of steel from austenitizing temperatures in a quench medium. Successful hardening depends on the geometry of the part, the hardenability of the steel, and the quenching practices employed in the industry.[11] The most critical information relating to the hardening process is the rate of heat transfer from the work piece to the quenching medium. When the work piece first comes into contact with the quench medium, a stable vapor phase is formed around it and this vapor blanket acts as an insulator decreasing the heat flow from the metal to the quench medium as shown in Fig. 2(B). This stage is followed by nucleate boiling and convection stages. The cooling rate is maximum in the nucleate boiling stage. To adequately analyze a quenchant system, it is necessary to model the metal/quenchant interfacial heat transfer during various stages of quenching. The heat flux densities during quenching have been used to characterize the cooling behavior of various types of quench media.[12] Furthermore, the metal/quenchant heat flux transients govern the temperature gradients inside the work piece subjected to quenching and, hence, play a major role in the evolution of thermal stresses. A lumped heat capacity method is a simple approach to determine the metal/quenchant interfacial heat transfer coefficients. In this method, the temperature is assumed to be uniform throughout the specimen. The method can be successfully adopted for thin specimens where the temperature gradients are negligibly small. However, for systems having appreciable temperature gradients, the correct method for getting the realistic metal/quenchant interface heat transfer properties is inverse modeling, which allows the determination of boundary conditions by the coupling of numerical methods with computer-aided temperature data acquisition.

Inverse analysis is, thus, a new research paradigm and is extensively used in materials modeling. However, the inverse heat conduction analysis is an ill-posed problem since it does not satisfy the general requirement of existence, uniqueness, and stability under small changes to the input data.[1] To overcome such difficulties, many techniques for solving inverse heat conduction problems have been proposed.[9] Furthermore, the output of an inverse solution to a heat conduction problem is very sensitive to measurement errors.

In the present work, an inverse model was developed and used to assess interfacial heat transfer during solidification and quenching. Heat flux transients were estimated during solidification against a chill and the study was extended to determine the heat transfer coefficients during quenching of steel specimens.

## ESTIMATION OF INTERFACIAL HEAT FLUX

Beck's nonlinear estimation technique[13,14] for determination of heat flux was adopted in this work. The one-dimensional heat conduction equation

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) = \rho C_{\mathrm{p}}\left(\frac{\partial T}{\partial t}\right) \tag{1}$$

was solved subject to the following boundary and initial conditions.

$$T(L_1, t) = Y(t)$$

$$T(L, t) = B(t)$$

$$T(L, 0) = T_i(x)$$

To find the heat flux at $L = 0$, the following function based on least squares was minimized.

$$F(q) = \sum_{i=1}^{I=mr}(T_{n+i} - Y_{n+i})^2 \tag{2}$$

where $r$ = number of future time temperatures + 1 and $m = \Delta\theta/\Delta t$. $\Delta\theta$ and $\Delta t$ are the time steps for heat flux and temperature, respectively, $Y_{n+i}$ and $T_{n+i}$ are measured and calculated temperatures, respectively, at a location near to the surface where the boundary condition is unknown.

The unknown heat flux $q$ was represented by a vector of elements $q\,(q_1, q_2, \ldots q_N)$ and the heat flux $q(0, t)$ was approximated by $q_n$ by letting each one represent a step.

$$q(0, t) = q_n \quad \text{for} \quad \theta_{n-1} < t < \theta_n$$

The objective was to calculate $q_{M+1}$ using the present temperatures $T_{n+1}, T_{n+2}, \ldots T_{n+m}$ and the future temperatures $T_{n+m+1}, \ldots T_{n+i}$. The future temperatures are the calculated temperatures at time steps greater than the present time steps estimated using the known boundary condition $T(L, t)$ and the unknown heat flux approximated by $q_n$. The measured temperatures at location TC4 during solidification and at location T1 during quenching were used as the known boundary condition $T(L, t)$ in the present analysis. A key assumption used temporarily is to let $q_{M+2} = q_{M+3} = q_{M+r} \cdots = q_{M+1}$, which sets some future $q$s equal to $q_{M+1}$.

