Application of Inverse Methods to the Estimation of Boundary Conditions and Properties

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Abstract

Inverse methods can be used in solidification and related processes for the estimation of boundary conditions or physical properties of materials. For heat flow problems, these methods are based upon a minimisation of the errors between calculated and measured temperatures at given locations and times of the space-time domain, the calculated values being obtained from a numerical solution of the heat flow equation. In the present case, a *maximum a posteriori* technique has been implemented into a finite element code. This method is then applied to several situations for the determination of : *i)* the time-dependent heat-transfer coefficient at the surface of a steel rod which has been water-cooled after induction heating (non-stationary situation) ; *ii)* the space-dependent heat flow at the surface of a direct chill cast aluminium slab (stationary situation) ; and *iii)* the temperature-dependent thermal conductivity of aluminium-silicon alloys. In this latter case, the influence of the silicon concentration on the thermal conductivity is clearly revealed.

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Introduction

One of the main difficulty associated with numerical simulation of solidification processes is the lack of thermophysical properties and/or boundary conditions. However, using measurements made under well-defined conditions, numerical simulation can be used to deduce these missing data. These so-called *inverse methods* are well known, in particular through the two books written by Beck and co-workers [1,2] on this topic. The basic idea of these methods is equivalent to a standard least-squares method in which the analytical function is replaced by the numerical solution obtained from a *direct* finite element (FEM) or finite difference (FDM) calculation. For time-dependent boundary conditions problems, the problem is ill-posed and can lead to instabilities if the time steps are too small. For that purpose, several regularization methods have been devised [1].

For the determination of thermophysical parameters (e.g., thermal conductivity and/or specific heat), Milano and Scarpa [3] have modified the least-squares technique to include a *Maximum A Posteriori* (MAP) algorithm.

The purpose of the present contribution is to show how the MAP algorithm can be implemented easily into a direct FEM heat-flow code, in the present case *3-MOS* [4]. After a brief description of the theoretical background and of the numerical implementation, several examples will illustrate the potency of the technique to determine time or space-dependent heat transfer coefficients and temperature-dependent thermal conductivities.

Theory

Consider a domain, Ω, within which the heat flow equation has to be solved. This domain includes the solidifying ingot and the mould parts. A set of N_m thermocouples has been placed at well defined positions, $\mathbf{x}_j$ ($j = 1, N_m$), within this domain in order to measure the temperatures, T_{ij}^m, at a certain number of times, t_i ($i = 1, N_t$). These measured temperatures are used to deduce a set of N_β parameters $\boldsymbol{\beta} = \{\beta_1, \beta_2, \ldots, \beta_{N_\beta}\}$ via a minimisation of the function [3] :

$$S(\boldsymbol{\beta}) = \sum_{i=1}^{N_t} \sum_{j=1}^{N_m} \frac{1}{\sigma_T^2} \left[T_{ij}^m - T_{ij}^c(\boldsymbol{\beta})\right]^2 + \sum_{k=1}^{N_\beta} \frac{1}{\sigma_k^2} \left[\beta_k - \beta_k^o\right]^2 \qquad (1)$$

where $T_{ij}^c(\boldsymbol{\beta})$ are the calculated temperatures at time t_i and position $\mathbf{x}_j$. The standard deviation, σ_T, is a typical error associated with the temperature measurement whereas σ_k is a typical interval within which each of the parameter β_k is allowed to vary around an *a priori* (i.e. guessed) parameter, β_k^o. The MAP algorithm resumes to the standard least-squares method when the σ_k's are set to infinity. On the other hand, a parameter β_k will be fixed to the guessed value β_k^o if the corresponding deviation, σ_k, is made very small.

The parameters to be adjusted, $\boldsymbol{\beta}$, can be :

- Tabulated thermophysical properties, e.g., $\boldsymbol{\beta} = \{\kappa_1, \kappa_2, \ldots, \kappa_{N_\beta}\}$, where the κ_k's are the values of the thermal conductivity of the medium at some tabulated temperatures, T_k. The values of κ in each interval, $[T_k, T_{k+1}]$, are linearly interpolated.

