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# Thermal contact resistance in micromoulding

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## Abstract

This work outlines a novel approach for determining thermal contact resistance (TCR) in micromoulding. The proposed technique aims to produce TCR predictions with known confidence values and combines experimental evidence (temperature fields and contact angle measurements) with various mathematical modelling procedures (parametric representation of surfaces, finite element analysis and stochastic processes). Here, emphasis is made on the mathematical aspects of the project. In particular, we focus on the description of the parametric surface representation technique based on the use of partial differential equations, known as the PDE method, which will be responsible for characterizing and compressing micro features in either moulds or surface tools.

## 1 Introduction

The advances recently achieved on computer simulation of polymer processes are considerable. These include an improved understanding of the mechanical behaviour of polymer melts and the successful development of commercially available simulation software packages such as Autodesk Moldflow.

Nevertheless, there are areas in which the advances have not been as significant as required to fully understand and characterize polymer processes. In particular, the interface between the polymer and the process tooling, which is generally a metal/polymer interface and is mainly governed by heat transfer effects: the polymer melt is generally cooled when contacting a metal surface and, the flow characteristics together with morphology development are considerably influenced during the entire process. These phenomena are highly relevant to processes with big surface area to volume ratios, among which are thin-walled moulding and moulding of micro scale features and geometries. Here, the observed surface area to volume ratio of the components presents a tendency to be higher than those associated with conventional moulding.

Thermal Contact Resistance (TCR), or conductance, results from imperfections in the surfaces when two solids surfaces are brought in contact. This resistance generally depends on the applied pressure, which leads to the compression of asperities in the surface and therefore increases the true area of contact. TCR in processes such as injection moulding is known to be complex not constant with time over the whole process and depend on the temperature and the pressure. This has been experimentally demonstrated using infra red probes [1, 2]. However, software simulation packages compute temperature changes assuming a negligible or constant TCR [3]. This obviously leads to inaccurate results when simulating injection moulding processes at a design stage.

Thus, a truly predictive and more reliable simulation of melt processing is highly desirable and must include contact effects pertaining to the polymer/tool surface interaction. We propose to develop a mathematical model and support it with experimental evidence for characterizing TCR. Consequently, the project is divided into several stages of development in both the experimental and the mathematical modelling. The experimental stages include:

**Experimental measurement of thermal and surface properties**. A Battenfeld Microsystem 50 micro injection moulding machine (Figure 1 (a)) will be used to investigate cooling behaviour of polymer melts using an optimised injection mould tool design. A series of experiments will be performed whereby the cooling process behaviour is influenced by factors such as injection pressure, melt and mould temperatures and surface structure. Thermal measurements on filling moulds using tailored sapphire surfaces (sapphire was chosen due to its physical properties), and the associated calculation of TCR.

**Polymer melt contact angle measurements**. Contact angle measurements of molten polymer droplets resting on appropriate substrates will be made to generate data on the work of adhesion, required for the complete description of the heat transfer model. Optical measurements will be made on polymer droplets within a heated chamber, using  a First Ten Angstroms FTA 1000 Class B drop shape analysis system as the one shown in Figure 1 (b).


(a) (b)

Figure 1: Battenfeld 50, micromoulding machine (a), FTA 1000 Class B, drop shape analysis system (b).

**Development and realisation of an experimental set-up for capturing the effects of tool surface**. Calibration and real tool mimic surfaces will be designed to generate predictable levels of contact during the moulding process at intermediate pressures. Both types of surfaces are expected to be composed of 3D structures presenting nano and micro scale features, with surface quality better than 10 nm for the calibration surfaces, whilst the roughness of the mimicking ones is expected to vary from 0.07 - 1.5 µm Ra. A technology for 3D Focus Ion Beam (FIB) machining developed in [4, 5] is used to fabricate such surfaces in sapphire workpieces.