Then for the $l$th iteration, the Taylor's series approximation given by

$$T^{l}_{n+i} \approx T^{l-1}_{n+i} + \frac{\partial T^{l-1}_{n+i}}{\partial q^{l}_{M+1}} (q^{l}_{M+1} - q^{l-1}_{M+1}) \tag{3}$$

was used. For $l = 0$, an estimate of $q^0_{M+1}$ is the converged value of $q_M$. For $q^0_1$ one can use the value of unity.

The partial derivative in Eq. (3) is called the sensitivity coefficient and is a measure of change in the estimated temperatures with a small change in the boundary condition.

It can be calculated by using Eq. (4)

$$\phi^{l-1}_{i} = \frac{T_{n+i}(q^{l-1}_{M+1}(1+\varepsilon)) - T_{n+i}(q^{l-1}_{M+1})}{\varepsilon q^{l-1}_{M+1}} \tag{4}$$

where the numerator is the difference in temperatures calculated using an explicit finite difference scheme at the monitored node at the same time step for temperature ($\Delta t$), using the boundary conditions $q$ and $q + \varepsilon$. The denominator is the difference in the $q$ values, i.e., $\varepsilon$. $\varepsilon$ is a small number and was taken as 0.001 in the present investigation.

Minimizing Eq. (2) with respect to $q$ by setting the partial derivative to zero, the following equation is obtained.

$$\frac{\partial F(q)}{\partial q} = 0$$

i.e.,

$$\frac{\partial}{\partial q}\left(\sum_{i=1}^{I=mr} (T_{n+i} - Y_{n+i})^2\right) = 0 \tag{5}$$

Substituting Eqs. (3) and (4) in Eq. (5), we get

$$\frac{\partial}{\partial q}\left(\sum_{i=1}^{I} (T^{l-1}_{n+i} + \phi^{l-1}_{i}(q^{l}_{M+1} - q^{l-1}_{M+1}) - Y_{n+i})^2\right) = 0$$

which gives

$$\sum_{i=1}^{I} \phi^{l-1}_{i}(T^{l-1}_{n+i} - Y_{n+i} + \phi^{l-1}_{i}(\nabla q^{l}_{M+1})) = 0 \tag{6}$$

Rearranging the above equation, the correction term for heat flux was obtained as

$$\nabla q_{M+1}^{l} = \frac{\sum_{i=1}^{I}(Y_{n+i} - T_{n+i}^{l-1})\phi_i^{l-1}}{\sum_{i=1}^{I}(\phi_i^{l-1})^2} \tag{7}$$

where $\Delta q_{M+1}^{l} = q_{M+1}^{l} - q_{M+1}^{l-1}$

The procedure was then repeated for a new heat flux value. The iteration was continued until

$$\frac{\nabla q_{M+1}^{l}}{q_{M+1}^{l-1}} < 0.005 \tag{8}$$

The final iterated value of $q$ was used as the initial heat flux for estimating the heat flux for the next time step. The calculation of the heat flux was continued till the desired period. In the estimation of temperatures during quenching, cylindrical coordinates were used in place of cartesian coordinates. To minimize the effects of measurement errors, a regularization technique was employed. In this procedure, an augmented sum of squares function given by

$$F(q) = \sum_{i=1}^{I=mr}(T_{n+i} - Y_{n+i})^2 + w_0\sum_{i=1}^{n_p}\beta_i^2 \tag{9}$$

was minimized. In the above equation, $\beta_i$ and $n_p$ are the parameters to be estimated and the number of parameters, respectively; $w_0$ is the zeroth order regularization parameter and was taken as 0.001 in the present investigation. The regularization method modifies the least squares approach by adding factors that are intended to reduce fluctuations in the unknown surface heat flux.[1,2] These fluctuations are not of physical origin but are inherent in the ill-posed problem of estimating the boundary heat flux by inverse modeling. An integral weighting function was hence used to control the characteristics of the surface condition over some interval of time. The aim is to reduce the measurement errors and make the inverse problem more tractable.

## EXPERIMENT

Figures 3 and 4 show schematic sketches of the experimental set-up used for the determination of interfacial heat flux transients during solidification of tin against a steel chill and quenching of medium carbon steel, respectively. The thermocouple sensors are located at finite difference nodal locations. All of the thermocouples were connected to a portable temperature data logger. The thermal data acquired, was input to the inverse model, which estimated the interfacial heat flux transients.