- Coefficients of a temperature-dependent thermophysical property function, e.g., $\kappa = \beta_1 + \beta_2 \cdot T + \beta_3 \cdot T^2 + \ldots + \beta_{N_\beta} \cdot T^{N_\beta - 1}$.
- Temperature-dependent boundary conditions at a given boundary, e.g., $\boldsymbol{\beta} = \{h_1, h_2, \ldots, h_{N_\beta}\}$, where the h_k's are heat-transfer coefficients for a set of given temperatures, T_k.
- Time-dependent boundary conditions at a given boundary, e.g., $\boldsymbol{\beta} = \{Q_1, Q_2, \ldots, Q_{N_\beta}\}$, where the Q_k's are the values of the heat flow leaving a given boundary at tabulated times, t_k.

In the present case, no distinction has been made between time- and temperature-dependent boundary conditions, assuming that the tabulated times, t_k, are much more spaced than the times used in the direct heat flow computations (i.e., equivalent to regularization). However, if the indices, k, of the tabulated heat flow are identical to the time steps, i, used for the direct computations, a different procedure can be used : the summation over the time steps in Eq. 1 can be eliminated and the heat flow at any future time step, Q_{i+1}, is then calculated from the temperature variations measured between (i) and (i+1) [5].

In order to minimise $S(\boldsymbol{\beta})$, one writes :

$$\frac{\partial S}{\partial \beta_l} = \sum_{i=1}^{N_t} \sum_{j=1}^{N_m} \frac{-2}{\sigma_T^2} \left[T_{ij}^m - T_{ij}^c(\boldsymbol{\beta}) \right] \cdot X_{ijl} + \frac{2}{\sigma_l^2} \left[\beta_l - \beta_l^o \right] = 0 \tag{2}$$

where X_{ijl} is the *sensitivity coefficient* :

$$X_{ijl} = \frac{\partial T_{ij}^c(\boldsymbol{\beta})}{\partial \beta_l} \cong \frac{T_{ij}^c(\beta_1, \ldots, \beta_l + \delta\beta_l, \ldots, \beta_{N_\beta}) - T_{ij}^c(\beta_1, \ldots, \beta_l, \ldots, \beta_{N_\beta})}{\delta\beta_l}. \tag{3}$$

$\delta\beta_l$ is an a priori variation of the parameter β_l which is used to calculate the sensitivity coefficients. An iterative procedure is used to find the solution $\boldsymbol{\beta}$ minimising $S(\boldsymbol{\beta})$. In this procedure the calculated temperatures, $T_{ij}^c(\boldsymbol{\beta}^{\nu+1})$, at the next iteration (ν+1) are also linearized :

$$T_{ij}^c(\boldsymbol{\beta}^{\nu+1}) \cong T_{ij}^c(\boldsymbol{\beta}^{\nu}) + \sum_{k=1}^{N_\beta} X_{ijk} \cdot \Delta\beta_k \tag{4}$$

The increments, $\Delta\boldsymbol{\beta}$, of the parameters are then found at each iteration as the solution of the set of linear equations :

$$[\mathbf{A}] \cdot \Delta\boldsymbol{\beta} = \mathbf{f} \qquad \text{or} \qquad \sum_{k=1}^{N_\beta} A_{lk} \cdot \Delta\beta_k = f_l \tag{5a}$$

with :

$$A_{lk} = \sum_{i=1}^{N_t} \sum_{j=1}^{N_m} \frac{X_{ijk} \cdot X_{ijl}}{\sigma_T^2} + \frac{\delta_{lk}}{\sigma_l^2} \tag{5b}$$

$$f_l = \sum_{i=1}^{N_t} \sum_{j=1}^{N_m} \frac{1}{\sigma_T^2} \left[T_{ij}^m - T_{ij}^c(\boldsymbol{\beta}^{\nu}) \right] \cdot X_{ijl} - \frac{\beta_l^{\nu} - \beta_l^o}{\sigma_l^2} \tag{5c}$$

(δ_{lk} is the Kroneker symbol).

