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#### ABSTRACT

## INVESTIGATION OF THERMAL CONTACT RESISTANCE AT A PLASTIC-METAL INTERFACE IN INJECTION MOLDING

#### by

#### Lakshminarayanan Sridhar

Thermal contact resistance (TCR) at the plastic-metal interface is one of the parameters required for the simulation of plastic processing techniques such as injection molding. However, the available data is both unreliable and insufficient due to the difficulties involved in measuring this parameter. The effects of thermal contact resistance on the heat transfer in plastics processing with particular reference to injection molding of thermoplastics is investigated using combined experimental measurement techniques, parametric studies and numerical analysis.

TCR under steady state conditions has been determined experimentally at typical thermoplastic-mold metal interfaces for an amorphous and a semi-crystalline polymer using a one-dimensional heat meter type apparatus. However, a parametric study established that TCR in injection molding is a time and space (location on the part surface) dependent parameter. The analysis shows that the thickness direction shrinkage is the cause of the disparity between the steady state experimental data and data from an injection molding experiment available in literature. The gap at any location on the part surface is a function of the thickness direction shrinkage and the deformation due to unbalanced cooling and non-uniform shrinkage. A finite element analysis was used to

study the heat flow across a typical interface in injection molding, and to establish the basis for an analytical solution to the heat equation. This solution was used to develop a model for an effective time dependent TCR which can be utilized to improve the simulation of injection molding. An improvement of up to 20% in the cooling time predictions is expected with the use of the improved model of TCR.

The parametric study, using computer simulation of the injection molding process, was also undertaken to analyze the effect of TCR on the simulation and to determine the effect of injection molding processing parameters, such as hold pressure, on the physical mechanism affecting TCR.

An inverse method was developed and tested with simulated data for the determination of thermal conductivity and TCR from transient temperature measurements.

## INVESTIGATION OF THERMAL CONTACT RESISTANCE AT A PLASTIC-METAL INTERFACE IN INJECTION MOLDING

by

Lakshminarayanan Sridhar

A Dissertation Submitted to the Faculty of New Jersey Institute of Technology In Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy

**Department of Mechanical Engineering** 

January 1999

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## APPROVALS PAGE

## INVESTIGATION OF THERMAL CONTACT RESISTANCE AT A PLASTIC-METAL INTERFACE IN INJECTION MOLDING

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Padma

& my family

In the life of a man, his time is but a moment, his being an incessant flux, his senses a dim rushlight, his body a prey of worms, his soul an unquiet eddy, his fortune dark, and his fame doubtful. In short, all that is of the body is as coursing waters, all that is of the soul as dreams and vapours; life a warfare, a brief sojourning in an alien land; and after repute, oblivion. Where, then, can man find the power to guide and guard his steps? In one thing and one alone: the love of knowledge.

Marcus Aurelius, Meditations

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## NOMENCLATURE

- g temperature jump distance (m)
- k thermal conductivity (W/m-K)
- $R_{,}R_{g}$  thermal resistance (m<sup>2</sup>-K/W)
- t time (s)
- T temperature (°C)
- x length variable
- $\Delta l$  shrinkage (m)
- $\alpha$  linear thermal expansion coefficient (m/m/°C)
- δ gap (m)
- v specific volume (m<sup>3</sup>/Kg)

## subscript

- 1,2 denotes the two surfaces in contact
- av average
- g gas

#### **CHAPTER 1**

#### INTRODUCTION

#### 1.1 Motivation

Plastic processing techniques generally require the polymer to be heated and cooled. The heat transfer during the processing plays a key role in the design of the mold and in determining the productivity and quality of the part formed. Injection molding is one of the most widely used polymer processing techniques and its market share has been growing with new techniques being developed to handle exotic materials and complex shapes. Injection molding is very well suited for large volume manufacturing as it permits a high degree of automation.

One of the important components in injection molding is the mold, which has to be designed for strength, longevity and to provide the requisite part quality. Traditionally, the mold design and manufacture goes through an iterative process where it is modified based on actual testing, to improve the heat transfer characteristics and to set the processing control parameters. Recently, Computer Aided Engineering (CAE) software have entered the market which enable the simulation of the process and, hence, reduce the testing and modification of the mold with very significant savings in the cost. The success of the simulation depends on the accuracy with which the software can model the molding process and considerable work is currently being done on this including better characterization of the thermal, flow and mechanical properties, and a more realistic modeling of the flow/heat transfer process.

1

In the simulation of heat transfer in injection molding, one of the parameters that has been included is the thermal contact resistance at the plastic metal interface in the mold cavity (Chiang et al., 1993). This resistance to the heat flow influences the cooling time and other process related parameters. Recent investigations (Rhee et al., 1994; Yu et al.,1990) have shown that predictions of cooling time and pressure decay by simulation software indicate trends different from those obtained from experimental measurements. Investigations were carried out using both temperature measurements during injection molding and from steady state experiments to evaluate the magnitude of TCR for use in the simulation. The results were, however, inconclusive as they were not able to effectively link the magnitude of TCR to the processing/simulation variables (Yu et al.,1990). Furthermore, there was a large difference in the reported values of TCR obtained from steady state experiments and those obtained from temperature measurements during injection molding. The current investigation is an attempt to explain both the discrepancies in the TCR values obtained under the two experimental conditions and to understand the mechanism of TCR in injection molding with respect to the time dependent nature of shrinkage. This requires a study of TCR at plastic-metal interfaces in general.

#### **1.2 Thermal Contact Resistance**

Thermal contact resistance is a resistance to the flow of heat at the interface between two bodies in contact. The resistance is due to the imperfect nature of contact at any real interface (Madhusudhana,1996; White,1991) as illustrated in Fig. 1.1(a) which shows a



(a) Imperfections at the surface



Figure 1.1 Imperfections at contact surfaces that cause TCR. Also shown to the right in (a) is the temperature drop due to TCR.

magnified cross sectional view of a typical interface. The graph on the right in the figure shows the temperature gradient in the two bodies and the additional temperature drop at the interface. Studies on metal-metal contacts have shown (Bowden and Tabor, 1950; Madhusudhana,1996) that the actual area in contact is a small fraction of the nominal interface area in contact even at moderately high contact pressures. While the actual contact area is larger when one of the surfaces in contact is soft, as in plastic-metal contact, it is still less than the nominal area of contact. The TCR then manifests itself as a jump in the temperature at the interface as illustrated in Figure 1.1(a). If  $\Delta T$  is the temperature difference between the two surfaces and q the heat flux crossing the interface, then the TCR, R<sub>c</sub> is given by

$$R_{c} = \Delta T / q \tag{1.1}$$

The inverse of the TCR, h (h= $1/R_c$ ) is the thermal contact conductance. The TCR can be thought of as a combination of the thermal resistance to heat flow through constricted contact points (solid contact resistance) and thermal resistance to heat flow across the gaps (gap resistance) in a parallel thermal circuit. If it were possible to obtain the two resistances separately, and if the two surfaces can be assumed to be isothermal, then TCR for the joint,  $R_c$ , may be expressed as

$$R_{c}^{-1} = R_{C|solid contact}^{-1} + R_{c|gap}^{-1}$$
(1.2)

The TCR is a surface effect in that it depends on surface characteristics such as the topology. It is also a volume effect as the disturbance to the heat flux lines occurs within the two bodies at some distance from the contact plane and not at the surface alone. The TCR is, therefore, a function of surface parameters and material properties and the significance of any particular parameter in determining the magnitude of R<sub>e</sub> depends on the nature of contact and the type of heat transfer. In general, TCR depends on the surface characteristics, thermal conductivity of the bodies in contact, interstitial fluid (fluid filling the gaps at the contacting plane) characteristics, contact pressure and nature of heat transfer (steady/unsteady/periodic). A larger R<sub>e</sub> can reduce the heat flow between the surfaces significantly. There are applications where TCR needs to be increased, such as in thermal insulation using laminations, as well as applications where TCR has to be minimized, such as in heat exchangers, electronic chips etc. The TCR affects both the process characteristics (for example by reducing the heating time) as well as the process efficiency (by requiring a higher temperature difference to drive a given heat flow).

As the TCR depends to a large extent on the nature of the surface, which is defined statistically, it has been studied on a case by case basis. Experimental, analytical and modeling methods have been developed that address the specific applications. The major fields of application in which TCR has been investigated to date include aerospace, nuclear energy, electronic packaging, metal processing, tribology, medicine, building heat transfer, thermal energy storage and heat transfer in thermal power applications (Fletcher, 1988; Madhusudhana, 1996; Madhusudhana and Fletcher, 1986).

TCR also plays a role in heat transfer in many plastic processing techniques. The commonly used processes include extrusion, injection molding, compression molding,

transfer molding, blow molding, film blowing, thermoforming and pultrusion. Of these TCR plays a more significant role in heat transfer in injection molding, thermoforming, compression molding, transfer molding and pultrusion. In extrusion and film blowing, a complementary parameter, the heat transfer coefficient is considered. In early studies, the TCR effect was considered to be negligible in processing of plastics. The one main reason for this assumption is the low thermal conductivity of plastics ( of the order of 0.2  $W/m^2K$  compared to >10  $W/m^2K$  for most metals). However, the need for accurate simulation of polymer processing methodology has shown that TCR is of significance in injection molding and possibly, in other processing methods. In the present research, we have considered the effects of TCR in injection molding as it is one of the most widely used processes for the manufacturing of plastics products.

#### **1.3 Injection Molding**

In injection molding, the molten plastic is injected into a mold which contains a cavity in the shape of the part to be produced. Figure 1.2 shows a schematic of a typical injection molding machine (McCrum et al.,1992).

The polymer in the form of pellets is plasticized in the extruder. The required heat is supplied partly by electric heaters and partly by shear heating as the extruder's screw rotates. The molten polymer collects in front of the extruder screw which then stops rotating at a preset time and, acting as a piston, pushes the molten polymer into the cavity under very high pressure(10-150 MPa). This stage is called the filling stage.

The molten plastic starts to cool as soon as it comes in contact with the cavity



Figure 1.2 Sectional diagram of a reciprocating screw injection molding machine showing salient processing features (McCrum, 1992, after Ogorkiewicz).



Figure 1.3 Various stages of the injection molding cycle time.

walls causing it to shrink. After the cavity is filled the pressure in the extruder is maintained so that more molten polymer enters the cavity to make up for the reduction in volume caused by shrinkage. The pressure in the extruder at this stage is called the holding or packing pressure and is removed after it ceases to push any more polymer into the cavity. The packing pressure provides a degree of control on the shrinkage phenomenon. The part is then allowed to cool to a temperature where it becomes sufficiently rigid so that it can be ejected from the mold without undue deformation. This stage, from the end of filling until ejection of part is called the post filling stage. A finite amount of time is required for the part to be taken out of the mold and this is called the mold open stage. Figure 1.3 illustrates the three stages (the post-fill stage has been subdivided into the packing/holding and cooling phases) and their typical duration as a fraction of the injection molding cycle time (C-MOLD,1997).

Heat transfer takes place in the mold during all three stages. Once the part is ejected the mold is closed and the entire process is repeated a large number of times. This causes the mold metal to be subjected to a periodic heat transfer during each cycle while the part is subjected to transients with steep temperature gradients. On ejection, the part cools slowly to room temperature. Figure 1.4 shows the typical variation in temperature at the mold wall and in the center of the cavity during an injection molding cycle obtained from a simulation.

A number of variations of the basic injection molding process have been developed to address the needs of special products. These include gas assisted injection



**Figure 1.4** Variation of temperature with time in the part and in the mold wall corresponding to a specific location in the part (from simulation).

molding, reaction injection molding, foam injection molding etc. TCR effects in the conventional injection molding is the main subject of this study. It is expected that the results can be modified for the other processes.

#### 1.4 Objectives and Thesis Organization

This research included the following components

- 1. To conduct a parametric investigation into the significance of TCR in injection molding and to study the effect of processing variables on TCR in injection molding.
- 2. To experimentally determine the TCR at selected plastic-metal interfaces.
- 3. To investigate the discrepancy in the values of TCR obtained from steady state experiments and the reported results from measurements performed during injection molding, and to propose a model that will explain the mechanism of TCR in injection molding.
- 4. To develop a model for the effective TCR to be used in injection molding simulation which incorporates both the material properties and the effect of processing variables.
- 5. To propose a method for experimental determination of thermal conductivity and TCR from transient temperature measurements during injection molding.

The thesis is organized in three sections in line with the above objectives. The parametric investigation and its results are presented in chapter 3, the experimental study and its results are discussed in chapter 4 and chapter 5 contains the procedure and results relating to the modeling of an effective TCR for use in injection molding simulation. The

results of the chapters 1 and 2 are self contained and hence the sections include their discussion. The results of these two chapters are then used to develop the modeling strategy and chapter 3 contains the subsequent results and discussion. A method that uses transient temperature measurements to evaluate TCR as well as thermal properties of a polymer sample has been developed and tested in simulation and its results are presented in chapter 4.

#### CHAPTER 2

#### LITERATURE SURVEY

#### 2.1 Reviews

A very large volume of literature is available on TCR investigations spurred on by research in aerospace heat transfer, nuclear energy use and electronic packaging. Recently, TCR has also been studied in various processing applications, for example in metal casting, rolling and plastic processing.

Madhusudhana (1996), Fletcher (1988), Madhusudhana and Fletcher (1986), and Yovanovich (1986) have provided reviews of developments in the area of contact heat transfer in the recent past. While the review of Yovanovich discussed the various contact conductance correlations that have been developed, Fletcher (1988) and Madhusudhana and Fletcher (1986) reviewed the various areas in which contact heat transfer has been studied. Fletcher (1993) provided an overview of the experimental methods currently in use with typical results. Madhusudhana (1996) has recently published a monograph which reviews the various aspects of contact heat transfer in a systematic way starting from idealized constriction models. The book also briefly discusses experimental techniques and provides a number of references.

#### 2.2 Steady State TCR Measurement and Modeling

Due to the statistical nature of TCR, a very large number of experimental studies have been carried out with results specific to a particular type of interface. Earlier TCR studies

were mainly concerned with metal-metal contacts and the applications were in product design and in heat transfer calculations where the contact resistance measured from steady state experiments could be applied. Snaith et al. (1986) presented a review of results of TCR in connection with pressed metal contacts primarily to assist designers in understanding the factors involved. Recent steady state investigations of interest are those of Marotta and Fletcher (1998) regarding aluminum and stainless steel contacts, Sridhar and Yovanovich (1996) on interfaces in tool steels in connection with machining, Lambert and Fletcher (1995) on electroplated silver coatings, McWaid and Marschall (1992) on pressed metal contacts in vacuum, and Tauchert et al. (1988) on layered steel vessels. A number of modeling techniques have been employed to obtain generalized models to describe the experimental results. One of the earliest models to provide a good correlation with experimental data was that of Cooper et al. (1969), which was based on the plastic deformation theory of asperities. Mikic (1974) proposed a model based on elastic deformation of the asperities as experiments had shown that good correlation with plastic models was obtained only for the initial loading at the interface. When the cyclic load was applied to the bodies the elastic models for TCR gave a better estimation of the experimental results though the actual nature of deformation was hypothesized to be a combination of elastic and plastic deformation. Yovanovich (1981) developed a correlation for TCR at conforming, rough, metal-metal contacts which was experimentally verified (Yovanovich and Hegazy, 1983). Song and Yovanovich (1987) further refined Yovanovich's model and introduced an explicit expression for computing the microhardness. The elastic deformation theory of Greenwood and Williamson (1966) was modified by McCool (1986), and verified experimentally by McWaid and Marschall

(1992) for certain types of metallic contacts in vacuum. This experiment showed that the deformation at the interface is neither purely elastic nor purely plastic but a combination of both. Sridhar and Yovanovich (1996) have extended the application of the model presented by Song and Yovanovich (1987) by presenting a correlation between the microhardness and Brinell hardness for tool steels. Marotta and Fletcher (1998) reported on the results of investigation into TCR at aluminum and stainless steel interfaces and found that, contrary to expectation, the elastic model gave better estimates of the measured TCR in case of aluminum-aluminum contacts compared to the plastic models. Marotta (1997) provides a detailed review of the various models proposed for thermal contact resistances at metal-metal contacts and compares their predictions with special reference to coated surfaces.