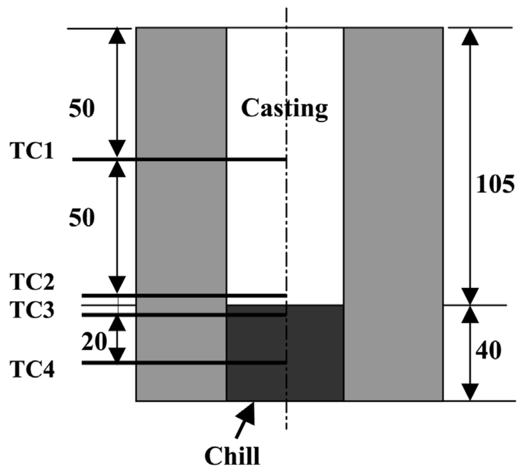


***Figure 3.*** Sketch of the experimental set-up for solidification against a chill.

## RESULTS AND DISCUSSION

The thermal history recorded during upward solidification of pure tin against a steel chill is shown in Fig. 5. Figure 6 shows the thermal history inside a medium carbon steel specimen during quenching in water. The temperature data were used as an input to inverse analysis module for estimating the casting/chill interfacial heat flux. The casting/chill and the metal/quenchant interfacial heat flux transients are shown in Fig. 7.

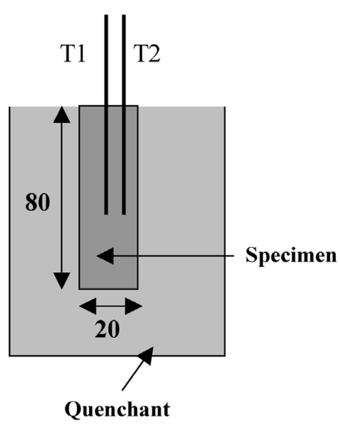


***Figure 4.*** Sketch of the set-up for quenching experiments.

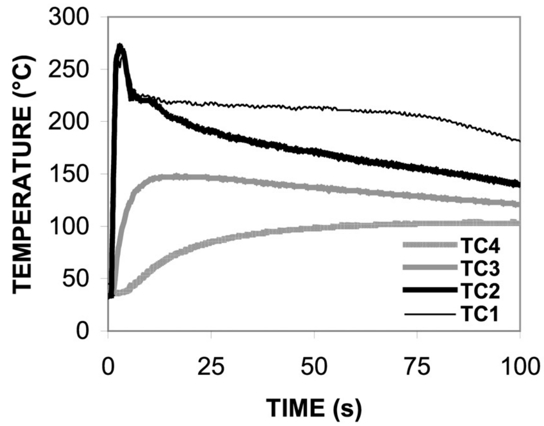


***Figure 5.*** Thermal history during solidification of tin against a steel chill.

In order to account for the lag between the heating of the chill surface and the subsequent response of the thermocouple sensor at a location near to the interface, future temperatures were taken into account in the inverse solution. Numerical experiments were carried out for future temperatures of 1–5, keeping all other parameters constant. The effect of number of future temperatures on the heat flux transients during solidification of lead against a copper chill is shown in Fig. 8. It was found that the effect of increasing the number of future temperatures was to smoothen the output, thereby, reducing the sensitivity of the algorithm to measurement errors. However, the sudden changes in heat flux, which may be due to the true nature of the problem, could be missed due to smoothing. For example, the peak in the heat flux transients during solidification indicates the transition in the interfacial region from a conforming contact to a nonconforming contact. This is shown by the heat flux