The implementation of the MAP inverse method (Eqs. 5) can be done in a direct program that calculates $T^c_{ij}(\beta)$ once the parameters, β, are known. From guessed initial values of $\beta^{(v=0)}$ the temperatures $T^c_{ij}(\beta^v)$ and sensitivity coefficients X_{ijl} (Eq. 3) are calculated at each iteration v. Knowing these values, equations 5 are solved in order to obtain the increments $\Delta\beta$ until convergence is reached. Please note that, within each iteration, $(N_\beta+1)$ direct problems are solved with the direct code. This might be CPU-intensive especially if : *(i)* the problem is 3-dimensional, *(ii)* the number of parameters N_β is large and *(iii)* the convergence is slow. In two dimensions, this problem is less critical and the MAP algorithm has been implemented as a main program calling the direct FEM heat-flow code *3-MOS* considered as a subroutine.

Results and Discussion

Temperature-dependent heat transfer estimation during transient cooling

The cooling curves measured at different locations of a small Ck45 steel cylinder are shown in Fig. 1, together with an insert indicating the position of the thermocouples. Four thermocouples were placed at the centre of the ingot and at 15, 19 and 22 mm from the centre. (These three last thermocouples were duplicated in order to test the assumption of an axisymmetric configuration). The top and bottom faces of the cylinder were insulated with ceramics. The cylinder was first heated to a nearly uniform temperature with induction heating and then its lateral surface was sprayed by a set of water nozzles arranged in a nearly axisymmetric configuration ("shower"). As can be seen, the cooling curves clearly reveal the ferrito-perlitic reaction upon cooling (near $T \cong 620$ °C), especially for the curve measured at the centre of the cylinder. The small temperature increase noticed for this thermocouple at $t < 10$ s also indicates that the temperature was not yet totally uniform at the end of the heating stage.

Using the measured cooling curves shown in Fig. 1, an inverse calculation of eight temperature-tabulated heat transfer coefficients was performed. The result of such a calculation is displayed in Fig. 2 as a function of the surface temperature of the steel cylinder for various water flow rates. As can be seen, the heat-transfer coefficient, h, is an increasing function of the water flow rate and of the surface temperature, at least up to 150 °C. Above this value, the errors on the h-values are quite large due to the very short time interval over which these values apply (typically less than 2-5 s) and to the diffusion time (e.g., the first thermocouple located at 3 mm below the surface is characterised by a diffusion time equal to 1.2 s). Nevertheless, the trend is in agreement with previously reported values [6] and the agreement between the re-calculated and the measured cooling curves (see Fig. 1) is fairly good. (It seems that the thermal conductivity used in the calculation for the temperature interval [0, 400°C] is too large). It is to be noted from the shape of the cooling curves that the direct code also accounts for the solid-state transformations, using an equivalent c_p-method.