Holman and Gadja (1984) and Beckwith et al. (1993) provide the background information on the basic measurement procedures in heat transfer while Fletcher (1993) reviews the latest trends in TCR measurement and some pertinent results

In summary, well-established TCR models and accurate experimental methods are available for certain metal-metal and coated metal surface contacts encountered in common engineering applications. However, special applications still have to rely on empirical values of TCR and the experiments will need to be designed suitably.

## 2.3 Processing and Plastic Applications

Recently attention has been focused on TCR in processing applications where the heat flux as well as the contacting surfaces may generally not be in steady state. This interest

stems from increasing demand for accurate numerical simulations to improve productivity and design quality.

Seyed-Yagoobi et al. (1992) investigated the effect of TCR in paper drying processes and determined an experimental correlation for TCR in terms of the contact pressure and moisture content of the paper sample. They used a regression method to compute the TCR value by varying the contact pressure and calculating the total thermal resistance of the sample from the measured temperatures. The use of such a method was feasible because, according to these authors, the thickness of the paper sample did not vary significantly with load to introduce error. Their correlation was subsequently incorporated in a numerical code to simulate the drying process (Asensio and Seyed-Yagoobi, 1993).

Attia and Osman (1993) investigated the effect of TCR in solidification of metal casting while Ruan et al. (1994) proposed a method to measure the contact heat transfer coefficient, during the solidification of a binary alloy casting, by an inverse method. In their method Ruan et al. used an FEM procedure to compute the temperatures in the melt. The results were obtained with simulated temperatures and with the assumption that the TCR is uniform over the entire surface. Wang and Matthys (1996) studied the variation of contact conductance during the solidification of a splat of liquid metal on a colder substrate and showed that the computed contact conductance varied by more than an order of magnitude as the characteristics of the interface changed during the solidification process. The procedure used transient temperatures measured by pyrometers. As in the case of Ruan et al. the TCR was considered uniform over the entire surface. They obtained TCR values of  $2.5 \times 10^{-4} \text{ m}^2\text{-K/W}$  at the instant when the melt had solidified but

reported that in some cases the computed TCR of the partially solidified melt was lower than that of the fully liquid melt. They used a novel method to compute the TCR which involves comparing the profile of the measured transient temperatures with profiles computed using a mathematical model for the heat transfer process. Chien et al. (1997) have proposed a similar method to compute on-line process control parameters from measured quantities during injection molding of plastics.

Mohr et al. (1997) investigated the TCR at paper-elastomer surfaces for two different types of elastomers. The two elastomers studied had nearly the same surface roughness but the *surface waviness* of one contact surface was an order of magnitude higher. They used the data from the work of Seyed-Yagoobi et al. (1992) to obtain the thermal conductivity of paper, and showed that the TCR for the sample with higher waviness was considerably larger even at high contact pressures. They concluded that for soft surfaces such as elastomers, TCR appears to depend on the waviness rather than surface roughness.

In the case of plastics, Hall et al. (1987) carried out investigation of plastic interfaces in connection with the measurement of thermal conductivity (k). They reported that different methods of preparing the contact surface resulted in different values of thermal conductivity which they attributed to TCR at the interface. They concluded that TCR in such measurements is not insignificant and its consideration could result in change in the value of k by 6.5-12.1%. From their results a TCR value in the range of  $1.4 \times 10^{-4}$  m<sup>2</sup> K/W at a polystyrene-metal interface can be deduced. Peterson and Fletcher (1988) carried out more systematic studies at thermoset-metal interfaces of the type encountered in electronic packaging and found that the TCR could be modeled using the
correlation developed by Song and Yovanovich (1987). They used comparatively large samples in which the thermocouples were inserted in the thermoset specimen, and the measurements were conducted in vacuum. The interface between the thermoset and metal was formed by the method normally used to thermally bond electronic component heat spreaders to their plastic cover. Their work did not account for the contact resistance between the thermocouple and the plastic sample. The TCR values obtained by them while in the range of those obtained by Marotta and Fletcher (1996), are much larger than those obtained at thermoplastic-metal interfaces in the current investigation and by Rhee et al. (1994) and Hall et al. (1987).

Scialdone et al. (1992) studied the contact conductance at a metal-metal interface where different polymeric materials with relatively high thermal conductivity were used as interstitial media. The use of these materials (an elastomer and a conductive silicon) resulted in significant reduction in the TCR.

Rhee et al. (1994) studied the effect of TCR on the filling stage cavity pressure predictions in the simulation of injection molding. They evaluated the TCR at a thermoplastic-metal interface from steady state experiments where the plastic-metal interface was formed when the plastic was in a softened state similar to that obtained in the filling stage of injection molding. They, and Narh and Sridhar (1997) reported values of the order of  $6-9x10^{-5}$  m<sup>2</sup>-K/W for such interfaces and concluded that this value of TCR is in order for the filling stage simulation. Marotta and Fletcher (1996) investigated the TCR at polymer-metal (aluminum) interfaces for a selected group of polymers. The samples were thick and contact surfaces were machined. Marotta and Fletcher obtained values for TCR in the range of  $0.15x10^{-3} - 2x10^{-3}$  m<sup>2</sup>-K/W. They further found that their

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results do not show good agreement with either the plastic or the elastic models proposed essentially for metal-metal contacts, while the data of Peterson and Fletcher (1988) showed good correlation with the plastic model of Yovanovich and Hegazy (1983) and Song and Yovanovich (1987).

Yu et al. (1990) reported on the study of the evolution of TCR during injection molding. Their results showed that the TCR increased from a very low value during the filling stage to a high value in the post fill stage. Their results fit in well with our proposed mechanism of shrinkage driven TCR. However, they could not generalize their results as the data was obtained for a particular part geometry and the TCR values obtained by them were much larger than those obtained by Rhee et al. and Narh and Sridhar from steady state experiments. Furthermore, their method, like that of Peterson and Fletcher, did not account for contact resistance between the plastic and thermocouple or for the lag in temperature response of the thermocouple. Yu et al. recommended average values of TCR for different materials, and for different thickness and showed that the use of these values improved the cooling time simulation results significantly. This gives a degree of confidence in their results, but as shown by us (Sridhar and Narh, 1998), an average value of the magnitude recommended by Yu et al. may result in errors in the simulation result. The assumption implicit in their analysis is that the TCR is uniform over the part surface at any instant of time. The tabulated TCR data proposed by them is inconvenient to incorporate in simulation software as it treats TCR as another material property to be stored in the data base. The TCR would then have to be experimentally determined for each material and thickness.

All the results reviewed above, except that of Yu et al. and Wang (1996), were based on steady state experiments. While Yu et al. did use transient measurement, their technique required a number of assumptions, the most significant being (i) that the measured temperature represented the part temperature accurately, (ii) that the part temperature distribution was uniform about the centerline, (iii) that the TCR was uniform at all locations in the part and (iv) that the thermal conductivity values from resin manufacturers were accurate.

Transient temperature measurements were used by Moses and Johnson (1989) to compute TCR. They measured TCR at periodically contacting surfaces by a quasi-steady state method and showed that the temperature profile reached a steady shape after a few cycles. They proposed that this information could be used to compute TCR from instantaneous temperature values. In an interesting analysis, Beck (1988) used the data of Moses and Johnson to compute TCR by an inverse method. He also analyzed the uncertainty in his results and showed good agreement between the TCR values obtained by him and those obtained by Moses and Johnson. In an earlier work, Beck (1969) had proposed an inverse method for calculating TCR. However, no experimental results were available in literature based on this method due probably to the high degree of accuracy required in the temperature measurements, the difficulties in designing the experiment and the relatively intensive computation. Recently, inverse method based techniques, such as that proposed by Beck are being used, increasingly, for computing thermal properties from transient temperatures (Scott and Beck, 1992; Scott and Saad, 1993; Taktak et al., 1993). Methods of the type used by Wang (1996) used pattern recognition technique, a form of inverse method, to determine TCR. Such a technique could prove

advantageous for on-line measurements during plastics processing as brought out by Chien et al. (1997).

In summary, TCR has been investigated for a number of interfaces including some plastic-metal interfaces. However, none of the results explained the mechanism of TCR in injection molding process or gave a basis for the use of available experimental data in plastic processing and product design. Furthermore, there are no established techniques for measuring the TCR in injection molding, reliably, from transient temperature measurements.

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### CHAPTER 3

## **PARAMETRIC STUDIES**

### 3.1 Objectives

Thermal contact resistance in processing is a difficult parameter to measure in situ as it requires accurate measurement of the temperature of the material being processed. At the same time it is difficult to obtain an interface in controlled experiments similar to that obtained during the processing, especially in applications such as injection molding, casting solidification etc. It is, therefore, important to study the significance of TCR on the injection molding simulation results before undertaking an evaluation of its magnitude. It is also important to investigate the injection molding process based on the understanding of TCR from literature to determine the effect of process variables on the TCR during injection molding. This has been done by a parametric investigation detailed in this chapter.

### 3.2 Analysis Strategy

The parametric study was conducted by simulating the injection molding process using the finite element based software, C-MOLD<sup>1</sup>. This software is used by a number of leading engineering companies. The simulation predicts the pressure, velocity and temperature distributions and shrinkage of the part in the mold cavity during an injection

<sup>&</sup>lt;sup>1</sup> C-MOLD is a software by AC Technology, Ithaca, NY that simulates the filling, postfilling, mold cooling and shrinkage/warpage processes in injection molding (and certain other plastics processing techniques). It requires the part geometry, material properties and process conditions as input and generates the velocity, temperature, pressure and displacement fields in the mold cavity due to the flow of polymer.

molding cycle. The software accepts as input, the part geometry (in the form of a finite element mesh), the material properties (thermal conductivity, specific heat, viscosity, specific volume, coefficient of thermal expansion etc.) and process variables (max. injection pressure, fill time, post fill time, packing pressure and profile, ram speed profile, holding time, mold/coolant temperature etc.). A constant TCR value is specified as a default, which can be modified by the user. This value does not consider the resistance due to gaps. The analysis steps have been briefly described in Sridhar and Narh (1998); details are given in the software user's manual (C-MOLD, 1997).

# 3.2.1 Finite Element Modeling

Five commonly encountered part geometries were selected for our study. These range from simple to complex shapes. We used amorphous as well as semi-crystalline polymers for the study. The salient analysis conditions of the parts and their identifying codes are given in Table 3.1 and the part geometries are shown in Figs. 3.1(a)-(e). Solid models of the parts were created using the solid modeling software Pro-Engineer. The solid models were then converted to mid-plane mesh as required by C-MOLD. Runners, gates, cooling channels and parting plane were modeled in the modeler module of C-MOLD in accordance with mold design practices (Buckleitner, 1995). Tool steel P-20, with constant thermal properties, was used for the mold material. Figures 3.1(a)-(e) also show the node and element locations in the cavity where the temperature and pressure data were obtained from the simulation for subsequent analysis. The process conditions were based on recommendations of the software supplier.

Model	Polymer	Max. Thk. (mm)	Melt Temp. (°C)	Eject. Temp. (°C)	Fill time (s)	Hold Press.*	Hold Time <sup>+</sup>	Mold Temp. (°C)	Gate Size (mm dia.)
A	PS	3.2	220	100	0.93	100/50	10	60	2.2
B	PS PS	5.1	220	100	1.1	100/50	30	60	3.7
С	PP	2.5	240	95	0.9	100/50	10	50	1.5
D	PC	5	300.5	120	1.8	100/50	25	100	3
Е	HDPE	5	218	95	1.3	100/50	30	45	3

Table 3.1 Process parameters and the models used in the analysis

\* as % of max injection pressure

+ as % of cycle time

Note: Part A was analyzed with two thickness.

Table 3.2         Summary of results and process	sing condition modifications
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Model/	Estimated	Max.	Modified process variables
Run	Cooling Time <sup>†</sup>	Injection	(analysis code indicated within
	(s)	Pressure	parantheses )
		(MPa)	
A / A1	21	15	(A1): thickness =3.2mm;
Al/Ala	61	16	(A1a): thickness =6.2mm
A / A2	21	15	Hold time = 20s
A / A3	21	15	Mold temp.=80°C; Hold time=20s
A / A4	21	14	Melt temp.=250°C; Hold time=20s
A / A5	21	14	Gate size=3.2mm diameter ; Hold
			time=20s
A / A6	26	15	$TCR=10^{-3} m^2 - K/W;$
A6a	70		(A6): thk=3.2mm; (A6a): thk=6.2mm
B / B1	66	29	
B /B2	74	29	
C / C1	25	25	
D / D1	65	7.5	
E/E1	54	17	

† cycle time = filling time + cooling time



Figure 3.1(a) Model A: model of an ASTM tensile test specimen showing the mid-plane mesh, cooling channels, runner and gate. For line a-a consult text 'Simulation Results/Shrinkage Analysis'.



Figure 3.1(b) Model B: model of a box with partitions and showing the runner system. For line b-b consult text 'Simulation Results/Shrinkage Analysis'.



Figure 3.1(c) Model C: model of a cup showing the runner and gate.



Figure 3.1(d) Model D: Model of a plastic lid showing the runner and gate.



Figure 3.1(e) Model E: Model of an electronic remote controller cover showing the runner

## 3.2.2 Effect of TCR

Models A, B and E were used to study the effect of TCR on injection molding simulation of a simple and complex geometry, respectively. Mold cavity filling, mold cooling and postfilling analyses were performed using TCR values of  $4x10^{-5}$  m<sup>2</sup>-K/W (C-MOLD default) and  $10^{-3}$  m<sup>2</sup>-K/W (in the range of values recommended by Yu et al. (1990) for polystyrene(PS)).

# 3.2.3 Effect of Process Variables

Models A-E were used to study the effect of process variables on the evolution of TCR. The analysis consisted of filling, mold cooling and post filling. Table 3.2 gives the details of the process parameters that were varied and the corresponding analysis identification codes.

The main controllable processing variables in injection molding are the injection pressure, the melt temperature, the coolant inlet temperature (i.e. the mold temperature), the packing/holding pressure and the holding time. Since the contact resistance is due to imperfect contact (i.e. presence of gaps at the interface), then for a given mold and polymer, the thermal contact resistance in injection molding can be taken to be a function of both the surface deformation and the contact pressure. Thus, the effect of the controllable processing variables on the contact pressure and the surface deformation were studied.

*Cavity Pressure*: The contact pressure is assumed to be equal to the cavity pressure (although there may be some variation between the pressure at the mid-plane as computed by the software, and the contact pressure, this should not affect the conclusions

as brought up under "discussions"). The cavity pressure variation is affected by the maximum injection pressure, the mold metal temperature, the holding pressure, the holding time and the melt temperature. Another factor that affects the cavity pressure is the gate size which, while not a process variable, has been considered as a variable for the purpose of this analysis.

### 3.2.4 Shrinkage Analysis

The surface deformation is due to shrinkage/warpage which are affected mainly by the holding pressure/time and non-uniform cooling of the part. However, in this study part shrinkage at only one processing condition is considered sufficient to represent the effect on TCR as illustrated in the results section. Models A, B and E were used to study the effect of shrinkage/warpage with the processing conditions A1, B1 and E1 of Table 3.2, respectively. This analysis consisted of the filling, mold cooling, postfilling and shrinkage/warpage calculations.

The simulation is carried out on a mid-plane mesh as, in general, injection molded parts are thin and can be modeled reasonably accurately by considering their mid-plane. Thus, while the effect of the part thickness is considered in the solution of the energy and momentum equations, the part deformation is only computed on the mid-plane. Although the deformation along the two major axes (of a rectilinear coordinate system) is much larger than in the thickness (gapwise) direction, the latter is critical to the development of the gap and, hence, the TCR. The surface deformation can then be studied as a superposition of the mid-plane deformation and the thickness direction shrinkage.