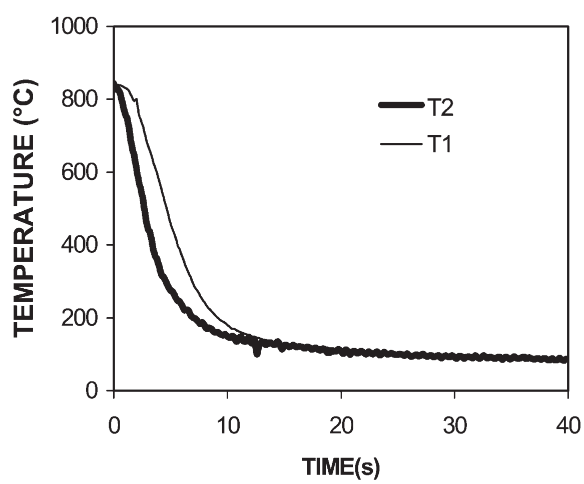


***Figure 6.*** Thermal history inside a steel specimen during quenching.

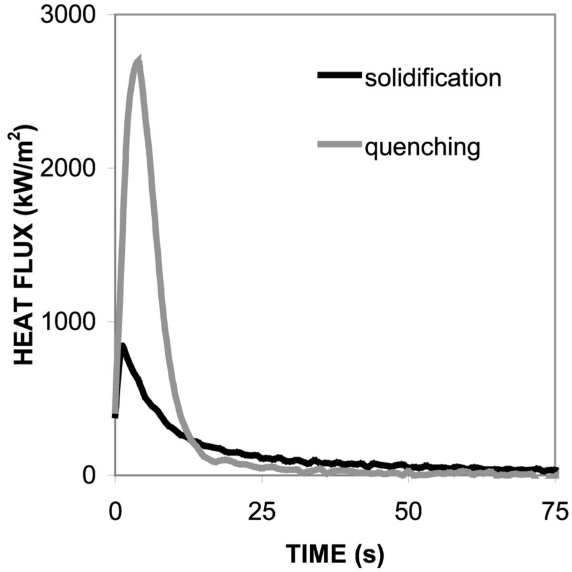


*Figure 7.* Heat flux transients estimated by inverse analysis during solidification and quenching.

transient curve in Fig. 8 computed using a future temperature of one, which shows a clear peak corresponding to a heat flux of 2510 kW/m$^2$. However, with an increase in the number of future temperatures the transition was not very clear. Hence, it is essential to strike a balance between two opposing conditions of minimum sensitivity of heat flux to measurement errors and adequate tracking of heat flux variation with time. Hence, a choice has to be made on the number of future temperatures to be used for the particular problem based upon the accuracy of data. In the present investigation, a future temperature of one was found to be suitable, because the noise

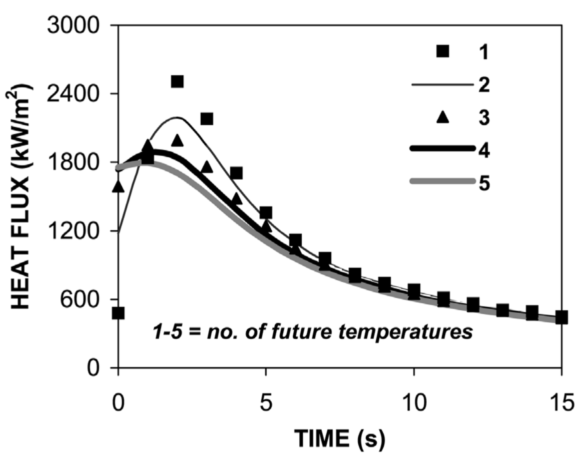


*Figure 8.* Effect of future temperatures on casting/chill interfacial heat flux transients.

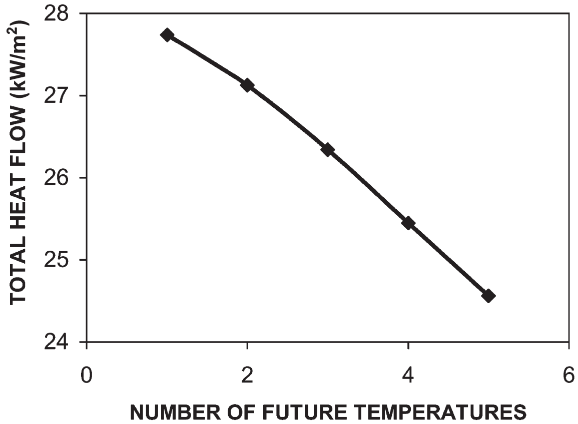


***Figure 9.*** Effect of future temperatures on total heat flow at the casting/chill interface.

due to the measurement errors in the input data was filtered before being used as an input to the inverse model. The effect of future temperatures on the total heat flow at the interface is shown in Fig. 9. The increase in the number of future temperatures resulted in a decreased heat flow at the casting/chill interface.