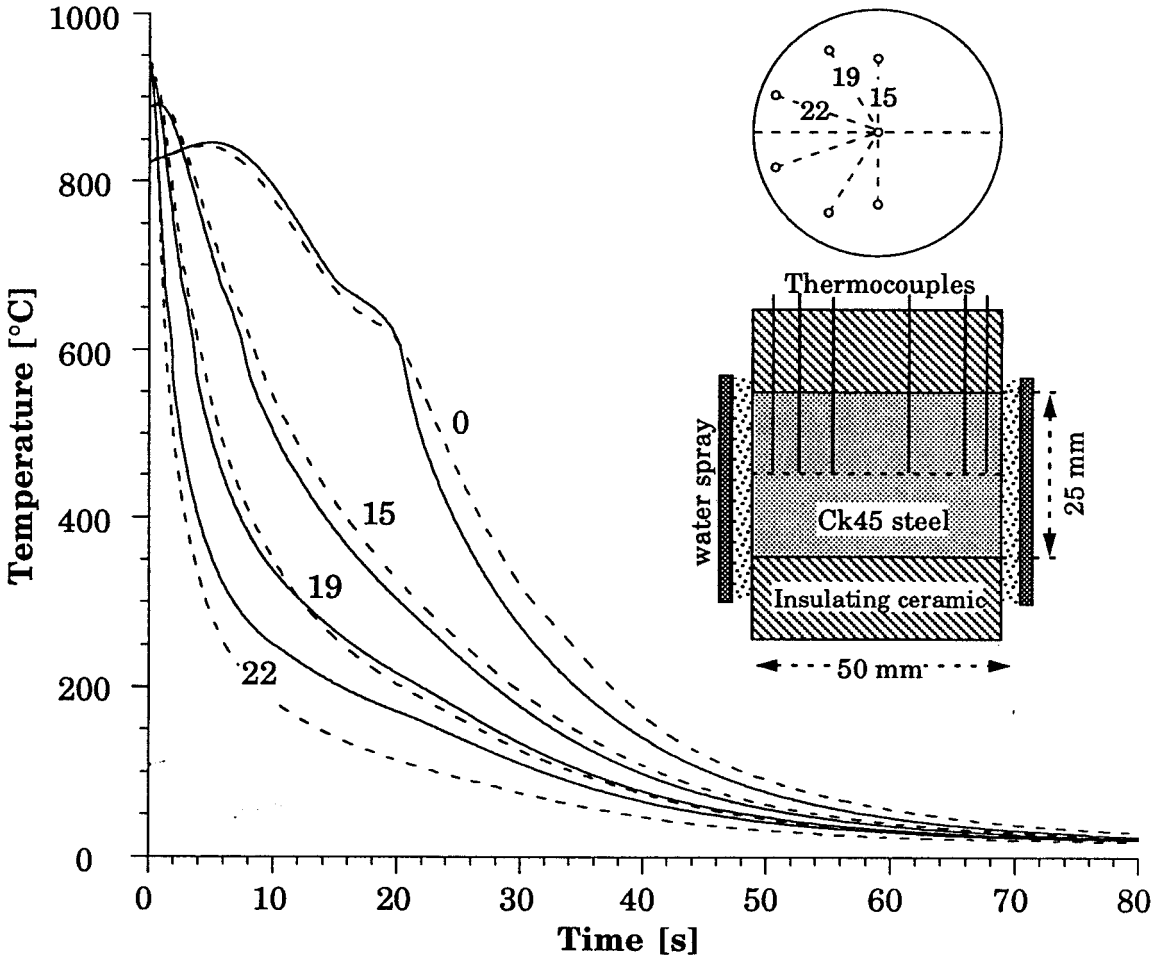

Figure 1 : *Measured (dashed lines) and calculated (continuous lines) cooling curves at various points of a Ck45 steel cylinder which was induction heated and then cooled down by water spraying. The position of the thermocouples is indicated in the insert. Water flow rate : 45 l / min.*

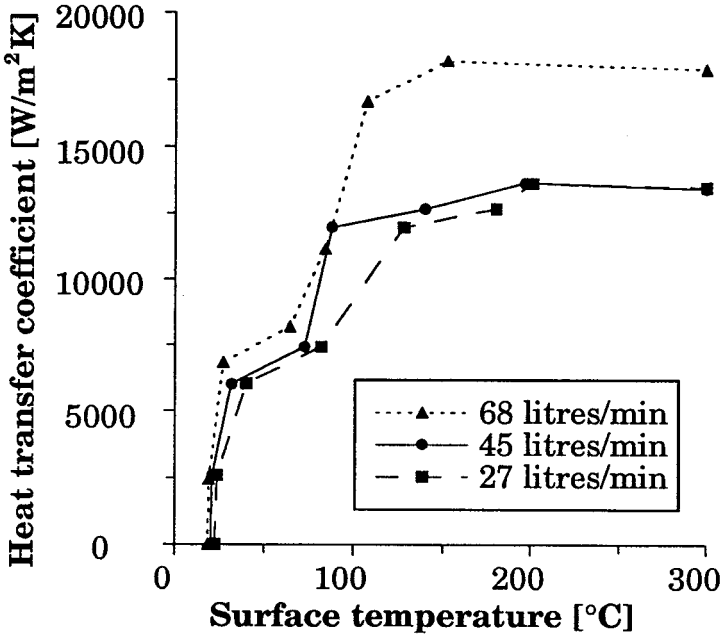

Figure 2 *: Temperature-dependent heat-transfer coefficient calculated by inverse modelling for a steel cylinder cooled down by water spraying with various flow rates.*

Space-dependent heat flow estimation for DC casting

The cooling curves were measured at the mid-plane of direct chill (DC) cast aluminium ingots. After a nearly steady-state regime was obtained, five thermocouples were immersed from the top in the melt pool at various distances from the lateral surface of the ingot. The thermocouples being moved with two long rods already trapped by the solid part of the ingot, they were translated at the same speed as the withdrawal rate of the ingot. The details of the experimental set-up are given in Ref. 7. After the measurement, the cooling curves measured at each thermocouple location were converted into temperature profiles along the height of the casting (stationary situation). These profiles are displayed in Fig. 3 for an AA3104 aluminium alloy.