### 3.2.5 Computation of Gap and Gap Resistance

The thickness direction shrinkage was computed from the simulated thickness direction average temperature and from the actual temperature distributions at a location on the mid-plane of the selected model. Eq. (3.1) computes the gap based on the average temperatures  $T_{av}$  while equation (3.1a) uses the thickness direction temperature distribution computed by C-MOLD. At any instant, if the melt velocity is zero, Eq. (3.1a) is expected to give a more accurate result for the shrinkage.

$$\Delta I_{t} = \int_{0}^{1} \alpha(T) [T_{av}(v) - T_{av}(v - \Delta v)] dv$$
(3.1)

$$\Delta l_{t} = \int_{0}^{t} \int_{0}^{1} \alpha(T)(T(x, v) - T(x, v - \Delta v)) dx dv$$
(3.1a)

where  $\Delta l_t$  is the total shrinkage in the thickness direction at time t (time 0 corresponds to the instant when the macroscopic gap starts to form), T (x,v) and T(x,v-dv) are the temperatures at location x along the thickness axis at times t and t-dt respectively, T<sub>av</sub> is the thickness direction average temperature, 1 is the total thickness and  $\alpha$  is the coefficient of linear thermal expansion (or contraction) calculated from the specific volume variation with temperature for the polymer assuming isotropic behavior. For polystyrene, the specific volume was computed from the relation (Orwoll, 1996)

$$v = (1.067 - 5.02 \times 10^{-4} \mathrm{T} - 0.135 \times 10^{-6} \mathrm{T}^2)^{-1}$$
(3.2)

which is a power series curve fit for the temperature range 79°-320°C at atmospheric pressure.  $\alpha$  is then given by

$$\alpha = \left(1 - \left(\frac{\nu_t}{\nu_{t-dt}}\right)^{1/3}\right) (T_{t-dt} - T_t)^{-1}$$
(3.3)

For gaps of 6 mm or less, and for the range of interfacial temperature drops encountered in injection molding, the heat transfer through a medium with Grashof<sup>1</sup> number ~2000 (air for example) is essentially by conduction (Lang, 1962; Madhusudhana, 1993). Assuming the gaps are filled with air and no mold release agent is present, the thermal resistance of the gap can then be calculated by the following equation (Madhusudhana, 1996)

$$R_{g} = (\delta + g_{1} + g_{2}) / k_{g}$$
(3.4)

where  $\delta$  is the gap in meters,  $k_g$  is the thermal conductivity of the interstitial medium and  $g_1$  and  $g_2$  are the temperature jump distances (in meters) for air. The temperature jump distance is a measure of the efficiency of energy transfer between the gas molecules and solid surface; the temperature jump increases the temperature difference in the gap compared to the temperature difference due to the thermal conductivity of the gas alone.

<sup>&</sup>lt;sup>1</sup> Grashof number Gr= g  $\beta$  (T<sub>w</sub>-T<sub> $\infty$ </sub>)  $L^3/v^2$ ; where g is gravitational constant,  $\beta$  is the volumetric thermal expansion coefficient, Tw and T<sub> $\infty$ </sub> are the wall and ambient temperatures, L is the length scale and v is the kinematic viscosity.

For the results presented here, the interstitial medium is considered to be air at atmospheric pressure and 350K.

### 3.3 Simulation Results

The results of the simulation are presented below for the three aspects investigated. A separate discussion combining all three results is then presented.

#### 3.3.1 Effect of Thermal Contact Resistance on Heat Transfer in Injection Molding

Figure 3.2 shows the thickness direction average temperature in models A and B, from the start of filling until the plastic has reached a temperature close to its ejection criterion, for the two different values of TCR. Most injection molding results are presented in terms of the bulk temperature. The bulk temperature is defined as the velocity weighted average temperature in the thickness direction; when the velocity goes to zero the bulk temperature is the average temperature in the thickness direction. As this study is concerned with the shrinkage phenomenon which affects the surface displacement *only after the fluid velocity has become zero*, the average temperature is thought to be a better indicator of shrinkage characteristics. The figure shows that a higher value of TCR increases the time taken by the part to reach a given average temperature, i.e. the cooling time is increased. The cooling time obtained with the TCR value of  $10^{-3}$  m<sup>2</sup>-K/W is about 25% longer than that obtained with a TCR value of  $8x10^{-5}$  m<sup>2</sup>-K/W for model A with a part thickness of 3.2mm. Figure 3.2 also shows the bulk temperature curves for model A with an increased part thickness of 6.2 mm and for model B which has a larger volume



**Figure 3.2** Thickness direction average temperature in models A (for two different values of part thickness) and B at a specified location, plotted at different instants in the molding cycle with the two values of TCR (the values are the default value of CMOLD,  $4x10^{-5}$  m<sup>2</sup>-K/W, and the exerimental values of Yu et al, 1990). Refer to Table 3.2 for model designations. The broken horizontal line corresponds to 110 °C - a typical ejection temperature for PS. Note the differences in the cycle time for the two values of TCR used (broken vertical lines).



Figure 3.3 Thickness direction temperature distribution in models A and E at the end of filling and at the end of postfilling for the two values of TCR.  $R_c$  values are in m<sup>2</sup>-K/W. For model A, end of filling and end of postfilling are at 0.93s and 22s of the cycle time respectively, and for model E, the end of filling and end of postfilling are at 1.3 and 55s of the cycle respectively.



**Figure 3.4** Plot of bulk temperature at the end of filling and at 16.84s of cycle time (postfilling stage) for different values of TCR.

and a more complex geometry than model A. Figure 3.3 shows the temperature distribution in the thickness direction, at the end of filling and at an instant in the postfilling stage for models A and E respectively. The temperature distributions again correspond to the two different values of TCR used in Fig. 3.2.

It is seen from Fig. 3.2 that the use of a higher value of TCR does not significantly affect the average temperature at the end of filling compared to its effect on the average temperature at the end of the postfilling stage. However, Fig. 3.3 shows that the temperature distribution at the outer layers of the part at the end of the filling stage is quite different for the two values of TCR; the higher value of TCR causes the outer layer temperatures to be higher by about 15° to 80 °C for the two cases shown.

Figure 3.4 is a plot of the bulk temperature in the part at end of filling and at 16.84s into the cycle (i.e. later stage of postfilling), for different values of TCR. It is seen that the bulk temperature at the end of filling does not show significant variation with TCR. However the bulk temperature in the postfilling stage increases with TCR with the increase not being linear.

#### 3.3.2 Effect of Process Variables on Cavity Pressure

Figures 3.5 (a and b) and 3.6 show the effect of varying the controllable process variables on cavity pressure. Figure 3.5(a) shows the gate and cavity pressures at different instants in the cycle time for all the models, with hold times and hold pressures as given in Table 3.1. The hold pressures and times are selected to minimize the part shrinkage. It can be seen that the cavity pressure decays rapidly at the end of filling. The cavity pressure has been plotted at locations closer to the gate; at locations farther from the gate the decay is







**Figure 3.5(b)** Plot of the variation of gate and cavity pressure against normalized cycle time (normalized with respect to total cycle time). Solid lines represent the gate pressure and dashed lines represent the cavity pressure at the indicated nodes.



Figure 3.6 Plot of the cavity pressure against cycle time for model A for different processing conditions (refer to Table 3.2). Solid lines represent the gate pressure and dashed lines represent the cavity pressure at the indicated nodes.

steeper and this data has not been included. Figure 3.5(b) shows the cavity pressure normalized with respect to the maximum injection pressure and plotted against a time scale normalized with respect to the estimated cycle time for the particular model given in Table 3.2. It is seen that the cavity pressure decays to atmospheric in 20-50% of the cycle time. As the decay occurs faster in locations farther away from the gate, we can conclude that for over more than 50% of the part surface area the contact pressure is very small (ideally zero). This corresponds to 50-80% of the cooling time. Comparing models A and B, it is seen that the decay in cavity pressure is faster in the more complex geometry even though it has a larger thickness and longer cooling time.

Figure 3.6 shows the effect of process variables and gate size on the pressure variation in the cavity for model A (refer to Table 3.2 for the process variables modified in each run compared to the base values of Table 3.1). The cavity pressure decay is slowed down by an increase in the hold pressure time; the magnitude of the hold pressure does not affect the decay as long as it is above the cavity pressure at any instant. The rate of pressure decay in the cavity is also slowed down by an increase in the mold and melt temperatures but there is also a related increase in the cycle time. An increase in the gate size also results in a slower pressure decay and, in fact, has the most significant effect on the freezing of the gate. An increase in the gate size slows down gate freeze off time and extends the high cavity pressure regime in the cavity. The above results can be summarized as follows: changing processing parameters such as hold pressure, mold temperature, melt temperature and hold time has the effect of altering the cavity pressure decay time by about 20% of the cycle time.

# 3.3.3 Shrinkage Analysis

Figure 3.7 shows the results of the shrinkage analysis using CMOLD. The analysis predicts the shrinkage at the end of the postfilling stage in terms of the displacement of nodes on the mid-plane mesh when the part is ejected from the cavity. The results are plotted for the nodes along the lines a-a, b-b and c-c for models A, B and E respectively. For each model the displacement normal to the selected surface is shown, i.e. Y, X and Y displacements for models A, B and E, respectively. Figure 3.7 shows that a plate-like part deforms such that one of its surfaces is concave outwards (and hence the opposite surface deforms convex outwards). While the analysis predicts the displacements at the end of the cycle, the tendency of the part to deflect starts right from the moment the cavity pressure starts to decay. Thus the surface of the part would tend to move towards the mold wall on one surface and away from the mold wall on the other - based on the nonuniform heat transfer from the part surface. The magnitude of the movement varies with the location on the part surface. Figure 3.7 also shows that the magnitude of the displacement normal to the surface is greater for box like sections viz. models B and E. For a mold that has been designed to provide balanced cooling, variation of the controllable processing variables such as the holding pressure/time, does not affect the mid-plane displacements qualitatively, and hence their effect has not been brought out here.

### **3.3.4 Gap Formation Analysis**

As explained under "analysis strategy", the shrinkage analysis considers deformation along the two major dimensions of the part's surface. The thickness direction shrinkage





was calculated using Eqs. (3.1)-(3.3) and from the temperature data obtained from the simulation using a TCR value of  $8 \times 10^{-5}$  m<sup>2</sup>-K/W for model A (run A1), and from Eqs (3.1a)-(3.3) for model B. It is assumed that the thickness direction shrinkage causes surface displacement only when the cavity pressure has decayed to atmospheric; this is discussed further below.

Figure 3.8 shows the thickness direction shrinkage in terms of the gap formed between the part surface and mold wall at a location on the mid-plane, assuming that the shrinkage is uniform about the mid-plane. The figure shows that the gap has a magnitude of 4-5 µm within 3s of the cavity pressure decaying to atmospheric pressure. The computed gap increases monotonically till mold opening, reaching a maximum value of about 27µm and 49µm for models A and B respectively, based on the temperature distribution. The computed shrinkage based both on the average temperature (as shown in Fig. 3.7) and thickness direction temperature distribution (similar to that in Fig. 3.8 for different time intervals in the postfilling phase) is shown for model A. The calculated gap based on the thickness direction temperature distribution is expected to be more accurate and is of a slightly smaller magnitude than that based on the average temperature. The corresponding computed gap resistance using Eq. (3.4) is also shown in Fig. 3.8. In the latter case the gap resistance is assumed to be zero as long as the cavity pressure is above atmospheric. The gap resistance reaches a maximum value of about 10<sup>-3</sup> m<sup>2</sup>-K/W for model A which is comparable with the average TCR value measured by Yu et al. Furthermore, the gap resistance increases with increased part thickness with the resistance of model B attaining a maximum value of about  $1.65 \times 10^{-3}$  m<sup>2</sup>-K/W.



**Figure 3.8** Formation of gap and evolution of the gap resistance plotted against the cycle time for the temperature data obtained from analysis for model A (A1) and B. The computation is done at the node indicated on the mid-plane in Figs 3.1a and b.

# 3.4 Discussion

In this section we discuss the implications of the results presented above starting with the significance of TCR in injection molding simulation followed by a phenomenological description of the injection molding process and the effect of process variables and shrinkage on the TCR.

The analysis of the effect of different values of TCR on the simulation show that the value of TCR to be used in both the filling as well as the postfilling stages is of importance. If the TCR variation during an injection molding cycle is of the order investigated in our analysis, then a constant value of TCR will lead to incorrect results in either the filling or postfilling stages. The use of an incorrect value of TCR during the filling stage will not have a significant effect on averaged variables like bulk temperature and average melt velocity and will affect variables computed layer-wise like the gap-wise temperature distribution and frozen layer fraction. In the postfilling stage the effect is on both the layer-wise computed as well averaged variables.

We now discuss the results of the process variables and shrinkage analysis. As the molten plastic enters the mold cavity, the thin outermost layers freeze instantaneously due to the lower temperature and high diffusivity of the mold. This is seen from the temperature distribution at the end of filling shown in Fig. 3.3 for the TCR value of  $4\times10^{-5}$  m<sup>2</sup>-K/W. Even during the filling stage *the contact is, therefore, between a thin but flexible layer of frozen plastic and the mold wall.* Neglecting the elastic effect of the frozen shell of plastic, it can be assumed that the cavity pressure at the mid-plane is equal to the contact pressure between the plastic surface and the mold metal. Therefore, as long as the cavity pressure is above atmospheric, the flexible outer layer of the cooling plastic

would be in good contact with the mold metal (Battey and Gupta, 1997). In the initial postfilling phase, as the cooling plastic begins to shrink, the pressure at the gate supplies additional molten plastic into the cavity to make up for the shrinkage. This additional material combined with the cavity pressure ensures that there is no displacement of the part surface relative to the mold wall.

Our analysis results show that in a typical injection molding cycle, the cavity pressure is atmospheric for a major portion of the cooling time, the actual period depends on the part and the process variables. The results presented can be utilized to understand which process variable has a significant effect on the pressure decay for a given part geometry. Thus, once the cavity pressure drops to atmospheric, the part surface should be able to pull away from the mold wall and the interface should consist of macroscopic gaps (defined as gaps of thickness larger than the surface roughness).

In an ideal case, and in the absence of mid-plane deformation, the gap would be uniform over the entire part surface at any instant in the postfilling phase (the magnitude may vary marginally depending on the actual temperature distribution at different points on the mid-plane). However, factors such as part weight, adhesion between plastic and mold wall, machine vibrations etc. would cause the part to be in contact with the mold wall over certain portions of its surface. Furthermore, the thickness direction shrinkage provides some freedom for the part to deform as a result of mid-plane deformation caused by unbalanced cooling and non-uniform shrinkage. Thus, the actual gap at any point at any instant in the postfilling stage will be a superposition of the surface movement due to thickness direction shrinkage, mid-plane deformation and displacements due to part weight and vibrations etc. All these factors may be affected by plastic-mold adhesion



Figure 3.9 A simulation of the part surface and mold wall showing the non uniform gap due to superposition of mid-plane shrinkage on the thickness direction shrinkage.

phenomenon. The resulting interface between the part and mold wall will then be a combination of nominally contacting regions and gaps. This is conceptualized in Fig. 3.9 for the case of model B.

The above discussion also shows the difficulties involved in determining TCR from experimental observations during injection molding. Determining the temperature at a single location on the surface (even if it could be done very accurately) would only result in determining the TCR at that spot which, as shown above, could be a region of contact or gap. The same difficulty applies to determination of gap as reported by Wang et al. (1996). As of now, it appears that the available ultrasonic techniques can only identify the onset of gaps but the ability to evaluate the size of gap accurately could only be done by validating the simulation models for TCR and part shrinkage.

### **CHAPTER 4**

# **EXPERIMENTAL INVESTIGATION**

#### 4.1 Objectives

Measurement of thermal contact resistance from temperature measurements during injection molding is difficult due to the difficulty in measuring the temperature of the molten polymer. An experimental investigation was therefore undertaken to measure the thermal contact resistance from steady state conditions at plastic-metal interfaces formed under conditions closely approximating those obtained during injection molding. Two different thermoplastic polymers, one amorphous and another semi-crystalline were selected and interface formed with a typical mold steel surface of the type used in injection molds. A Kline and McClintock (1953) type analysis was undertaken to estimate the uncertainty in the experimental results. A method was also developed to utilize transient temperature measurements to measure the thermal contact resistance and thermal conductivity for a polymer sample.