The mathematical aspect of the project is mainly divided into three stages. These are:

**Efficient representation of surface topography through the PDE method**. A surface generation technique based on the use of partial differential equations (PDEs), known as the PDE method will be used to produce geometric representations of the mould surfaces. This surface generation technique has been recently developed as a tool of polymer surface characterization [6, 7] by associating key design parameters with the coefficients describing the analytic representation of the corresponding PDE-based surface. Thus, the representations of tailored sapphire surfaces will be used directly to generate meshed surfaces suitable for analysis. However, processing tool surfaces are in practice subject to statistical variation, and therefore, appropriate statistics that relate to the surface features will be gathered from the PDE-based surface data.

These data is obtained from characterizing a number of samples for each surface type, which can generate surfaces stochastically, with predetermined statistical distributions of parameters, using a Monte Carlo approach. The resulting PDE-based surfaces are used in the finite element model.

**Development of a finite element (FE) model for contact and heat transfer**. A three-dimensional finite element model of heat flow at the interface, using stochastically generated surfaces, to produce representative (ensemble average) TCR values for given melt temperature, melt pressure and time will be developed using Abaqus.

The physical phenomena involved in the contact process include wall friction and slip [8], surface tension and surface energy of the polymer melt [9]. The contacting polymer melt must realistically respond to the filling pressure by conforming, with an increasing proportion of the rigid surface (tool or mould surface). The heat transfer mechanism will be assumed to be conduction both at contact points and air-filled gaps (which are small enough so that convection effects in them can be ignored). Radiation across gaps will be neglected as the temperatures are assumed to be less than 700K [10].

The use of coupled thermal/mechanical analyses will be essential, and will require temperature-dependent properties as input data. For the sake of efficiency, the models will be as small as possible. Models of irregular surfaces need to be of sufficient size for all the physical effects to be represented. The dimension normal to the surface must be sufficient to give a valid coupled thermal/ mechanical analysis. The mechanical model will be verified by comparison of predictions of the contact area with the experimental results.

**Demonstration of the new techniques within a process modelling environment**. Once the model has been developed, it will be coded in a high-level language. The subroutine will be implemented within Autodesk Moldflow and applied to a number of benchmark problems, both in micromoulding and at a larger scale and the simulation results will be compared against the corresponding experimental set up.

## 2 Mathematical foundations of the PDE method

The PDE method was firstly applied to the area of computer aided geo- metric design as a technique suitable for blending surfaces [11] and its use has expanded to different areas and applications. This technique regards parametric surface representations of objects as the graphic representation of the solution to an elliptic PDE (the Laplace and the Biharmonic equations fall into this category). Thus, shape representation is transformed into a boundary-value problem whereby relevant features associated with a given geometry are described by the boundary conditions responsible for finding a unique solution to the PDE. The general form of an elliptic PDE over a two-dimensional parametric domain is given by

$$\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}\right)^{2n} \mathbf{X}(u, v) = 0\,, \tag{1}$$

where $u$ and $v$ are the parametric surface coordinates, which are then mapped into the physical space; that is, $X(u, v) = (x(u, v), y(u, v), z(u, v))$. The order of the PDE is represented by $2n$.

A closed form analytic solution to Equation (1) can be found when the boundary conditions and the parametric domain are restricted to some conditions. Such a solution is given in terms of an infinite series, and for computational purposes, needs to be approximated by a finite one whereby the first N terms are considered and a remainder term, responsible for satisfying the boundary conditions exactly, is introduced. The approximation is given by,

$$\mathbf{X}(u, v) = \mathbf{A_0}(u) + \sum_{n=1}^{N} [\mathbf{A_n} \cos(nv) + \mathbf{B_n} \sin(nv)] + \mathbf{R}(u, v)\,, \tag{2}$$

where the vector-value polynomials $\mathbf{A_0}(u)$, $\mathbf{A_n}(u)$, $\mathbf{B_n}(u)$ and the remainder term $\mathbf{R}(u, v)$ (when the order of the PDE is equal to 4) are determined by