Since the software *3-MOS* can account for an advection term, these temperature profiles were then used to deduce by inverse modelling the height-dependent heat flow extracted at the lateral surface of the ingot by the chill and by the water spraying system underneath. The results are shown in Fig. 4. As can be seen, a heat flow of a few hundreds kW/m^2 is extracted from the ingot during the initial contact with the chill but the heat flow almost vanishes as soon as an air gap forms. At the location of the water spraying impingement, the heat flow is maximum (nearly 4 MW/m^2). It decreases then to lower values as water flows and evaporates along the side of the ingot. The temperature profiles calculated with the boundary conditions of Fig. 4 are compared with the measured profiles in Fig. 3.

Thermal conductivity estimation

Cylindrical castings of aluminium alloys were solidified under one-dimensional heat flow conditions using the experimental set-up described by Ampuero et al [8]. This set-up has the advantage to prevent any convection associated with pouring effect since the ceramic mould and the metal are first preheated together in a furnace. Once a uniform temperature is reached, the furnace is removed and an instrumented water-cooled copper chill is applied to the bottom surface of the mould. The latter is made out of a thin aluminium-nitride plate having a high thermal conductivity. Seven thermocouples were placed at various heights of the aluminium ingots (20, 40, 60, 80, 100, 120 and 140 mm from the chill). The first thermocouple near the chill was taken as a boundary condition to determine by an inverse calculation the temperature-dependent thermal conductivity of four aluminium-silicon alloys using the six remaining cooling curves. An adiabatic boundary condition was set at the lateral and upper surfaces of the ingot, since the ceramic mould is made of a very low thermal diffusivity material (Promat™).

The results of such inverse calculations are shown in Fig. 5 for four alloys : pure aluminium, Al-3 wtpct Si, Al-7 wtpct Si and Al-11 wtpct Si. As can be seen, the inverse modelling calculations are in good agreement with thermal conductivities previously reported in the literature. In particular, the thermal conductivity of pure aluminium is very close to the values given by Pehlke [9], except for the small peaks (wiggles) observed just above and below the melting point. These peaks could be due to the transformation kinetics (i.e., departure from equilibrium) which is not accounted for in the direct calculation. Furthermore, the concentration-dependence of the thermal conductivity estimated for the solid phase seems to be in agreement with the values obtained using a different technique by Gündünz and Hunt [10] for Al-1.67 wtpct Si and Al-12.5 wtpct Si alloys.