### 4.2 Steady State Measurement Technique

Thermal conductivity measurements are generally performed using both steady state and transient methods, while thermal contact resistance measurements are generally conducted by steady state methods. Measurement techniques for thermal conductivity include steady state methods such as the guarded hot plate method, and methods using heat flux meters Holman and Gadja (1984), and transient techniques such as the line source method for thermal conductivity of polymers (Lobo and Cohen, 1990) and the TC

probe method (Mathis Instruments,1998). Experimental measurements of thermal contact resistance are, generally, performed at a steady state (Mohr et al.,1997; Narh and Sridhar,1997) or quasi-steady state (Moses and Johnson,1989) using temperature measurements, taken at some distance from the interface, to extrapolate to the interface temperatures and to calculate the heat flux crossing the interface. The method used here is described briefly in Hall et al.(1987).

# 4.2.1 Theory

For a material obeying Fourier conduction, the thermal resistance it offers to one dimensional heat transfer is a linear function of its thickness (everything else remaining constant). The total resistance  $R_t$  of such a sample with identical surface characteristics on both sides, when sandwiched between two contact surfaces is given by the equation:

$$R_{t} = R_{s} + 2R_{c} \tag{4.1}$$

where  $R_s = t_h/kA$  is the thermal resistance of the sample,  $t_h$  the specimen thickness, k thermal conductivity and A the cross sectional area. This relation can be used to determine both the thermal conductivity and the contact resistance by a regression procedure depending on the number of independent parameters that are varied during the measurement. Using Fourier's law, the total resistance can be expressed as:

$$R_t = \Delta T/q \tag{4.2}$$

where  $\Delta T$  now denotes the temperature drop between the two contact surfaces between which the specimen is sandwiched. Then for the case of one dimensional steady state heat flow the total resistance becomes a linear function of thickness:

$$R_{t} = (1/kA)t_{h} + 2R_{c}$$
(4.3)

The total thermal resistance can be computed for specimen of different thickness at the same mean temperature. The slope of a line fit through the points ( $R_{t,}t_{h}$ ) yields the thermal conductivity and the intercept is equal to  $2R_{c}$ . The thermal conductivity of the sample is assumed to be constant in the range of temperatures across the sample, or the thermal conductivity determined can be considered as the effective thermal conductivity at the mean temperature of the sample.

### 4.3 Apparatus

Fig. 4.1 shows a schematic drawing of the apparatus used. It consists of a cylindrical block made of mold steel (DME steel P20) which is attached to a thick rigid steel plate using a Bakelite bracket. The bracket houses an electrical heater, and a load cell is attached to the top of the plate to record the applied load. The plate is supported on a steel frame which permits it to move up and down while maintaining the parallelism between the bottom surface of the top steel block and the top surface of the lower steel block. The lower steel block, also fabricated from the same mold steel, is mounted on a copper


Figure 4.1 Schematic of the TCR measuring apparatus.

Material	Туре	Manufacturer/ Grade	T <sub>m</sub> (°C)	T <sub>g</sub> (°C)
Polystyrene (Ps)	Amorphous	Dow Styron 615 Apr	-	100
Polyehtylene Terepthalate (Pet)	Crystallizable	Eastman Kodak Pet 9921	250	80

jacketed heat sink which is attached to the lower steel plate of the frame. A constant temperature bath maintains the temperature of the sink at a set value of a circulating heat transfer oil. The steel blocks have holes drilled perpendicular to the axis to permit J-type thermocouples to be inserted till the centerline. A thermal compound is used to ensure good contact between the thermocouple tip and the mold steel. The entire apparatus is then placed in a rigid steel frame which permits application of a constant load on the top of the load cell. The thermocouple readings are recorded through a data acquisition system consisting of an isothermal terminal block, multiplexer/signal conditioner and a data acquisition board in the computer.

## 4.4 Measurement Procedure

The TCR obtained is greatly dependent on the nature of interface. In the experimental procedure followed here, the plastic specimen surface is modified by heating it after placing it in the apparatus. This additional sample preparation step is done to achieve an interface that more closely resembles the one formed during injection molding.

# 4.4.1 Sample Preparation

Polystyrene (refer Table 4.1 for material data), an amorphous plastic, was initially used in this study as its thermal and physical properties have been extensively studied and thus can be used as a reference to establish the accuracy of our data. Polystyrene disk samples of 38.2 mm diameter were compression molded. A brass shim was used to obtain uniformity of thickness to within 25  $\mu$ m. The thickness of the sample was measured by taking readings along the periphery as well as at the center. In the present study the effect

of varying the surface roughness has not been considered. Hence, to bring all samples to the same state at the contact plane in the apparatus, each sample was heated to approximately 100°C between the steel blocks on the apparatus and maintained at this temperature for 25 minutes. The steel blocks and the sample were then brought to the temperature at which measurements were to be made. A similar procedure was followed for the PET samples except that the initial heating was carried out at approximately 90°C instead of 100°C, to avoid excessive softening and deformation.

The sample was placed between the two steel block faces as shown in Fig. 4.1 and insulation was placed around it. Once the sample was heated to 100°C (90°C for PET) as described above, the temperature of the sink was adjusted and the heater input controlled using a rheostat to obtain a temperature gradient of about 10°C between the heater and the sink. The TCR measurements were conducted at average specimen temperatures of 75° and 65 °C. The heater and bath settings were first adjusted to obtain the required mean sample temperature and the required temperature gradient. For each heater and bath settings were taken when steady state was reached. Steady state was generally reached after 1 hour from the instant the heater setting was changed. For subsequent load changes steady state was reached in about 20 minutes. The temperature measurements consisted of recording the temperatures indicated by the eight thermocouples located on the steel blocks (four in the upper block and four in the lower block).

The thermocouple readings are plotted against the axial distance as shown in Fig. 4.2



**Figure 4.2** Thermocouple readings for a typical steady state measurement with plastic sample. The figure shows the apparatus schematic for reference- dotted lines on the schematic represent thermocouple locations. Boundaries A and B pertain to the transient temperature measurement method.

shown here for a PS sample, and the gradient of the least squares best fit line multiplied by the known conductivity of the steel block gives the computed heat flux, q. The intercept of the two lines (temperature profiles in the two steel blocks) with the block surfaces in contact with the plastic specimen gives the temperature of that contact surface. The total thermal resistance,  $R_t$ , of the specimen is then computed using Eq. (4.3). In our case, we measured the total resistance of a number of specimens of at least four different thicknesses and same area at a constant pressure and temperature. For each thickness, measurements were taken for at least two samples. The total resistance was then plotted against the specimen thickness as shown in Fig. 4.3. The TCR and thermal conductivity are then calculated as the intercept and slope respectively of the best fit straight line.

Measurements for different loads were carried out at two different mean temperatures. The maximum temperature at which the experiment could be performed was limited by the temperature at which the specimen showed signs of deformation. In the case of PS measurements could be done at 85 C but with PET the maximum temperature was limited to 75 C. The sample thickness were measured at the end of the experiment when the apparatus had reached room. No corrections were made to the values of thickness of the sample to account for the strain effects under load as the computed strain in these range of loads was less than the variation in sample thickness. However, the sample thickness was measured before and after the experiment to check that undue deformation did not occur.



**Figure 4.3** A typical plot of total thermal resistance as a function of plastic specimen thickness from steady state measurements for a PS sample at different contact pressures. Note the proximity of the data points for the higher contact pressures of 3.16 and 6.77 Mpa

During measurements with PET, the specimen would be expected to crystallize. In fact, the specimen at the end of the experiment showed an increased opacity. The extent of crystallization was not measured.

# 4.5 Experimental Results and Discussion

Fig. 4.4 shows sample plots for TCR as function of contact pressure for at different mean sample temperatures. Fig. 4.6 shows the corresponding thermal conductivity as a function of contact pressure.

As seen in Fig. 4.4 the value of TCR dropped initially and then tended to a limiting value as the pressure was increased. This effect is observed for both PS and PET samples. The initial drop in the value of TCR as the load is increased appears steep due to the scale used but is not as steep as in the case of metals as seen in the results of Fletcher (1993). For PS the TCR values varied in the range  $2x10^{-5}$  to  $10^{-4}$  m<sup>2</sup>-K/W while those of PET varied in the range  $10^{-5}$  to  $9x10^{-5}$  m<sup>2</sup>-K/W. The PET runs at the higher mean temperature of 80 °C are in the vicinity of the material's T<sub>g</sub> and possibly result in higher deformation. Furthermore, the TCR values reach a plateau for a relatively small increase in load compared to metal-metal contacts. The measured values of TCR show little dependence on temperature within the range of measurement. The uncertainty analysis (refer Appendix A) gives a total uncertainty of approximately 20% which is considered within allowable limits for this type of experiment (Madhusudhana,1996 ;pp 74). In Figs. 4.4 and 4.6 the points described as "disturbed" are discussed in the last paragraph of this section (ref. page 66).



Figure 4.4 Plot of TCR as a function of interface contact pressure from steady state measurements for PET and PS interfaces with mold steel.



Figure 4.5 Plot of TCR as a function of interface contact pressure from steady state measurements : comparison of results with literature. Note that the data points in the range of  $10^{-5} - 10^{-4}$  m<sup>2</sup>-K/W are from the present study.



Figure 4.6 Plot of thermal conductivity of PS and PET samples as a function of contact pressure from steady state measurements.

Figure 4.5 shows the results obtained in the current investigation along with those obtained by other investigators for comparison. Results of interest plotted here are those obtained by Marotta and Fletcher (1996), Mohr et al. (1997), and Peterson and Fletcher (1988). Marotta and Fletcher studied the TCR at a number of plastic-metal interfaces including polypropylene (PP), polyvinyl chloride (PVC), polycarbonate (PC), Teflon (PTFE), acrylonitrile butadiene styrene (ABS) and high density polyethylene (HDPE) in contact with aluminum surfaces. However they used thick, machined samples with no thermal preparation of the type used in the current investigation. Thus, the measured surface profile parameters, roughness, waviness and flatness, have large magnitudes as reported by them with root mean square roughness values of 1-2 µm, waviness of 2-60µm and flatness deviation of 12-196µm. They reported that the maximum TCR of about  $7x10^{-3}$  m2-K/W, was observed with ABS (with a waviness of 55.9µm and flatness of 195.8 $\mu$ m). In general the TCR measured by them is in the range of  $7x10^{-3} - 6x10^{-4}$  m<sup>2</sup>-K/W compared to  $1 \times 10^{-5} - 10^{-4}$  m<sup>2</sup>-K/W measured during the current investigation. The lower values obtained in this work are attributable to the special interface forming technique employed by us. In our case the surface roughness values were those measured for the steel block surfaces (0.44 µm) and the method of specimen preparation along with the thin specimen used ensured that the waviness and flatness parameters could be assumed to be negligible.

Figure 4.5 shows the values obtained by Mohr et al. for a paper-metal interface and for two elastomer-paper interfaces. Their results show that the TCR for elastomer B interface is much smaller than for elastomer A, and approaches that of the paperaluminum interface at higher loads. While both elastomers had approximately similar roughness, elastomer A had a much larger magnitude for the waviness parameter. Even though elastomer B had a larger thermal conductivity than elastomer A, this could not explain the large difference in the TCR values and Mohr et al. concluded that the difference in waviness contributed mainly to the large difference in the TCR for the interfaces of the two elastomers with paper. Their results further show that the TCR value reaches a plateau for relatively small increases in contact load. This is clearly seen when compared to the data of Peterson and Fletcher (1988) who experimentally determined the TCR at thermoset-metal interfaces of the type formed in electronic packaging where the heat spreader metal is thermally bonded to the thermoset base or cover. Peterson and Fletcher found that their results could be predicted with a good degree of accuracy by the model of Song and Yovanovich (1987) which was developed for metal-metal contact. The two data points from their result are shown on a dashed line to indicate this agreement with the model. It can be seen that in this case the TCR value drops more steeply with an increase in load than in any of the other three results shown. Note that the Y axis of the plot is in log scale.

Figure 4.6 shows the measured values of thermal conductivity which shows a small increasing trend with temperature which is consistent with published results for PS and PET. The thermal conductivity of PS was in the range of 0.171 to 0.178 W/m-K and for PET in the range of 0.213 to 0.224 W/m-K both of which agree well with published values (Yang, 1996; Greene, 1992). The higher thermal conductivity of PET as compared to PS explains the slightly lower TCR measured at the PET-metal interface. However there no large difference in the magnitude of TCR obtained with the two different types of plastic.

To summarize the results of the steady state data available at polymer-metal interfaces, the interfaces formed with softer materials such as most thermoplastics, paper and elastomers show a small drop in TCR with load. The drop in TCR with temperature observed in certain cases is probably due to the variation of thermal conductivity with temperature. Based on the results of the current investigation and those of Hall et al. (1987) and Rhee et al. (1994), the TCR at conforming thermoplastic-metal interfaces appears to have a upper limit of 10-4 m2-K/W. The high values of TCR observed by other investigators is probable due to the effect of waviness. Furthermore, TCR at these interfaces is a weak function of pressure.

The values obtained in the current investigation are lower than those reported by Yu et al. (1990). To explain the difference between our values and those of Yu et al., we first postulated that the thermal contact resistance increased at the interface due the shrinkage of the plastic in the direction parallel to the interface plane. Such shrinkage would cause a break in the very good contact formed between the metal and plastic surface during the filling stages of injection molding when the soft plastic was pressed against the mold surface. To test this hypothesis, we performed a simple test; we measured the TCR after the interface was formed during the conditioning process described in the preceding sections. Then we repeated the measurements after the interface was disturbed by a slight rotation of the specimen about its vertical axis. The results of the second measurements (to be referred as disturbed interface results), are also plotted in Figs. 4.4 and 4.6. From Fig. 4.4, it is apparent that the movement of the interface has resulted in increased TCR, but to values that are still below those obtained by Yu et al for the later stages of the postfilling period. On the other hand the gap resistance values computed in chapter 3 show a striking similarity with the values of Yu et al. This along with the results of Marotta and Fletcher, whose samples had waviness values of magnitude much larger than the surface roughness, leads us to conclude that in the case of injection molding postfilling stage the gap resistance affects the TCR significantly.

# 4.6 Transient Measurement of TCR by an Inverse Method

This section describes an inverse method for the computation of TCR from transient temperature measurement. The method developed for measuring the TCR and thermal conductivity from transient temperature data has been tested in simulation and results are presented below. The method has the potential to determine TCR from transient temperature measurements without having to explicitly measure the part surface temperature.

In a heat conduction problem, the known thermal properties are used to solve the heat conduction equation and obtain the temperature distribution in a body. In the inverse problem, the temperature measurements at one or more locations are used to determine either the unknown properties or unknown boundary condition coefficients. If the property has a single value in a given experiment, the problem is called parameter estimation (for instance determination of isotropic thermal conductivity which is independent of temperature). When the quantity to be determined is a function of time, temperature, or space, then the problem becomes one of evaluating a function and is known as function estimation or an inverse problem.

The inverse method consists of selecting the appropriate conduction model for the process or experimental set up and developing a procedure to solve it for a given set of properties and boundary conditions. The quantity to be estimated is defined as a discrete or continuous function and given an initial value which may be arbitrary or an estimated value based on prior data. The heat conduction model is then solved and the temperature at a given location is obtained as the output. The temperature is then measured at discrete time intervals at the same location in the experimental set up, for the same boundary conditions as those used in the solution of the heat conduction equation. An objective function (which is essentially the difference between the calculated and measured temperatures) is then used to determine a correction to the function to be estimated. The unknown quantity is thus corrected iteratively until the minimum of the objective function is reached and convergence obtained.

## 4.1.1 Inverse Formulation

The inverse problem formulation follows the method outlined in Beck and Arnold (1974) and Jurkowski et al. (1989). The apparatus of the type illustrated schematically in Fig. 4.2 was considered as an approximate model of an injection mold cavity. The apparatus is subjected to a transient temperature environment by means of a heater/heat sink arrangement near the two boundaries. The temperature distribution over a period of time is measured at a location near the interface, and at boundaries A and B. In the inverse method for estimating the unknown thermal conductivity of a specimen, an objective function  $S(\beta)$  is defined as

$$S(\beta) = \left[\mathbf{T} - \eta(\beta)\right]^{\mathrm{T}} W\left[\mathbf{T} - \eta(\beta)\right] + \left(\nu - \beta\right)^{\mathrm{T}} \mathbf{V}^{-1} \left(\nu - \beta\right)$$
(4.4)

where  $\eta(\beta)$  is the vector of temperature values at the location near the interface as obtained from a physical (numerical) model of the apparatus, and **T** is the vector of temperatures measured at that location over a particular interval of time. The vector  $\beta$ consists of the parameters to be estimated and has the form  $[\mathbf{k}^{\mathsf{T}}\mathbf{R}^{\mathsf{T}}_{\mathsf{cl}}\mathbf{R}^{\mathsf{T}}_{\mathsf{cl}}]^{\mathsf{T}}$ , where  $\mathbf{k}$ ,  $\mathbf{R}_{\mathsf{cl}}$ and  $\mathbf{R}_{\mathsf{c2}}$  are again vectors whose components are the values of the parameters at each instant of time at which the temperatures are measured.