$$\mathbf{A_0}(u) = \mathbf{a_{00}} + \mathbf{a_{01}}u + \mathbf{a_{02}}u^2 + \mathbf{a_{03}}u^3\,, \tag{3}$$

$$\mathbf{A_n}(u) = (\mathbf{a_{n1}} + \mathbf{a_{n3}}u)\, e^{anu} + (\mathbf{a_{n2}} + \mathbf{a_{n4}}u)\, e^{-anu}\,, \tag{4}$$

$$\mathbf{B_n}(u) = (\mathbf{b_{n1}} + \mathbf{b_{n3}}u)\, e^{anu} + (\mathbf{b_{n2}} + \mathbf{b_{n4}}u)\, e^{-anu}\,, \tag{5}$$

$$\mathbf{R}(u, v) = \mathbf{r_1}(v)e^{wu} + \mathbf{r_2}(v)e^{-wu} + \mathbf{r_3}(v)ue^{wu} + \mathbf{r_4}(v)ue^{-wu}\,. \tag{6}$$

The value of the constant vectors $\mathbf{a}_{ij}$, $\mathbf{b}_{ij}$, and $\mathbf{r}_i(v)$ are determined by the specified boundary conditions, and the value of w has been conveniently chosen as $w = a(N + 1)$.

In summary, the PDE method offers analytic surface representations of complex geometries via a well defined mathematical function. This provides a mechanism for compressing massive data sets whilst providing the possibility of reproducing the characterized data set at different levels of detail by simply changing the resolution with which the parametric domain is discretized. Further details on the PDE method can be found in [11, 7].

Examples of the different PDE-based surface representations are shown in Figure 2. The boundary curves used to solve the boundary-value problem are shown at the left of each respective surface. These examples correspond to some of the surface features analyzed in [7].

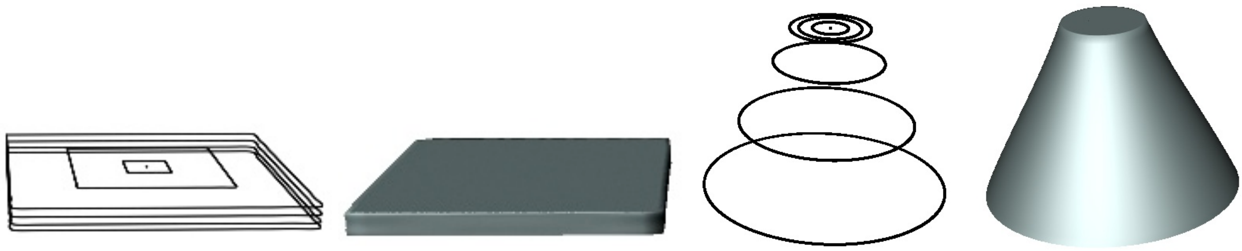

Figure 2: PDE-based surface representations of various objects. The boundary curves are outlined at the left whereas the corresponding PDE surface is shown at the right in each case, extracted from [7].

For the purposes of illustrating the procedure with which the PDE method is used for characterizing surfaces typically encountered in polymer processes, experimental data obtained using Atomic Force Microscopy (AFM) corresponding to a 30 nm thick layer of poly(N-isopropylacrylamide), on a Sylgard (TM) silicone elastomer substrate (PNIPA surface henceforth) has been described as a PDE-based surface [7]. The boundary curves required have been extracted so that the entire profile is described. This helps to preserve the original features of such a profile . Thus, a total of 31 curves were extracted equidistantly along the profile. This set of curves gives rise to a PDE-based surface representation composed of the solution to 10 different PDEs (this is explained in more detail in [7]).

Figure 3 presents the AFM data set representing a PNIPA surface (a), the corresponding boundary curves (b) and the resulting PDE-based surface representation (c). The surface area of the PDE-based representation has been found using numerical techniques and has been found equal to 6.07 x 108 nm2. Thus, the PDE method has proven to be useful for characterizing important physical properties of complex profiles for which their surface area can be accurately quantified. Furthermore, these results suggested the PDE method could potentially provide excellent means for multi-scale analyses of more complex surface profiles.