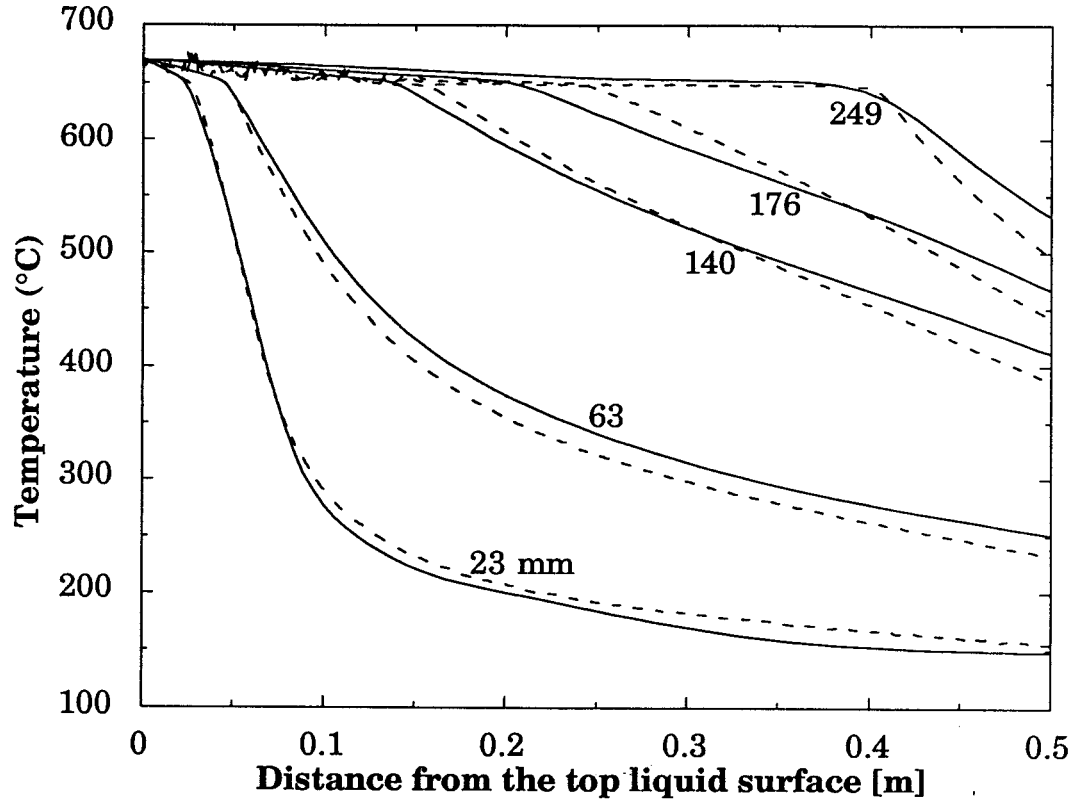

Figure 3 : *Measured (dashed lines) and calculated (continuous lines) temperature profiles along five vertical lines within a DC cast AA3104 aluminium ingot. The numbers indicate the position of the thermocouples from the lateral surface of the ingot whereas the horizontal axis corresponds to the distance from the top of the ingot.*

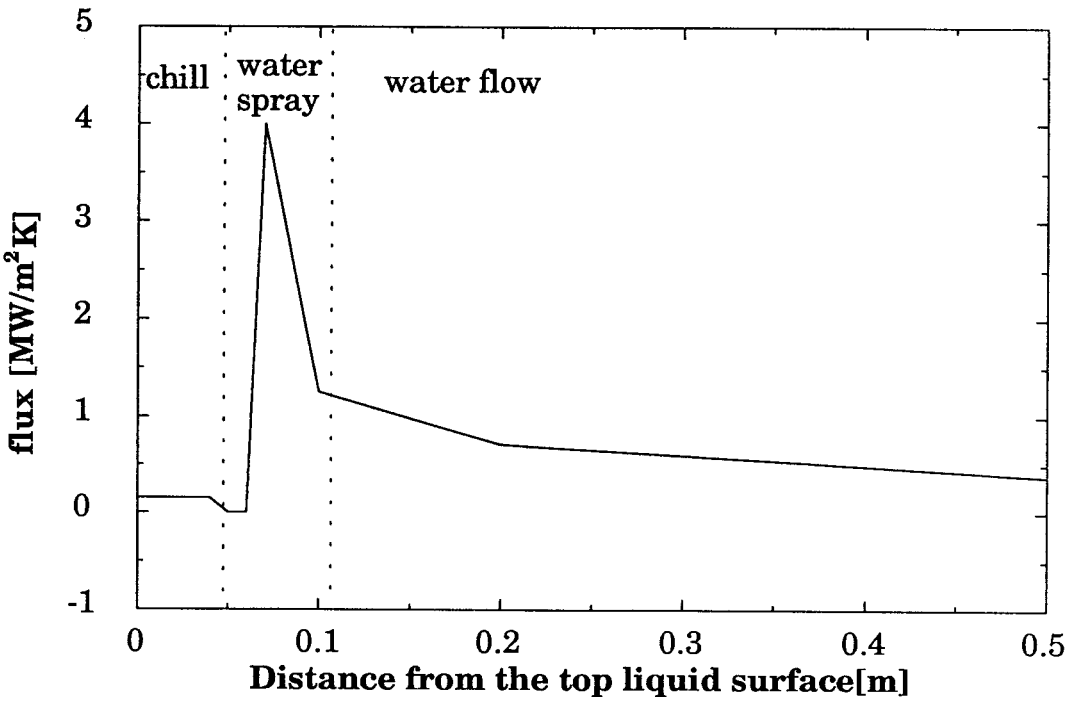

Figure 4 : *Height-dependent heat transfer coefficient in DC casting calculated by inverse modelling using the measured temperature profiles shown in Fig. 3.*