The objective function is minimized by iteratively generating new values of the parameter vector starting with an initial guess. The Gauss method of linearization has been used here to generate the new iterates, as simulation shows that it provides reasonably quick convergence. The new set of parameter values are then obtained from

$$\beta_{j+1} = \beta_j + \left[ \mathbf{X}^{\mathsf{T}} \mathbf{W} \mathbf{X} - \mathbf{V}^{-1} \right] \left[ \mathbf{X}^{\mathsf{T}} \mathbf{W} \left( \mathbf{T} - \eta(\beta_j) \right) + \mathbf{V}^{-1} (\nu - \beta_j) \right]$$
(4.5)

where **X** is the sensitivity matrix, and is a measure of the variation in the temperature distribution for a small variation of the components of  $\beta$ ,  $\beta_j$  is the value of  $\beta$  at the start of the jth iteration, and  $\beta_{j+1}$  denotes the new value of the parameter vector used to start the next iteration. Each iteration requires the solution of the numerical model of the apparatus with the latest value of  $\beta$ . Assumptions in this formulation are that the errors in the temperature measurement are additive and normally distributed, with zero mean and constant variance.

Due to the insulation provided in the radial direction, the apparatus used essentially provides a one dimensional heat flux across the plastic specimen sandwiched between two steel blocks. Thus the one dimensional heat conduction equation

$$\frac{\partial}{\partial \mathbf{x}} \left( \mathbf{k} \frac{\partial \mathbf{T}}{\partial \mathbf{x}} \right) = \mathbf{C} \left( \frac{\partial \mathbf{T}}{\partial \mathbf{t}} \right) \tag{4.6}$$

was used to model the apparatus and generate the vector  $\eta(\beta)$  for each new set of values of  $\beta$ . At each interface the continuity of heat flux condition was applied as

$$-k\frac{\partial T}{\partial x}\Big|_{x=-0} = \frac{\left(T_{x=-0} - T_{x=+0}\right)}{R} = -k\frac{\partial T}{\partial x}\Big|_{x=+0}$$
(4.7)

The heat conduction equation was solved by an implicit finite difference algorithm with a prescribed temperature initial and boundary condition and known values of thermal conductivity and heat capacity of the steel blocks. A finite difference method was employed to compute the sensitivity matrix  $\mathbf{X}$ .

# 4.6.2 Inverse Procedure

In the results presented here the temperature distribution has been generated from a numerical simulation of the apparatus described in section 4.3 above. The location of boundary nodes and the node for generating the components of  $\mathbf{T}$  correspond to locations

1,8 and 4 in the apparatus (see Fig. 4.2) respectively. The thermal conductivity and heat capacity of steel blocks were taken as that for P-20 tool steel (a commonly used mold material) at a mean temperature of 80°C, as the diffusivity of the steel blocks was assumed to be constant in the temperature range of the simulation. The apparatus was modeled as a one dimensional heat conducting region as expressed in Eq. (4.6) and the heat flow at the interface was modeled by Eq. (4.7). The Crank-Nicholson type finite difference algorithm used to solve the model numerically requires a one dimensional spatial grid and a temporal grid. The spatial grid for the numerical simulation extended from boundary A (thermocouple location 1) to boundary B (thermocouple location 8 in Fig. 4.2) - a distance of 41.4mm. The locations A and B correspond to the locations of the two extreme thermocouples in our apparatus. The spatial grid used a spacing of 1mm in the steel blocks and smaller spacing of 0.1mm in the specimen and regions adjoining the interface. A spatial node point was located at either side of each interface between the specimen and the steel blocks and the temperatures obtained at these nodes were used as  $T_{+0}$  and  $T_{-0}$  in Eq. (4.7). The temporal grid was uniformly spaced.

#### 4.6.3 Simulation

The simulations were performed by generating the temperature distribution in the apparatus with an assumed value of the parameter vector  $\beta = [k_{i=1,p} = 0.17, R_{c1; t=1,120} = 0.0001, R_{c2; t=1,120} = 0.0005]$  where the index p is the number of intervals into which the total temperature range of the simulation is divided. The value of the thermal conductivity corresponds to a typical value for polystyrene, a widely studied plastic. The contact resistance values are in the range of the values from our experimental

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measurements and shown in Fig. 4.4. The contact pressure, thermal conductivity and the thermal contact resistance were assumed constant with time. This assumption of constant TCR was based on the temperature range used in the simulation - for a plastic well below its glass transition temperature (100°C for polystyrene), the surface hardness of the plastic material has reached an approximately constant value, and the TCR at a constant contact pressure can be assumed to be constant with time. Thermal conductivity has been considered as a constant to reduce the computation time. It can, however, be estimated as a function of temperature (see the results and discussion on the sensitivity coefficients later). The simulation was started with an initial temperature distribution as shown in Fig. 4.7 which corresponds to actual temperature measurements in a steady state experiment. Simulation runs were carried out for several cases for the same value of  $\beta$ . Table 4.2 lists six of these runs. The prescribed temperature boundary conditions were formed from the temperatures at the two outermost nodes (at locations 1 and 8 of Fig. 4.2) from time t = 0to time t = 120 s (80s for Case 2). Figure 4.8 shows the boundary conditions corresponding to cases 1, 3-6 of Table 4.2 used in the simulation. Shown in this figure also are the components of the temperature vector  $\mathbf{T}$  generated by simulation for case 4.

## 4.6.4 Inverse Procedure Solution

The inverse method was used to estimate the value of  $\beta$  from the known initial and boundary conditions and the temperature distribution at the location of measurements for T generated from the simulation. The temperature vector T consisted of the temperatures generated at a node located at a distance of 0.002 m in the steel block from interface 1;



**Figure 4.7** Temperature distribution (at t=0s) at nodes in the numerical model of the TCR measuring apparatus. These temperatures were used as initial conditions in the solution of Eqs. (4.6) and (4.7).



**Figure 4.8** Components of vector T and temperatures at boundaries A and B (Fig. 4.2) as functions of simulation time. The temperatures at boundaries A and B were used as boundary conditions for the numerical solution of Eqs. (4.6) and (4.7).

this corresponded to the location of the thermocouple closest to the interface in the experimental apparatus. Normally distributed random noise, generated with zero mean and standard deviation as indicated in Table 4.2 was added to the temperature vector **T**. The parameter vector was initialized with a guess set of values for the optimization to commence. Each iteration of the optimization loop involved the solution of Eqs. (4.6) and (4.7) with the value of  $\beta$  at the start of the iteration. The resulting temperature distribution was used to generate the matrix **X**. A new set of parameter vector values was calculated using Eq. (4.5) at each iteration. The iteration was continued until the maximum change in any element of the parameter vector in successive iterations was less than 0.5%.

# 4.6.7 Simulation Results

Figures 4.9, 4.10 and 4.11 show the results of the inverse procedure. A total of six cases as listed in Table 4.2 were analyzed. The inverse procedure was started with a guess value of the vector  $\beta$ , as indicated in Table 4.2. The initial guess for  $\beta$  has to be a vector

Case	Simulation	Standard	Temperature	Temperature	Initial (guess)	
	Time	deviation of	drop at	drop at	value of	
	(s)	noise added	boundary A	boundary B	$\beta = \begin{bmatrix} k & R_{c1} & R_{c2} \end{bmatrix}$	
		(K)	(K)	(K)		
1	120	0	20	60	$[0.1 \ 0.001 \ 10^{-5}]$	
2	80	0.005	20	60	[0.5 0.01 0.01]	
3	120	0.005	20	60	[0.5 0.01 0.01]	
4	120	0.01	20	60	[0.5 0.01 0.01]	
5	120	· 0.01	20	60	$[0.1 \ 0.001 \ 10^{-5}]$	
6	120	0.005	10	30	$[0.1 \ 0.001 \ 10^{-5}]$	

**Table 4.2** List of various cases analyzed by the inverse procedure.

with components of order of magnitude similar to the correct solution, as discussed later. Case 1 represents the condition of no noise being added to the temperatures used to generate T. In case 2 the simulation time was reduced to 80s in an attempt to determine the minimum simulation time required to estimate the parameters by the inverse procedure. Cases 3 and 4 show the effect of varying the magnitude of noise. Cases 4 and 5 show the effect of the variation in the initial guess for  $\beta$ . Case 6 shows the effect of varying the gradient at the boundary.

Figure 4.9 shows the values of thermal conductivity component of the parameter vector for the various cases. For the noiseless case, convergence to a value of 0.169 W/m-K was obtained in 10 iterations. To determine the effect of simulation time for data with noise on the convergence of the estimation procedure, the simulation time for case 2 was set at 80s with the lowest magnitude of noise (standard deviation = 0.005 °C). The result for case 2 in Fig. 4.9 shows that the inverse procedure did not start converging even after 10 iterations and was therefore stopped. Increasing simulation time period in steps of 20s, a total simulation time of 120s was found to give satisfactory convergence. Cases 3 and 4 in Fig. 4.9 show the effect of increasing the magnitude of noise. Convergence to a value of 0.168 W/m-K was obtained in both cases in approximately 12 iterations. The number of iterations shown in the figure are greater than this value due to the rather stringent closure criteria. Case 5 shows that the procedure gave good convergence with a substantially different starting guess. Case 6 represents the estimation with a shallower gradient - convergence was again obtained in approximately 10 iterations.



Figure 4.9 Thermal conductivity of the specimen versus number of iterations for the cases in Table 4.2. Consult text for details.

Figure 4.10 shows the estimation of  $R_{c1}$  for the various cases. Convergence in the case with zero noise was obtained in about 12 iterations. Case 2, again, did not give correct estimation while the time period of 120s gave satisfactory estimates with noise in **T**. Reduction in the temperature drop at the boundary resulted in a poorer estimate (case 6).

Figure 4.11 shows the estimation of  $R_{c2}$ . For the cases 3-6, with noise in T, the estimates are better than those for Rc1. This is attributable to the larger magnitude of the TCR at interface 2 and the larger temperature drop at boundary B. Figure 4.12 shows the normalized sensitivity coefficients  $\beta_i \frac{\partial \eta_j}{\partial \beta_i}$ , for the three parameters plotted as a function of time. Results for case 4 only are plotted as the sensitivity coefficients did not show large variation in magnitude between cases 1, 3-6. Absolute values of normalized sensitivity coefficients in a well designed experiment are expected to be of the order of the maximum temperature difference in the experiment. However this criterion is not always attainable (Beck, 1988). As seen in Fig. 4.12, the maximum magnitude of the sensitivities in the present case are well below this criterion except for the thermal conductivity. Analysis of the normalized sensitivity curves shows that the curves for Rcl and  $R_{c2}$  are not correlated. Therefore the procedure has estimated two different TCR values at the two interfaces. Hence, there appears to be no need to make the assumption that the two interfaces have the same TCR (made in Jurkowski et al., 1989) as was required in our steady state procedure. It should thus be possible to study two different interfaces in a single experiment. Furthermore, the magnitudes of the sensitivities increase with the simulation time. This is due to the increasing temperature difference



Figure 4.10 Plots of thermal contact resistance,  $R_{c1}$ , versus the number of iterations for the cases in Table 4.2.  $R_{c1}$  is the TCR at interface 1 (see Fig. 4.2).



Figure 4.11 Thermal contact resistance,  $R_{c2}$ , versus the of number of iterations for the cases in Table 4.2.  $R_{c2}$  is the TCR at interface 2 (see Fig. 4.2).

between boundaries A and B with time. Increasing the temperature difference can thus lead to better results but the maximum temperature difference, particularly in the case of plastics, has to be carefully designed due to the possibility of plastic softening. The magnitudes of the normalized sensitivity of k are substantially higher than those for the TCRs (except at time t=0). Thus, the present experiment is designed more optimally with respect to the estimation of k. It should, therefore, be possible to obtain satisfactory estimates of k as a function of temperature as the inverse procedure is more sensitive to variations in k.

Figure 4.13 shows the magnitude of the objective function S at the end of each iteration step for case 4 in Table 4.2; other cases showed a similar trend. In cases 1, 3-6, estimates for k converged earlier than those for  $R_{c1}$  and  $R_{c2}$ . The initial drop in magnitude of S can therefore be associated with the estimation of k.

In these simulations, we used initial estimates (guesses) for  $\beta$  that were close to the exact solution (within one order of magnitude, or less, of the exact solution in the case of k, and two orders of magnitude in case of R<sub>c1</sub> and R<sub>c2</sub>). When the initial estimates for  $\beta$  are not that close, the value of S may increase. In such cases, the procedure was terminated when the value of S did not decrease within the next two iterations. This is one of the drawbacks of the Gauss method and Dulikravich and Martin (1997) present some hybrid strategies which can be used to overcome this defect. However, in the present study (and in many parameter estimation problems),, where the range of k and TCR values were approximately known, the Gauss method provided satisfactory estimates.



**Figure 4.12** Plot of the normalized sensitivity coefficients  $\beta_i \frac{\partial \eta_j}{\partial \beta_i}$ , for thermal conductivity and TCRs as functions of simulation time for Case 4 in Table 4.2.



Figure 4.13 A plot of the magnitude of the objective function versus the number of iterations for case 4 in Table 4.2.

The effect of the location of the temperature vector **T** node on the convergence of the estimation procedure was studied by varying the location of the node from the interface to a location at a distance of 0.002 m from the interface. This range represents a typical location of the thermocouple in the apparatus nearest to the interface. In this range, the location of this node did not affect the convergence and results similar to those in Figs. 4.9-4.11 were obtained.

To conclude, an inverse method based procedure has been developed that can be used to measure TCR from transient temperature measurements. While the method is sensitive to the noise in the measurements, it provides a means to compute TCR without having to measure the temperature of the plastic.

# **CHAPTER 5**

#### **MODELING OF EFFECTIVE TCR**

#### 5.1 Objectives

In this chapter, an analytical study is presented which leads to a mathematical model for the TCR for use in injection molding simulations. The actual effect of TCR in injection molding is highly non-linear and depends on a number of factors for which measurement techniques are yet to be developed. Therefore, some simplifying assumptions have been made in this study which allow an analytical solution. The purpose of this solution is to show the dependence of TCR on the various processing variables and material properties.

# 5.2 TCR Models from Literature

Models for TCR are available in the published literature for certain metal-metal interfaces (Antonetti et al.,1993; Clausing,1966; Cooper et al.,1969; Yovanovich,1981). The models have, in general, been derived from the concept of thermal constriction resistance in which heat is assumed to flow in *flux tubes* (similar to the concept of streamlines). At the interface the flux tubes are assumed to take a tortuous path such that the heat transfer is mainly through the actual contact spots between the two surfaces (Madhusudhana and Fletcher,1986). This assumption is valid as long as the fluid in the interstitial gap has a thermal conductivity much lower than that of the two bodies in contact, which is true for most cases. The constriction resistance is the additional resistance due to the longer path taken by the heat flux tubes. The constriction resistance is computed by assuming some regular geometry for the asperities, and by solving the heat equation for the bodies in

contact. The constriction resistance obtained for one contact is then added in parallel with the other contacts assuming a statistical distribution of the contacts. Some of the earliest solutions of this type are presented by Mikic and Rohsenow (1966) and Cooper et al.(1969). The irregular geometry of the asperities and their random distribution requires that any analytical solution be modified based on experimental data. Furthermore, the effect of contact pressure needs to be incorporated into the solution obtained purely from heat transfer considerations.