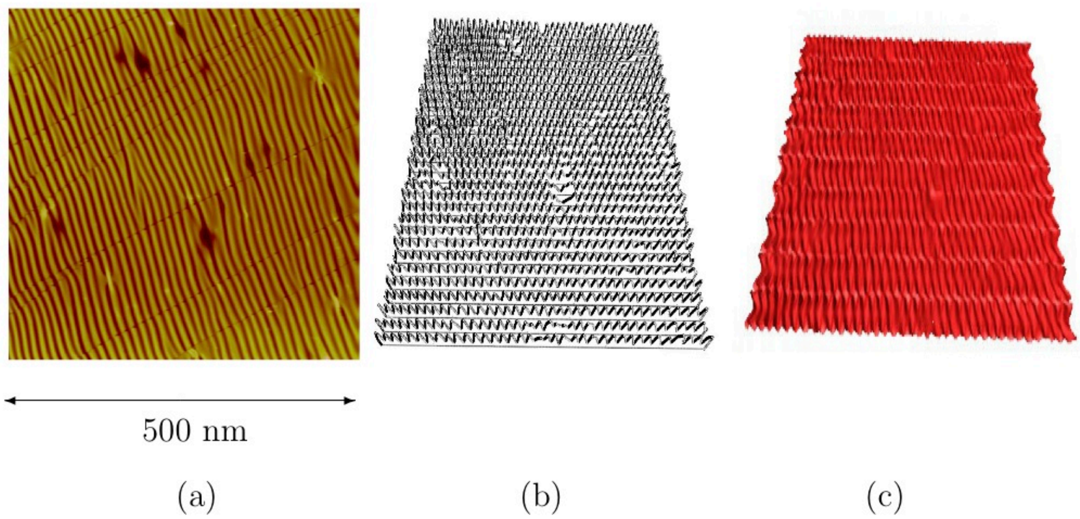


Figure 3: Experimental data obtained using atomic force microscopy rep- resenting a PNIPA surface (a), the extracted boundary curves (b) and the resulting PDE-surface representation (c).

The examples presented so far have aimed to illustrate the underlying procedure associated with the PDE method. Next, a set of preliminary results pertaining to typical tool surfaces are described.

## 3 Preliminary results

Experimental data describing the surface profile of a steel tool surface has been obtained using white light interferometry (WLI). A two-dimensional representation of such data is presented in Figure 4. It is often the case that when using WLI, the height of some points in the square grid is undefined. The height of the undefined points has been determined by using a biharmonic average of the neighbouring points. Afterwards, a full three-dimensional representation of such a profile was then produced in the form of a point cloud. A total of 97 boundary curves were extracted from such a point cloud leading to a PDE-based surface representation composed of 31 different PDEs.

Figure 5 shows the three-dimensional representation of such a point cloud (a), the corresponding extracted boundary curves (b) and the resulting PDE- based surface representation (c). It must be stressed that PDE-based surface representation has been obtained using a resolution similar to the original one and that the compression ratio is approximately 70%.