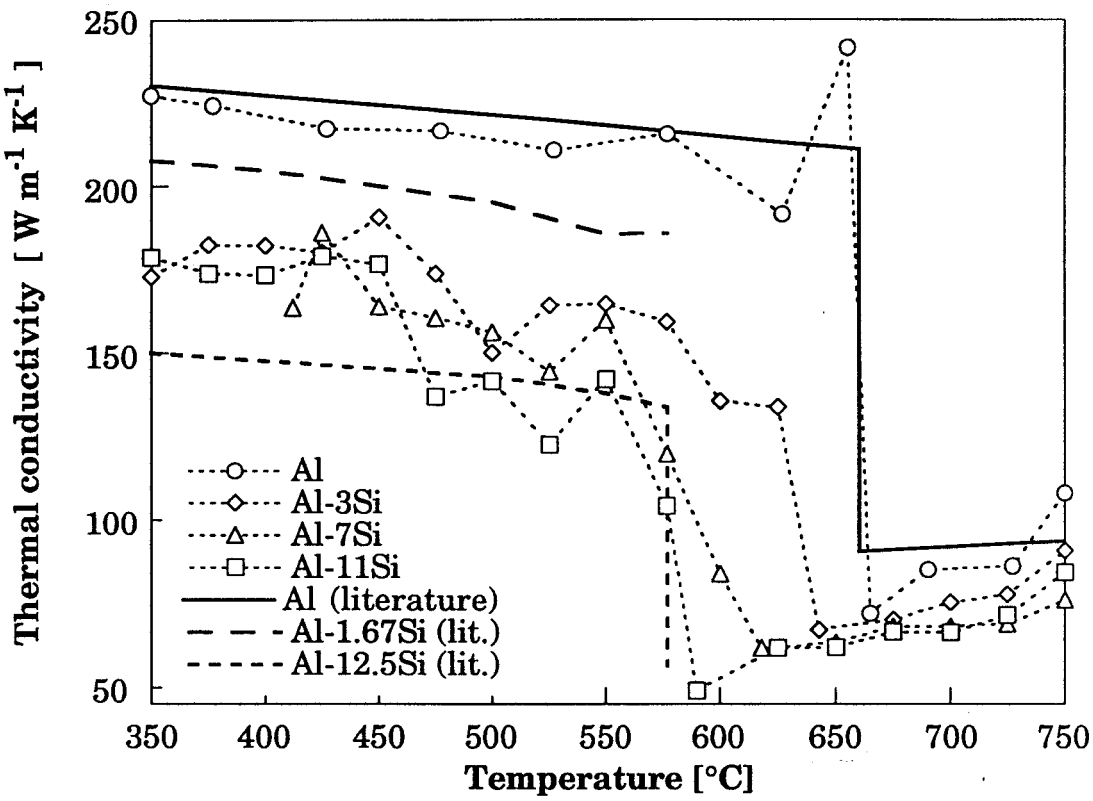

***Figure 5** : Temperature-dependent thermal conductivity of Al-Si alloys of various concentrations and of pure aluminium as deduced from inverse modelling using the temperatures measured in one-dimensional solidified ingots. These values are compared with three curves previously reported in the literature [9,10].*

Conclusion

The present contribution has demonstrated that a direct FEM heat-flow code can be used in an inverse way so as to deduce boundary conditions and/or thermophysical properties. If N_β parameters have to be determined, the inverse calculation is then equivalent to $(N_\beta+1)$ direct calculations in each of the iterations made to find the solution. The CPU-time associated with such inverse calculations therefore limits the problems that can be handled to two-dimensions. More important is the accuracy of the measurements and the precise control of the experimental conditions and of the other parameters entering in the simulation. For the determination of thermophysical properties, one-dimensional experiments with a precise knowledge of the boundary conditions are most preferable. Boundary conditions can be reasonably well predicted in real solidification of heat-treatment processes, providing the properties are known.

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