Experiments have shown that the effect of the number, distribution and shape of asperities on any surface could be related to surface profile measurements, in terms of the surface roughness, waviness and flatness. Experiments have further shown that for most metallic surfaces the asperities initially deform plastically, even for very small loads, when two surfaces are brought in contact. These two experimental observations were used to develop models that could predict the TCR for metal-metal contacts with a high degree of accuracy. One of the most widely used models is the model developed by Yovanovich (1981) and modified by Song and Yovanovich (1987) which is given by the equation

$$\frac{h_c \sigma}{(k \tan \theta)} = 1.25 \left(\frac{P}{H}\right)^{0.95}$$
(5.1)

where  $h_c$  is the contact conductance (= 1/TCR),  $\sigma$  is the root mean square (R.M.S) average of the R.M.S. roughness of the two surfaces, k is the harmonic mean thermal conductivity of the two surfaces,  $\theta$  is the included angle of the asperities and the tan $\theta$ term is obtained as the root mean square average of the slopes of the two surfaces, P is the contact pressure and H is a measure of the hardness of the harder material. The quantity H is determined from the Vickers microhardness tests by a procedure described in detail by Hegazy (1985). The model in Eq. 5.1 is a correlation for the complex analytical solution which is described by Yovanovich (1986).

Equation 5.1 is typical of the models that have been developed for TCR prediction, where the group of variables on the right form a dimensionless term called the dimensionless contact conductance  $C_c$ . Therefore the TCR models can be expressed in terms of a generalized equation of the form

$$C_{c} = A_{I} \left(\frac{P}{H}\right)^{n}$$
(5.2)

where  $A_1$  and n are constants that vary, depending on the type of interface. The above equation does not consider the heat transfer across the gaps as in many metal-metal interfaces the ratio of the heat flow through contacts to heat flow through gaps is large enough for the latter to be considered negligible. In cases where the gap heat flow is comparitively large, the total joint conductance is given by

$$\mathbf{h}_{j} = \mathbf{h}_{g} + \mathbf{h}_{c} \tag{5.3}$$

where  $h_c$  is the spot contact conductance given by Eq. 5.1 and  $h_g$  is the gap conductance given by the reciprocal of Eq. 3.4. The formulation in Eq. 5.3 assumes that the two surfaces in contact are isothermal and hence the conductances can be added in parallel using the electric analogy. The above background on the models available for TCR is then utilized in conjunction with the mechanism of TCR in injection molding to formulate a model for injection molding application.

#### 5.3 Heat Transfer Characteristics at a Plastic-Metal Interface

Before formulating the heat transfer problem, certain aspects of the heat flow at an interface between plastic and metal is presented. The study presented in this section was undertaken as the thermal conductivity of typical mold metal is high compared to that of a plastic, while its heat capacity is lower than that of a plastic. Thus the heat transfer at a plastic-metal interface can be expected to be different from that at an interface between similar materials.

For this study, a finite element analysis was performed using the software ANSYS. Due to the low thermal conductivity of plastics, the heat transfer in the plastic is mainly one dimensional while the heat transfer in the metal is three dimensional (Chiang et al.,1993). The analysis was carried out in two dimensions as the three dimensional analysis does not add to the qualitative nature of the results. Figure 5.1 shows the two dimensional mesh of two bodies in contact along an interface, used in the study. The figure shows the two bodies A1 and A2 in contact. The interface was modeled as three regions, A3, A4 and A5, of different contact resistances with the central gap (A4) having a high resistance  $(10^{-3} \text{ m}^2\text{-K/W})$  and the contacting surfaces (A3, A5) having a low contact resistance  $(10^{-4} \text{ m}^2\text{-K/W})$ . The values of the TCR selected were based on our results of gap and contact resistance obtained in chapters 3 (Fig. 3.8) and 4 (Fig. 4.4). The contact resistance was input as an equivalent thermal conductivity at the gap.

Specified Temperature Boundary



Specified Temperature Boundary

**Figure 5.1** Two dimensional finite element mesh of two bodies, A1 and A2 in contact. A3, A4 and A5 are the three sections into which the interface has been divided.

Table 5.1 Results of the FEM analysis

Case	Thermal Conductivity A1 (W/m-K)	Thermal Conductivity A2(W/m-K)	q <sub>f</sub> /q <sub>cal</sub> across A4	q <sup>f/</sup> q <sub>cal</sub> across A3,A5	$\frac{q_{cal}(A4)}{q_{cal}(A3)}$
1	20	20	0.98	1.48	0.15
2	20	0.2	0.23	1.73	0.77

•
The results of the steady state analysis, assuming constant temperature boundaries at the two ends and insulated sides, are shown in Table 5.1. The results show that for the case when materials A1 and A2 have the same high thermal conductivity, the ratio of the interface heat flux based on the FEM analysis,  $q_f$  to the heat flux computed using Eq. 5.3 (i.e. assuming the contacting surfaces were isothermal), q<sub>cal</sub>, is close to 1 (case 1 in Table 5.1) while the same ratio when material A2 has a much lower thermal conductivity, is not close to 1 (case 2 in Table 5.1). This means that the TCRs can be considered to be in parallel if the thermal conductivity of the materials is high and, hence, Eq. 5.3 gives a good estimate of the contact conductance. This, in turn, means that the surfaces in contact can be assumed to be isothermal. However, when the material on one side of the interface has a lower conductivity, then the resistances cannot be combined in the manner described. The result of case 2 in Table 5.1 also showed that the temperature on the contacting surface of material A1 varied by only 0.07% while the temperatures on the material A2 surface varied by about 8%. Thus, while the material A1 surface can be assumed to be isothermal, the surface of material A2 cannot. The other interesting result from this analysis is that in case 2 of Table 5.1, the heat flux is more uniform over the interface compared to case 1 which is seen from the ratio of the fluxes in the two regions given in the last column; ratio of nearly 1 indicates a uniform flux. On the other hand, the interfacial temperature difference is more uniform in case 1 compared to case 2.

## 5.4 Mechanism of TCR in Injection Molding

Based on the above investigations the following mechanism of TCR during injection molding processes is formulated.

As the molten plastic starts to fill the cavity it comes in contact with the cold mold walls and instantly starts to cool, forming a thin frozen layer at the surface. This layer is quite thin; its thickness at the end of the filling phase depends on the melt temperature, mold wall temperature, filling time and part geometry. The thin layer is very flexible, being above a transition temperature, and the high pressure of the still liquid polymer inside this skin layer keeps it in good contact with the mold wall. During this period, the part-mold wall interface will contain only microscopic gaps and the TCR can be said to be due to solid spot conductance (Madhusudhana, 1996). Microscopic gaps are defined here to be those of the order of the mold wall surface roughness typically of the order of 1 µm or less. Once the cavity pressure drops to atmospheric, there will be no pressure to counteract the effect of shrinkage and the plastic surface will start to pull away from the mold wall leading to the formation of *macroscopic gaps*. As the TCR will be mainly due to the constriction effect at the solid-solid contact (see Fig. 1.1(a)) its value should typically be small. This phenomenon continues beyond the filling period and into the postfilling phase because, even as the plastic cools and shrinks, more molten plastic enters the cavity due to application of hold pressure and pushes the skin layer back against the mold walls.

But once the gate (or any other section in the cavity) freezes, the part downstream of the frozen section experiences no further holding pressure and starts shrinking with no further make up flow of polymer. This causes the skin layer to pull away from the mold walls, the actual amount of separation depending on the materials pressure-volumetemperature (P-V-T) behavior of the polymer. In an ideal situation, the part should pull away uniformly on all sides and rest against the wall on only one side as dictated by gravity. In such a case, the heat transfer will be through the contact points on the one contacting surface, and through the gaps on the other five sides (assuming a box-like shape for the part).

In reality, however, the part will experience mid-plane deformation due to unbalanced cooling. Also, the gapwise shrinkage would be non-uniform due to temperature variation along the mid-plane, and the pulling away of the material from the mold wall will depend on the adhesion between the plastic and metal. The part will, therefore, make contact with the mold wall at certain points and there will be gaps over the rest of the surface. The TCR at any location on the part surface will thus depend on the nature of contact at that point. For a material with high thermal conductivity, an effective TCR can be computed by considering the gap and contact conductances to be in parallel. However, in case of low conductivity materials such as plastics, as shown in the previous section, considering the two resistances to be in parallel is only possible if the dimensions of the gaps are of a very low magnitude. If the gaps are large, then different values of TCR must be considered over different parts of the surface for an accurate estimation of the temperature profile in the plastic part. The gap conductance is strongly dependent on the gap thickness and if the gap increases with time the TCR at that location would vary significantly with time.

The above hypothesis is borne out by the results of Wang et al. (1996) who used an ultrasonic method to study the gap formation. They detected a period of good contact during the filling and initial postfilling phase followed by a period of poor contact at the location of the ultrasonic sensor. Furthermore, the period of good contact depended on the hold (or packing) pressure and lasted until the cavity pressure decayed to atmospheric. They have, however, not reported on dimensions of the gap.

The value of TCR due to solid spot conductance is expected to be of the order obtained from steady state experiments (Narh and Sridhar, 1997; Rhee et al., 1994) where the sample preparation assured essentially microscopic gaps in the interface. At the regions of macroscopic gaps, however, the TCR would be of the order shown in Fig. 3.8. This gap resistance is of considerably larger magnitude than the TCR obtained by us from steady state experiments for the plastic-metal interface. The computed gap resistance, based on the present analysis, approaches the measured TCR values reported by Yu et al. (1990).

#### 5.5 Modeling: Problem Formulation and Solution

The objective of this modeling is to obtain an analytical solution for an effective timedependent TCR at the interface of the plastic and mold in injection molding for a given planar part. A number of simplifying assumptions have to be made to obtain the analytical as against a numerical solution. The numerical solution, while capable of handling the complex shape and boundary conditions does not show the explicit relationship between the TCR and the process variables. Once such a relationship is established, the complexities due to geometry and boundary conditions can be incorporated numerically.





Figure 5.2 Deformation contour plot of a planar surface of a typical injection molded part. The deformation is in the direction perpendicular to the page and to the interface.

The assumptions made are as follows:

- (a) The TCR is derived for a planar part with uniform thickness. Figure 5.2 shows the deformation contour plot of such a part from the results of a simulation of the injection molding process.
- (b) The heat transfer is treated as a quasi-steady process and the TCR is evaluated at finite time instants. This is done as the TCR computation requires the a priori calculation of the surface deformation and the gap, which can be evaluated at specified instants in the molding cycle.
- (c) The thermal conductivity is taken to be independent of temperature.
- (d) The mold surface is considered to be isothermal; this follows from the results obtained in section 5.3.
- (e) The plastic part is considered as a semi-infinite medium. This assumption greatly simplifies the solution. The addition of the boundary conditions in the plastic only affects the functional form of the solution and this is not expected to affect the qualitative nature of the results.

The problem is then defined for the geometry shown in Figure 5.3 in which the zdirection is perpendicular to the interface. A radial coordinate system is considered because though the part geometry is rectangular the deformation profile as shown in Fig. 5.2 is circular. This is typical of the mid-plane deformation for flat parts during injection molding, and has been observed in all the models shown in chapter 3 (Figs. 3.1(a)-(e)). The governing equation to be solved is the steady state heat equation in radial coordinates

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} = 0$$
(5.4)



Figure 5.3 The geometry of the interface showing the radial coordinate system used for Eq. 5.4

Assuming a solution of the form T(r,z)=F(r) G(z), the separation of variables method gives two ordinary differential equations

$$\frac{\mathrm{d}^2 \mathrm{F}}{\mathrm{d}r^2} + \frac{1}{\mathrm{r}}\frac{\mathrm{d}\mathrm{F}}{\mathrm{d}r} + \lambda^2 \mathrm{F} = 0 \tag{5.5a}$$

$$\frac{\mathrm{d}^2 \mathrm{G}}{\mathrm{d}z^2} - \lambda^2 \mathrm{G} = 0 \tag{5.5b}$$

where  $\lambda$  is the eigenvalue. The boundary condition at z = 0 then becomes

$$-k\frac{\mathrm{dT}}{\mathrm{dz}} = \left(\frac{1}{\mathrm{R}_{i}}\right)\left(\mathrm{T} - \mathrm{T}_{\mathrm{M}}\right) = q_{i} \qquad a_{i} < r < a_{i+1} \qquad \text{and} \qquad 0 < a_{i} < b \qquad (5.6)$$

where b is the maximum value that r can take and  $T_M$  is the isothermal temperature of the mold surface. The specification of the above boundary condition divides the interface into n arbitrary annuli each with its own value of TCR, R<sub>i</sub>. Utilizing the formulation in the previous section, the TCR, R, over the regions of contact (i.e. microscopic gaps) can be considered to be constant with its value given by an equation of the form of Eq. 5.2. At regions of macroscopic gaps, R can then be calculated from the known average gap thickness for that annuli using Eq. 3.4. The solution of the above set of equations is then of the form

$$T = \sum_{i=1}^{n} \frac{(q_{i}a_{i})}{k} \int_{0}^{\infty} e^{-\lambda z} J_{0}(\lambda r) J_{1}(\lambda a_{i}) d\lambda / \lambda$$
(5.7)

where  $J_0$  and  $J_1$  are the Bessel functions of order 0 and 1 respectively, k is the material (plastic) thermal conductivity, and  $q_i$  is defined in Eq. 5.6. The evaluation of the above integral is described in Appendix C. The effective TCR for the surface is then computed by computing the average temperature,  $T_{av}$ , and the total heat flow, Q, over the region 0 < r < b, and using the equation

$$R_{c} = \frac{(T_{av} - T_{M})}{Q}$$
(5.8)

In the above equations, Eqs. 5.7 and 5.8, the effect of the material properties (i.e. the thermal conductivity, surfaces characteristics, hardness etc.) and the processing parameters is considered in terms of the evaluation of  $q_i$  which depends on the term  $R_I$  (Eq. 5.6) which in turn depends on the solid spot contact resistance equation (Eq. 5.2) and the simulation results used to calculate the gap formation.

### 5.6 Results and Discussion

Figure 5.4 shows the computed TCR using Eq. 5.8 for the geometry of the type shown in Fig. 5.2 with PS as the plastic material. The surface deformation and temperature profile was obtained by a simulation of the injection molding process using the software C-MOLD. The thickness direction gap was calculated using Eqs. 3.1-3.3, and this information was used to generate the time dependent values of the gap resistance R<sub>i</sub>. The



Figure 5.4 Results of the computation using Eq. 5.8 to calculate the TCR using deformation data from the simulation of the part shown in Fig. 5.2

solid spot contact resistance was assumed to be a constant with a value of  $6 \times 10^{-5}$  m<sup>2</sup>-K/W.

The model predictions are in line with those obtained from the gap resistance calculations shown in Chapter 3. They are also in line with the profile of the TCR measured by Yu et al. for most of the cycle time. The difference between the model results and the results of Yu et al. is in the latter stages of postfilling. The results of Yu et al. show an increasing trend even towards the end of the postfilling stage while our calculations tend towards a limiting value. The model predictions of Fig. 5.4 are in line with our simulation of the bulk temperature in the postfilling stages. According to the simulation, during the later stages of postfilling the rate of temperature drop slows down considerably. This, coupled with the fact that in most polymers the rate of increase in the specific volume is larger at higher temperatures suggests that at later stages in the postfilling stage the gap dimension should increase by a smaller amount and hence the TCR should tend towards a limiting value. The discrepancy between our results and those of Yu et al. can be explained in terms of the method used by them to measure the part surface temperature. It is likely that during the later stages of postfilling, the gap at the location where the insert was placed for the thermocouple changed to an extent that the contact between the part and insert was modified. As shown in Chapter 3, the part has a tendency to deform due to shrinkage and it is not possible to know for certain that an insert will make contact with the part surface.

A further aspect of Eq. 5.7 and 5.8 is that for parts with larger thickness, the TCR will show an increasing trend. This is because thicker parts will shrink more than thinner parts for the same bulk temperature. This is seen from Fig. 3.8, which shows that the gap

for the thicker part reaches a larger value at the end of the cycle than the thinner part. However, the part with larger thickness will show a smaller magnitude of gap at the same time from the start of the cycle. This is because the thicker part cools at a slower rate. Thus if an average TCR was to be calculated by integrating the area under the measured TCR curve of the type obtained by Yu et al., it is likely to show a smaller average TCR for a thicker part compared to a thinner part.