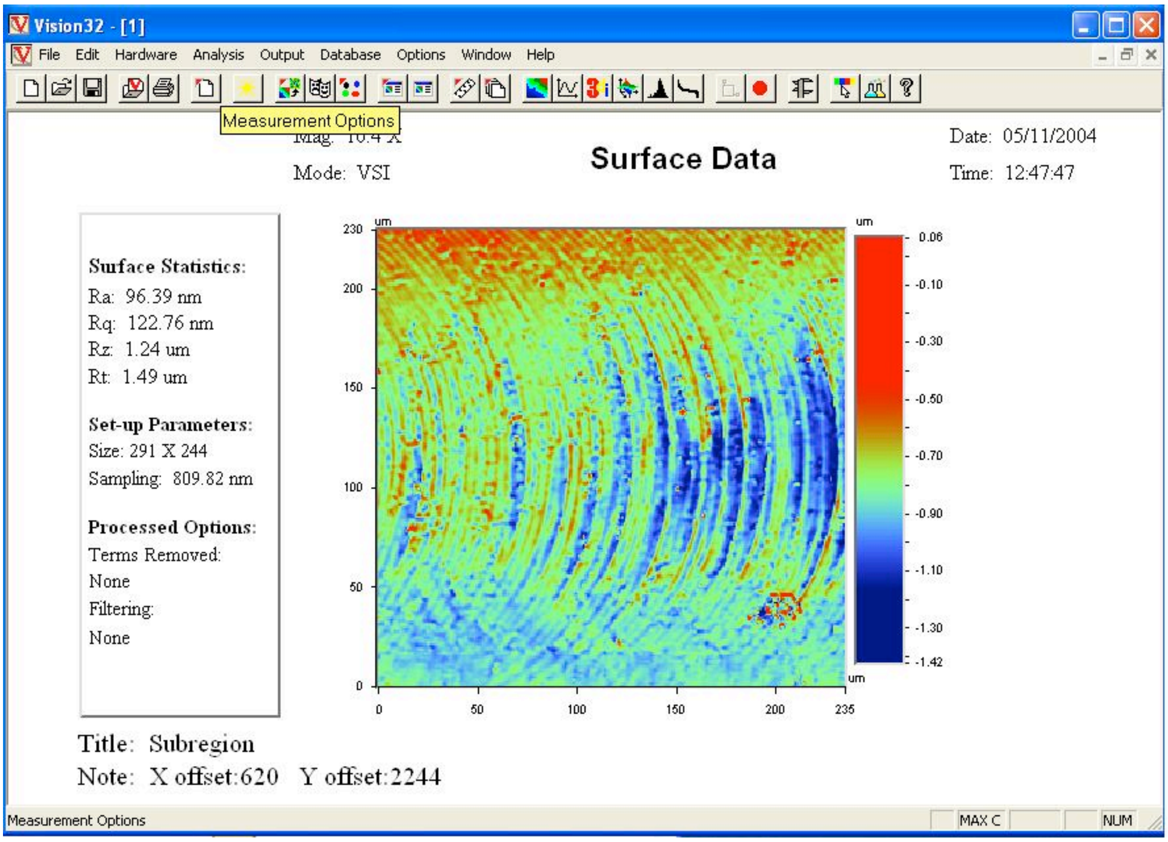


Figure 4: Two-dimensional representation of a steel tool surface.

## 4 Discussion

The compression ratio could be potentially improved by describing the remainder term as a piecewise polynomial functions and also by taking into consideration that for the purposes of this work we are exclusively interested in describing the surface height; that is, a third of the information related to the PDE surface representation is required. A different PDE surface representation with a much lower resolution has been used to create a finite element solid representation of the tool surface and was used to solve the heat transfer problem in Abaqus. However, the correct material properties used in the solution remain to be determined and therefore, the results associated with this stage of the project are left to be presented at a later stage. In principle we have all the necessary mathematical tools for developing an algorithm capable of producing random surfaces. Notwithstanding careful considerations regarding the overall continuity of such surfaces should be made.

Figure 5: Three-dimensional point cloud associated with the profile of a steel tool surface (a), the extracted boundary curves (b) and the resulting PDE-based surface representation (c).

## 5 Conclusions

A general overview of a methodology combining mathematical modelling and experimental work for determining thermal contact resistance has been given. This work focuses on outlining the mathematical details of the surface characterization method, the PDE method, used to represent mould cavities and tool surfaces. The compressing capability and the analytic parametrization of complex surfaces offered by the PDE method facilitate the generation of finite element solid models at different levels of detail and also enable the possibility of producing random surfaces with an stochastic distribution of surface features commonly found in micromoulding. The project is at an early development stage and preliminary results obtained to date in surface characterization are presented.

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