The solution of the inverse model was tested for grid size dependency by conducting numerical experiments for a set of experimental temperature data. A typical set of temperature data for lead solidifying against a chill was used to determine the effect. The numerical experiment was conducted for two grid sizes of 0.4 and 0.13 cm. The results are shown in Fig. 10. It was found that the effect of varying the grid size was negligible. For example, the heat flux values corresponding to 20 sec were 209.92 and 209.27 kJ/m$^2$ corresponding to chill surface temperatures of 208.84 and 209.05°C for grid sizes of 0.4 and 0.13 cm, respectively.

The effect of time step on temperature in the solution of the inverse model was studied in a similar manner. The numerical experiment was conducted for the

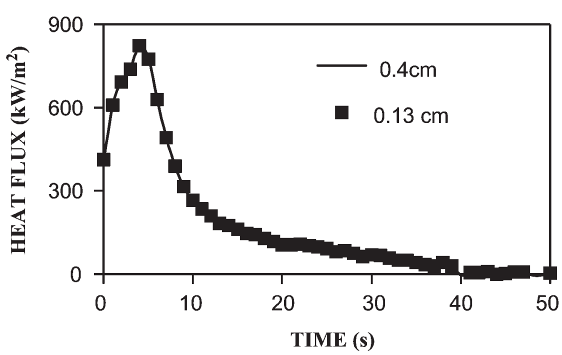


***Figure 10.*** Effect of grid size on heat flux transients.

data used for testing the grid size dependency. Time steps of 0.2 and 0.05 sec were selected. It was found that the effect of varying the time step was also negligible. For example, the heat flux value at a time of 20 sec was 209.167 kJ/m$^2$ for a time step of 0.2 sec and 209.924 kJ/m$^2$ corresponding to a time step of 0.05 sec. The corresponding total heat flow values were 19.099 and 19.124 MJ/m$^2$, respectively. The estimated chill surface temperatures were 209.05 and 208.85°C, respectively.

The combined effect of future temperatures and regularization was studied for data obtained without completely filtering the measurement errors from a quenching experiment. The heat flux transient was first found with only one future temperature and without any regularization term. The heat flux was estimated by using four future temperatures and zeroth-order regularization parameter of 0.001. This numerical experiment resulted in the smoothing of the heat flux and the effect is shown in Fig. 11.

The boundary heat flux transients estimated by inverse analysis would be extremely useful for modeling of heat transfer during solidification and quenching processes. For example, a solidification modeler can utilize the reliable data on casting/mold interfacial heat flux transients estimated by inverse modeling in simulation-based process design of castings to predict the temperature distribution and the occurrence of casting defects during solidification. In a similar manner, the metal/quenchant heat transfer data could be utilized for the judicious selection of quenchants for a particular grade of steel and to predict the thermal history and the evolution of thermal stresses during quenching.

## CONCLUSIONS

An inverse model to solve the boundary heat transfer problems during casting and quenching has been proposed. The model is capable of estimating the

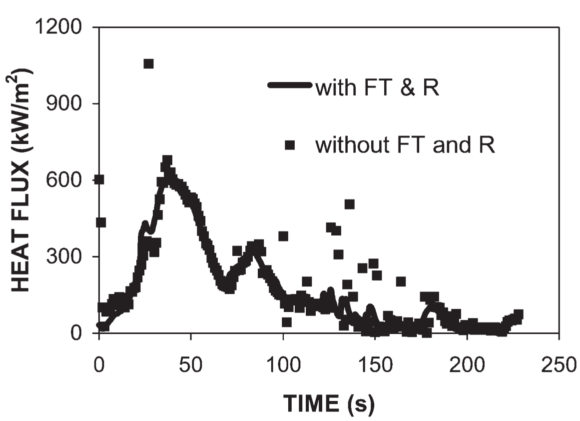


*Figure 11.* Effect of future temperatures (FT) and regularization (R) on estimated heat flux transients during quenching.

boundary temperatures and the interfacial heat flux transients during solidification and quenching. The effect of grid size and time step on the model output was found to be negligible. The response of the inverse heat conduction problem solution was significant to errors in temperature measurements. The use of future temperatures and regularization parameter considerably reduced the effect of data noise on the inverse solution. However, to represent the true nature of the problem, a judicious selection of future temperatures is needed to provide an accurate and stable inverse solution. The model could be extended to solve other contact heat transfer problems during materials processing.

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