The model presented in Eqs. 5.6 and 5.7 shows that the effective contact resistance in injection molding is dependent on the nature of mid-plane deformation and thickness direction shrinkage, both of which are used to compute the gap; on the mold and part surface characteristics which determine the solid spot conductance of Eq. 5.3; on the thermal conductivity of the plastic (both in Eq. 5.6 and in Eq. 5.2) and thermal conductivity of the mold (appearing in Eq. 5.2). Since the shrinkage deformation is dependent on complete thermal analysis for the injection molding cycle, the effective TCR is in effect a function of all the material and process variables used in the thermal analysis. The calculation of an effective TCR is therefore a complicated procedure and a method is outlined below for this purpose.

The use of the effective TCR requires that the simulation software have the capability to take the time dependent TCR values as input. The shrinkage analysis (or simulation) is to be carried out initially with a constant value of TCR. Using the part deformation information from the analysis the first set of effective TCR can be calculated for each planar surface of the part. The simulation is performed again with the new values of TCR. It is expected that convergence to the required degree of accuracy in terms of part temperature, should be reached in a small number of iterations.

Finally, it is interesting to compare the values obtained in Figs. 3.8, 4.4 and 5.4. values with those reported by Marotta and Fletcher (1996) who obtained TCR values in the range of  $6 \times 10^{-4}$  to  $7 \times 10^{-3}$  m<sup>2</sup>-K/W for selected thermoplastics at a plastic-aluminum interface, from steady state experiments at 20-40°C, and those obtained by Yu et al. (1990) from on-line measurements during injection molding. As mentioned earlier, Marotta and Fletcher used machined plastic samples so that the resulting interface was not of the conforming nature obtained by Rhee et al. (1994), and Narh and Sridhar (1997) and, consequently, the magnitude of TCR obtained by them was much larger. Yu et al. obtained very low values of TCR correcponding to those in Fig. 4.4 during the filling and early stages of postfilling. This suggests that the TCR at non conforming surfaces, such as those obtained during the later stages of postfilling. This suggests that the TCR at none conforming surfaces, such as those obtained during the later stages of postfilling, can have much larger magnitude than the TCR measured when the plastic surface closely conforms to the metal surface.

### **CHAPTER 6**

### **CONCLUSIONS AND FUTURE WORK**

### 6.1 Conclusions

The thermal contact resistance was investigated with respect to simulation of heat transfer at plastic-metal interfaces during injection molding. Due to the inherent difficulties in measuring TCR from experiments during injection molding, the investigation was carried out using computer aided parametric study and steady state experimental measurements. The parametric study established that TCR is an important parameter to be considered in both the filling and postfilling stages of the injection molding process simulation. In particular, the magnitude of TCR affects the simulation results. During the filling stage the effect of TCR is more on the temperature distribution than the average temperature. This affects the other parameters which are computed based on the temperature distribution, such as the frozen layer fraction and velocity profile. During the postfilling stage, TCR affects mainly the bulk temperature and other averaged parameters such as average velocity, as well. The processing variable on which TCR has a major impact is the cooling time which also determines the cycle time and, hence, the part cost and process economics.

The parametric study has further established that the thickness direction shrinkage leads to the formation of a gap at the mold-plastic part interface, and that this gap increases with time. Once the dimensions of this gap become larger than the dimensions of the asperities on the mold wall/plastic part surface, the use of TCR based on steady state measurements for numerical analysis (or simulation) is no longer valid at the

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interface. The resistance computed based on this gap, the gap resistance, is of the order of magnitude of the TCR measured by Yu et al. (1990), the only data available in the literature that used on-line arrangement to measure TCR during injection molding. The similarity is all the more remarkable as transient temperature measurements, in general, are more sensitive to measurement noise and calibration accuracy (the measurement errors include lag in thermocouple readings and effect of temperature drop across the thermocouple sheath). Yu et al. have not reported on any corrections that they have made for these effects. It, therefore, appears that the gap resistance contributes significantly to the TCR during the later stages of postfilling. However, our investigations have shown that the gap formation is affected by the mid-plane deformation of the part, caused by shrinkage and warpage - due to unbalanced cooling and non-uniform shrinkage. Thus, TCR is not uniform over the entire part surface. While TCR, in general, is a parameter that is an average measure of the resistance to heat transfer across an interface, in most applications, the interface can be divided into elemental areas. The resistance to heat transfer across the interface will vary within the elemental area where each of the areas will have essentially the same contact/gap resistance. In the case of injection molding, the elemental area for computing such an averaged TCR is the entire surface of a planar part. To summarize, an experiment of the type conducted by Yu et al. will give different results if the thermocouple is placed at different locations.

The experimental study has shown that the contact resistance between the plastic and metal fall in narrow band of TCR values for the conforming, thin, thermoplastic specimen used. Furthermore, the thermal contact resistance does not show a large dependence on the contact pressure which is in line with the results of other investigators. The materials used, PS and PET, are representative of an amorphous and a semicrystalline polymer. The slow crystallization kinetics of PET sets it apart from other easily crystallizable polymers such as polypropylene (PP) or polyethylene (PE). While the results presented are for PS and PET, the data shows that no significant difference is expected in the values of TCR at interfaces of mold steel with a conforming amorphous and with a conforming crystallizable plastic surface, in terms of its effect on the simulation. The results for PET can be extended to other fast crystallizing polymers as some degree of crytallinity was obtained in the PET during the steady state experiments. Therefore, the results can be generalized to cover thermoplastics which have similar thermal and mechanical properties, such as thermal conductivity, hardness, tensile and flexural modulus and glass transition temperatures, to those used in the present work.

The model proposed for the effective TCR for use in injection molding simulation basically establishes the causality between the TCR and the various process variables and material properties. Once such a dependence is established a more accurate correlation can be determined from numerical solutions and/or experimental results. This method has been followed in case of metal-metal interface, where the analytical solution was used by Yovanovich (1981) to establish a correlation based on experimental results.

While our research focussed on the contribution of TCR to the simulation of injection molding processes, a few interesting conclusions can be drawn regarding plastic-metal interfaces in general. Combining our results with those of Marotta and Fletcher (1996), it becomes apparent that neither the elastic nor the plastic model is a good fit for TCR at thermoplastic-metal interfaces. The results of Peterson and Fletcher (1988), who obtained a good fit for thermoset plastics indicate that the higher bulk and

surface microhardness associated with thermosets may have contributed to the observed results. It, therefore, appears that TCR at thermoplastic-metal interfaces depends more on the surface waviness, and the surface roughness may not be a significant parameter in the model. Thus Eq. 5.1 can be modified by substituting a surface waviness in place of the surface roughness ( $\sigma$ ) and the bulk hardness parameter (H) to represent the surface microhardness.

Our simulation results have established that the thermal contact resistance is a significant parameter to be used in the computer simulation of an injection molding process, and use of the correct functional form will lead to improved accuracy in the prediction of such quantities as the frozen layer growth and velocity distribution in addition to the cooling time. The magnitude of TCR may be of greater significance for materials whose morphology depends on the temperature distribution during the filling and postfilling stage, such as rapidly crystallizing polymers.

#### 6.2 Recommendations for Future Work

This investigation has revealed a number of open-ended questions that require further investigation for improving not only the quality of injection molding process but also can find applications in an on-line process control and design of plastc products. Among the areas that are suggested for future research are:

(a) Study of the deformation behavior of flat and non-flat surfaces during the postfilling stage and the development of a correlation between the gap formation and the final part displacement. This may involve both computer simulation and experimental measurements.

- (b) Investigation of TCR at polymeric blends (and composites) with metal interfaces along with a more detailed study of the effects of crystallinity and anisotropy.
- (c) Experimental measurement, and comparison of TCR values for thin (thickness in the range of the present work) and thick plastic specimen (thickness > 2mm) along with measurement of surface characteristics such as roughness, waviness, flatness, bulk hardness and surface microhardness. This, along with a rigorous FEM based analysis of the effect of gap formation on heat transfer across the interface, can be used to develop a general model for TCR at plastic-metal interfaces.
- (d) Use of inverse method to determine part surface temperatures from in-situ temperature measurements in the mold, and use of this for on-line process control.

#### APPENDIX A

# UNCERTAINTY ANALYSIS FOR THE STEADY STATE EXPERIMENT

The uncertainty in the value of TCR depends on the uncertainty in the values of the measured quantities in the experiment. The quantities, besides the temperature, whose uncertainties affect the TCR values, are the specimen thickness and the location of the thermocouple. Since the TCR is computed from a set of equations, these uncertainties are propagated through the calculations. The method of Kline and McClintock (1953) has been used to determine the propagation of uncertainty (Beckwith et al. (1993).

The method is based on the assumption that uncertainties in independent variables are related to the uncertainty of the dependent variable by the statistical equation

$$\sigma_{y} = \sqrt{\sum_{i} \left(\frac{\partial y}{\partial x_{i}}\sigma_{i}\right)^{2}}$$
(A1)

where y is the independent variable,  $x_i$  are the dependent variables in a linear function y = f(x<sub>i</sub>) and  $\sigma$  is the uncertainty associated with y and x<sub>i</sub>.

For the steady state experimental procedure described in chapter 4, the uncertainty in the TCR ( $R_c$ ) is found from Eq. 4.3. The uncertainty in the total thermal resistance ( $R_t$ ,) is found using Eq. 4.2 where, again, the uncertainty in the value of the computed quantity q, the heat flux, is found by propogating the uncertainty in the temperature measurement and the location of the thermocouple through the Fourier equation

$$q = k \frac{dT}{dx}$$
(A2)

The uncertainties in the thermocouple readings were computed by a series of calibration experiments. Since the computations depend on the temperature differences, the absolute error in the thermocouple readings does not introduce any error in the value of TCR. The absolute error will be reflected in the mean interface or sample temperature reported for a particular value of TCR. The uncertainty in the TCR value is affected by the error in the temperature difference between the thermocouple readings. Hence, the thermocouples were calibrated relative to each other. This was done by taking one thermocouple as a standard and calibrating all the other seven with respect to the readings of the standard thermocouple at two standard temperatures. The standard temperatures (0°C and 80°C) were established with a calibration type mercury thermometer. The calibration was further performed with all the thermocouple leads in place and with the thermocouples connected to the PC data acquisition system to reduce the effect of system errors due to thermocouple lead resistance and capacitance, noise between adjacent leads, other electrical noises in the apparatus area and errors in the data acquisition system. The uncertainty was computed by repeated measurements at the same temperature and calculation of the deviation of the sample readings. The uncertainty was then taken to be the standard deviation computed using the Students t-distribution formula and was of the order of 0.1°C.

The uncertainty in the specimen thickness was obtained from taking five readings at different locations on the specimen surface and calculating the deviation. The uncertainty in the specimen thickness comes out to the order of 10µm. The uncertainty in the location of thermocouples was based on the least count of the dial guage used in the imeasurement and comes out to 10µm.

Using the above values of uncertainty, the uncertainty in the value of TCR was calculated from Eqs. A1. The propagation of uncertainty through Eq. A2 was done in the ordinary least squares sense as the temperature gradient was computed by a least squares fit of the thermocouple readings in the reference steel blocks. The uncertainty in the measured value of TCR comes to 20%. This value, while large compared to uncertainties reported by some investigators for TCR at metal-metal contacts (typically of the order of 5-7% and even lower in case of vacuum environment; Lambert et al. (1995)) is considered acceptable for this type of experiment (Madhusudhana, 1996; pp 74).

### APPENDIX B

# INVERSE METHOD FOR ESTIMATING PARAMETERS FROM TRANSIENT TEMPERATURE MEASUREMENT

The inverse method described in Chapter 4 provides a powerful method of estimating parameters from processes that are highly non-linear. This is true of plastics processing and particularly of injection molding where one of the key problems is the determination of the part temperature, both at the surface and at the interior. The inverse method can be applied for this problem and is outlined here for the case of the part surface temperature.

As the inverse method depends largely on the accuracy of the modeling of the process, it is important to establish the numerical model and method to be used. As seen from the FEM analysis in Chapter 3, the heat transfer in the part can be considered to be one dimensional while that in the mold is two (or three) dimensional even for the case when the TCR is varying over the interface. Thus the mid-plane mesh model used in the simulation can be expected to provide an accurate modeling of the process. This assumes that the heat loss through the ends of the part (i.e. normal to the thickness) are negligible. However, the heat transfer model has to be modified to accommodate a TCR which varies with time and location and which needs to be defined separately for the two opposite surfaces. To accomplish this the surface has to be divided into elemental areas of appropriate size and a time dependent TCR specified for each elemental area. An a priori functional form can be defined for each elemental TCR based on the results of Fig. 3.8.

The temperature measurements have to be performed at more than one location on either mold plates. Temperature measurements on either halves of the mold are required as the TCR on the two surfaces will not be identical. The thermocouples should be located as close to the internal surface of the mold as possible. A mold interior lining of a material with high diffusivity like copper or the use of an aluminum mold would increase the accuracy of the measurements as the accuracy of the inverse method is highly dependent on the degree of change in the measured variables. As seen from Fig 1.4, the variation in temperature of the steel mold surface temperature is only of the order of 10-15°C for a plastic surface temperature change of 100°C over the cycle.

The numerical method used in Chapter 4 was based on the Gauss method of minimization. However, a sequential method using function estimation procedure (Beck et al. (1986)) is likely to yield better results. The unknown parameters in this analysis would be the part surface temperature as well as the TCR.

## Listing of Computer Program

The computer program used in the inverse method described in Chapter 4, Section 4.6, is given below. The program was written in MATLAB and executed on an Unix/CDE platform.

### Main Program:

%\*\*\* Inverse TCR problem- Apparatus simulation with linear heat conduction %\*\*\* OUTER PROGRAM %\*\*\* This algorithm performs the optimization of the parameter vector %\*\*\* using the Gauss linearization method and calls 1+4 inner programs %\*\*\* for the finite difference solution of the heat equation %\*\*\* Inner programs are: cn34.m, cn34in.m, cn34bc.m, cn34props.m, cn34geo.m %\*\*\* Thermal cond, TCR are considered as constant=> conduction equation is linear %\*\*\* and the number of parameters estimated are 3

%\*\*\* parameter estimation algorithm inputs

%\*\*\* input the number of measurement points(i.e the no of tc's for eg) nt=input('no. of measurement points= '); np=input('location of thermocouple(node)= '); sig=input('std. dev. of thermocouple rdgs= ');

```
%*** input the measurement vector yvec at the 11 time points
%*** at(location) metal contact surface node
for i=1:nt
yvec(i)=res(i); %***input('input measurement vector vvec= ');
end
%*** input the coefficients eps, delb (see the sum of squares function)
eps=input('coeff eps='); %*** default eps~1
                        %*** default delb=.01
delb=input('delta b = ');
%*** finite difference model inputs
cn34geo
%*** mesh coefficients(time step size and number of nodes)
k=r^{*}(h^{2});
              m=(t/k)+1; n1=round((11/h)+1); n2=(12/h)+1;
n3=round((13/h)+1);
n=n1+n2+n3;
nk=n;
if(np=-1), np=n1; end
%***generate the matrix w=I
w=inv((sig*sig)*eye(nt));
%*** generating the parameter vector byec
              %*** p=no of temp points at which kth is defined
p=1;
               %*** if you want to change this then kth generator
              %*** in the cn34.m file also has to be changed
bvec siz=p+2; %**m;
for i=1:bvec siz
       if i \le p
       bvec(i)=.1;
       else
                             % temp removed +m
               if i \le p+1
               bvec(i)=1e-5;
               else
               bvec(i)=1.5e-4;
               end
        end
 end
 bvec=bvec';
 %*** start the parabolic equation solver
 cn34
u1=u(np,1:m); %*** saving the solution for calculating the sensitivity matrix
```

<sup>%\*\*\*</sup> note u1 is the model vector(eta)

```
%*** gauss linear optimizer
```

```
bvecd=bvec; %*** arbitrary initialisation of the closure vector
count=1
while norm(bvecd,inf)>.5e-3 %*** using the inf norm as closure condition
```

```
%*** compute X(bm)
bvec ol=bvec;
for ix=1:bvec siz
       bvec(ix)=bvec(ix)+delb*bvec(ix);
       cn34
       bvec=bvec ol;
       dudx(ix,1:m) = (u(np,1:m)-u1)/(delb*bvec(ix));
       ix
       if ix==1, d store1(count,1:m)=dudx(ix,1:m);end
       if ix==1, d store2(count,1:m)=dudx(ix,1:m);end
       if ix==1, d store3(count,1:m)=dudx(ix,1:m);end
       %pause
end
%pause
%*** compute the new iterate b
clvec=dudx*w*(yvec-u1)';
       st=1
cu1= dudx*w*dudx';
       st=2
cu2=diag(diag(cu1));
       st=3
cu=cu1+cu2;
[ll,uu]=lu(cu);
c2vec=uu\(ll\c1vec);
bvec1=bvec+eps*c2vec;
%*** closure vector = percent change of each element of bvec
for ix=1: byec siz
       if bvec1(ix) < 0, bvec1(ix) = 1e-6; end
       if bvec1(1)>1.0, bvec1(1)=.15; end
       bvecd(ix)=(bvec1(ix)-bvec(ix))/bvec(ix);
end
bvec=bvec1;
bvec store(1:bvec siz,count)=bvec;
bvec1
```

```
sos(count)=((yvec-u1)*w*(yvec-u1)');
%pause
```

```
%*** calculate new model vector with new parameter vector
cn34
u1=u(np,1:m);
%*** temp. closure for large iterates
count=count+1
if(count>20)
count
break
end
```

```
end
```

```
if count<10
    finis=1
    else
    finis=0
end
%*** plotting
i=1:n;
j=1:m;
[I,J]=meshgrid(i,j);
mesh(u);
save inverse res</pre>
```

## Subroutine CN34.m

%\*\*\* Numerical algorithm Adjustable implicit scheme for the heat equation

```
%*** dirichlet b. conditions both ends(prescribed temp)
%*** Finite difference for dbc simulation of TCR apparatus
%*** 3 layer set with TCR at the interface
*****
%*** initial condition: u=cn34in (ie in the m file)
%*** boundary conditions: u(1,t)=from cn34bc.m
%***
             u(n,t)=from cn34bc.m
%*** NOTE: 1.program modified and is NO LONGER in dimensionless co-ords
%***
       2.using central differences for the neumann boundary
0/0***
      3.heat flow from lh to rh is positive
******
%*** This program is called from inv1. ic's, bc's and geometry are read only
%*** once in inv1. props file is read in this section during each iteration
******
```

%\*\*\* properties for the finite difference model

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```
%*** boundary conditions
f6r j=2:m
       cn34bc;
end
%*** init conditions
for i=1:nk
       if(i==1), ii=1; end
       if(i==n1+1), ii=1; end
       if(i=n1+n2+1), ii=1; end
       cn34in;
                              %*** change this func for diff init c.
       ii=ii+1;
end
%*** coefficients in the iteration are now to be calculated in the time loop
for j=2:m
       for i=2:nk-1
               ui=u(i,j-1);
               p1=21-floor(ui-80);%assuming kth2 is from 80 to 100 deg C
               \%if p1<=0,
               p1=1; %end
               if i>n1
                      if i \leq n1+n2
                      kth(i)=kth2(p1); %** +((kth2(p1)-kth2(p1+1))*(ui-(80+p1)));
                      diff(i)=kth(i)/(rho2*cp2);
                      end
               end
               if i==2;
                      a(i)=diff(i)*r*theta; b(i)=-(2*diff(i)*r*theta+1);
                      c(i)=diff(i)*r*theta;
                      al(i)=-diff(i)*r*thetab; b1(i)=2*diff(i)*r*thetab-1;
                      c1(i)=-diff(i)*r*thetab;
                      alph(i)=b(i);
       elseif i==n1;
               a(i)=2*diff(i)*r;
                                     b(i) = -(2*diff(i)*r+(2*k/(rho1*cp1*h*rc1))+1);
               c(i)=(2*k/(rho1*cp1*h*rc1));
               a1(i)=0;
                                     b1(i)=-1;
                                                                   c1(i)=0;
               alph(i)=b(i)-(a(i)*c(i-1)/alph(i-1));
       elseif i = (n1+1);
```

ch34props1

```
a(i)=(2*k/(rho2*cp2*h*rc1));b(i)=-
(2*diff(i)*r+(2*k/(rho2*cp2*h*rc1))+1);
               c(i)=2*diff(i)*r;
               a1(i)=0;
                                      b1(i)=-1;
                                                                    c1(i)=0;
               alph(i)=b(i)-(a(i)*c(i-1)/alph(i-1));
       elseif i==n1+n2;
               a(i)=2*diff(i)*r;
                                      b(i) = -(2*diff(i)*r+(2*k/(rho2*cp2*h*rc2))+1);
               c(i)=(2*k/(rho2*cp2*h*rc2));
               a1(i)=0;
                                      b1(i)=-1;
                                                                    c1(i)=0;
               alph(i)=b(i)-(a(i)*c(i-1)/alph(i-1));
       elseif i = (n1+n2+1);
               a(i)=(2*k/(rho1*cp1*h*rc2)); b(i)=-
(2*diff(i)*r+(2*k/(rho1*cp1*h*rc2))+1);
               c(i)=2*diff(i)*r;
               a1(i)=0;
                                      b1(i)=-1;
                                                                     c1(i)=0;
               alph(i)=b(i)-(a(i)*c(i-1)/alph(i-1));
               else
                       a(i)=diff(i)*r*theta; b(i)=-(2*diff(i)*r*theta+1);
                       c(i)=diff(i)*r*theta;
                       a1(i)=-diff(i)*r*thetab; b1(i)=2*diff(i)*r*thetab-1;
                       cl(i)=-diff(i)*r*thetab;
                       alph(i)=b(i)-(a(i)*c(i-1)/alph(i-1));
```

end

end

 $\%^{***}$  solve for each time step

# %j

i=2; %\*\*\* first calculate vector s (forward elimination) d(i)=a1(i)\*u(i-1,j-1)+b1(i)\*u(i,j-1)+c1(i)\*u(i+1,j-1)-a(i)\*u(i-1,j); s(i)=d(i);

```
for i=3:nk-1

d(i)=a1(i)*u(i-1,j-1)+b1(i)*u(i,j-1)+c1(i)*u(i+1,j-1);

s(i)=d(i)-(s(i-1)*a(i)/alph(i-1));

end
```

%\*\*\* next calculate solution vector u (backward substitution) for i=n-1:-1:2

$$u(i,j)=(s(i)-c(i)*u(i+1,j))/alph(i);$$

end

# Subroutine CN34bc.m

end

% \*\*\*Numerical Algorithm Boundary conditions file for algorithm in cn34.m

% \*\*\*note that the value of i,j are passed from the calling program

u(1,j)=85.7973-25\*((j-1)/(m-1));u(n,j)=81.984-12\*((j-1)/(m-1));

% u(1,j)=60;% u(n,j)=60;

% u(1,j)=ft(j);% u(n,j)=fb(j);

### Subroutine CN34in.m

% \*\*\* Numerical algorithm Initial conditions file for algorithm in cn34.m % \*\*\*note: the calling is for each initial mesh step- ie value of i % \*\*\*is from the calling program

%if i==2 %x=(asin(u(1,1)))/pi; ik=(x/h); end %u(i,1)= sin(pi\*(ik+i-1)\*h); % sinusoidal initial condition

```
%u(i,1)=1+(1-((i-((n-1)/2)-1)*h/2)^2)^.5;
%u(i,1)=1-(.5*(i-1)*h) %linear ramp initial condition
%u(i,1)=80+((85-80)/(n-1))*(i-1); %another ramp
%u(i,1)=100; %initial constant temperature condition
```

```
if(i \le n1)
```

```
u(i,1)=ict(ii);
end
if(i>n1)
if(i<=n1+n2)
u(i,1)=ics(ii);
end
end
if(i>n1+n2)
u(i,1)=icb(ii);
```

end

# Subroutine CN34props.m

%\*\*\* Numerical algorithm... Properties file for algorithm in cn34.m

rho1=7820; cp1=460; kth1=36.5; diff1=kth1/(rho1\*cp1); rho2=950; cp2=1700; kth2(1:p)=bvec(1:p); %\* diff2=kth2/(rho2\*cp2); %\*\*\* diff for the sandwich region is defined in cn34.m rho3=7820; cp3=460; kth3=36.5; diff3=kth3/(rho3\*cp3); theta=.5; thetab=1-theta; %\*\*\* default implicitness rc1=bvec(p+1); rc2=bvec(p+2);%\*\*\* NOTE: rc cannot have a value of 0

for i=	1:nk			
	if i<=n1	diff(i)=diff1;	kth(i)=kth1;	end
	%if i>=n1+1			
	%if i<=n2	diff(i)=diff2;	kth(i)=kth2;	end
	%end			
	if $i \ge n1 + n2 + 1 \operatorname{diff}(i) = \operatorname{diff3};$		kth(i)=kth3;	end
and d				

end

# Subroutine CN34geo.m

%\*\*\* Numerical algorithm Geometry and mesh inputs file for algorithm in cn34.m

geo=input('use default geometry? 1-yes, 0-no ');

if geo==0 l1=input('length of 1st section l1='); l2=input('length of 2nd section l2='); l3=input('length of 3rd section l3='); else l1=.0202; l2=.0009; l3=.0202; end

mes=input('use default mesh coefficients? 1-yes, 0-no ');

if mes==0
 t=input('time scale t = ');
 h=input('space step h = '); r=input('ratio r = ');
else
 t=150; h=1e-4; r=1e8;
end

## APPENDIX C

### **EVALUATION OF INTEGRAL IN EQUATION 5.7**

Equation 5.7 is given in the integral form, as evaluation of integrals containing Bessel Functions is not always a straightforward procedure. However in the present case the integral permits an analytical evaluation for the calculation of the average surface temperature of the plastic surface, as given in this appendix. The integral form of Eq. (5.7) is

$$T = \sum_{i=1}^{n} \frac{(q_i a_i)}{k} \int_{0}^{\infty} e^{-\lambda z} J_0(\lambda r) J_1(\lambda a_i) d\lambda / \lambda$$
(C1)

The average temperature of the surface, over the interval 0 < r < b (refer Fig. 5.3) is then given by

$$T_{av} = \sum_{i=1}^{n} \frac{1}{\pi b^2} \frac{(q_i a_i)}{k} \int_{0}^{b} \int_{0}^{c} (e^{-\lambda z} J_0(\lambda r) J_1(\lambda a_i) d\lambda / \lambda) 2\pi r dr$$
(C2)

where  $T_{av}$  is the average temperature. The average temperature at the surface is then given by setting z = 0 which removes the exponential term in the integral

$$T_{av} = \sum_{i=1}^{n} \frac{1}{\pi b^2} \frac{(q_i a_i)}{k} \int_{0}^{b} \frac{J_i(\lambda a_i)}{\lambda} \int_{0}^{c} (J_0(\lambda r) d\lambda) 2\pi r dr$$
(C3)

Interchanging the order of integration leads to

$$T_{av} = \sum_{i=1}^{n} \frac{1}{\pi b^{2}} \frac{(q_{i}a_{i})}{k} \int_{0}^{\infty} \frac{J_{1}(\lambda a_{i})}{\lambda} \left( \int_{0}^{b} (J_{0}(\lambda r) r dr) \right) 2\pi d\lambda$$
(C4)

Simplifying further

$$T_{av} = \sum_{i=1}^{n} \frac{2}{b^2} \frac{(q_i a_i)}{k} \int_{0}^{\infty} \frac{J_i(\lambda a_i)}{\lambda} \left( \int_{0}^{b} (J_0(\lambda r) r dr) \right) d\lambda$$
(C5)

The following identity results in evaluation of the inner integral

$$\int_{0}^{b} \left( J_{0}(\lambda r) r dr \right) = \frac{b J_{1}(\lambda b)}{\lambda}$$
(C6)

And hence Eq. (C5) becomes

$$T_{av} = \sum_{i=1}^{n} \frac{2}{b^2} \frac{(q_i a_i)}{k} \int_{0}^{\infty} \frac{J_1(\lambda a_i)}{\lambda} \frac{bJ_1(\lambda b)}{\lambda} d\lambda$$

or

$$T_{av} = \sum_{i=1}^{n} \frac{2}{b^2} \frac{(q_i a_i)}{k} \int_{0}^{\infty} \frac{J_1(\lambda a_i) b J_1(\lambda b)}{\lambda^2} d\lambda$$
(C7)

The infinite integral in the above equation can be represented in the form of Gamma and Hypergeometric functions, using the following relations available in the tables of integrals (Abramowitz and Stegun, 1964; pp487)

$$\int_{0}^{\infty} \frac{J_{\mu}(\lambda a) b J_{\nu}(\lambda b)}{\lambda^{n}} d\lambda = \frac{a^{\mu} \Gamma\left(\frac{\mu + \nu - n + 1}{2}\right)}{2^{n} b^{\mu - n + 1} \Gamma(\mu + 1) \Gamma\left(\frac{\nu - \mu + n + 1}{2}\right)} \Lambda$$
(C8)

where  $\Gamma$  is the Gamma function and the last term is a Hypergeometric function given as

$$\Lambda = {}_{s}F_{1}\left(\frac{\mu + \nu - n + 1}{2}, \frac{\mu - \nu - n + 1}{2}; \mu + 1; \frac{a^{2}}{b^{2}}\right)$$
(C9)

In general the Hypergeometric functions obey the following relations which are useful in simplifying the above expressions (the following relations also indicate the terminology used in defining Hypergeometric functions)

1. F(a,b;c;z) = F(b,a;c;z)

2. 
$$F(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b) \Gamma(c-b)} \int_{0}^{1} t^{b-1} (1-t)^{c-b-1} (1-tz)^{-a} dt$$
for Re (c) > Re (b) > 0

('Re' stands for the real part of the variable c and b)

Using Eqs. (C8) and (C9) and the above two identities for the hypergeometric function, the Eq. (C7) can be rewritten as

$$T_{av} = \sum_{i}^{n} \frac{q_{i}a_{i}}{bk} \left( \frac{a_{i}\Gamma\left(\frac{1+1-2+1}{2}\right)}{2^{2}b^{1-2+1}\Gamma(1+1)\Gamma\left(1-1+2+\frac{1}{2}\right)} \right)$$

$${}_{2}F_{i}\left(\frac{1+1-2+1}{2}, \frac{1-1-2+1}{2}; 1+1; \frac{a_{i}^{2}}{b^{2}}\right)$$
(C10)

which, on simplification leads to

$$T_{av} = \sum_{i}^{n} \frac{q_{i}a_{i}}{bk} \left( \frac{a_{i}\Gamma\left(\frac{1}{2}\right)}{4b^{o}\Gamma(2)\Gamma\left(\frac{3}{2}\right)} \right) \left( {}_{2}F_{i}\left(\frac{1}{2}, \frac{-1}{2}; 2; \frac{a_{i}^{2}}{b^{2}}\right) \right)$$

or

$$T_{av} = \sum_{i}^{n} \frac{q_{i}a_{i}}{bk} \left( \frac{a_{i}\Gamma\left(\frac{1}{2}\right)}{4\Gamma(2)\Gamma\left(\frac{3}{2}\right)} \right) \left( {}_{2}F_{i}\left(\frac{1}{2}, \frac{-1}{2}; 2; \frac{a_{i}^{2}}{b^{2}}\right) \right)$$
(C11)

Using the second relation for Hypergeometric functions given previously, the hypergeometric function in Eq. (C11) can be evaluated using the following expression

$${}_{2}F_{1}\left(\frac{1}{2}, \frac{-1}{2}; 2; \frac{a_{i}^{2}}{b^{2}}\right) = \frac{\Gamma(2)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{3}{2}\right)^{0}} \int_{0}^{1} t^{\frac{1}{2}-1} (1-t)^{2-\frac{1}{2}-1} (1-t)^{-\frac{1}{2}} dt$$
(C12)

Note that in the above expression, t is a dummy variable used for the integration. The integral on the RHS can be evaluated both numerically and analytically. The above

derivation shows the complexity involved in evaluating the integral even for the case where a number of simplifying assumptions had been made while obtaining the model.

•

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