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INVERSE HEAT TRANSFER ANALYSIS IN A POLYMER MELT FLOW WITHIN AN EXTRUSION DIE

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ABSTRACT

In forming processes like extrusion of polymer, the temperature profile in the polymer melt flow through the die can be quite sharp, due to high viscous dissipation and very low heat conductivity. To predict accurately the temperature rise, the inlet temperature profile has to be taken into account. It is generally unknown because for such creeping flow the temperature field is affected far downstream from the entrance of the die.

This numerical study aims to restore the temperature field within the polymer from temperature measurements taken inside the die. The polymer flow is assumed to be an incompressible steady laminar flow of a Newtonian fluid. The numerical solution of the inverse problem is computed by using a classical **C**onjugate **G**radient **M**ethod.

The analysis is important to decide of the location of the thermocouples in an experimental die. The feasibility of restoring the temperature profile is illustrated for different thermal and flow conditions.

NOMENCLATURE

u, w : Axial and radial velocity	T : Temperature
K : Consistence of fluid	U : Velocity
p^n : Direction of descent	Greek symbols :
J : Functional to be minimised	Ψ : Adjoint variable
c_p : Heat capacity	ρ : Density
$T_0(z)$: Inlet temperature	η_a : Dynamic viscosity
$\widetilde{Y}$: Measured temperatures	θ : sensitivity variable
Ns : Number of sensors	$\dot{\gamma}$: Shear rate
$F(T)$: Source term	α : Thermal diffusivity
	subscripts :
	w : wall
	f : fluid

NTRODUCTION

The extrusion process for plastic materials, consists usually of three sections: the feeding, conveying, and metering. In the metering section, the material is heated, pressured and homogenized [1]. The final product is obtained by pushing the molten material through the extrusion die. In order to obtain desired product quality and characteristics, the knowledge of the inlet thermal state of the die is very important. In order to perform a numerical simulation of polymer flows and heat transfer in the extrusion dies one has to specify inlet boundary conditions, which are generally unknown. Fortunately, for such a creeping flow the developing area for velocity field is very short. The inlet velocity profile could be chosen like fully developed. On the contrary, the inlet temperature profile develops quite slowly and affects temperature field far downstream. The problem which aims to specify the inlet temperature profile is referred to as a boundary inverse heat transfer problem, it belongs to the inverse heat conduction problems (IHCP) groups, which were considered by O. Alifanov [2], J.V. Beck [3] and others. These problems are known to be ill-posed, in contrast to the direct heat conduction problems (DHCP), The problem stated above is the problem of the initial temperature profile restoration. Whilst velocity field is known one could expect the uniqueness of the problem solution. If velocity field does not depend on temperature field, this equation is linear or quasi-linear. There are several reports on this subjects, for example: P. T. Hsu, &al. [4] A. J Silva Neto and M. N. Özizik, [5] estimated the inlet temperature profile in the laminar duct flow. Subsequent investigations by J.C. Bokar, and M. N. Özizik, [6]. C.H. Huaug and M.N. Özizik [7], H. A. Machado, and H. R. B. Orland, [8] examined various aspects of this problem, etc. Recently, Hsu et al. [9] presented a two-dimensional inverse least-squares method to estimate both inlet temperature and wall heat flux in a steady laminar flow in a circular duct. Ch.-H. Huang and W.-Ch. Chen [10] have solved a non-stationary Navier-Stokes equation, to provide coefficients for energy equation, but the velocity field itself does not depend on temperature. Among forced convection flows, the flow of complex fluid in a narrow channel is obviously the case when coupling between temperature field and velocity field may be very essential, because its viscosity strongly depends on temperature.

In the present study, a two-dimensional conjugate heat transfer model has been developed for a Newtonian and pseudo-plastic materials being processed in the extrusion die. The governing equations for the fluid and wall regions are solved at the same times, by using a finite volume numerical method (Aquilon) [11]. An iterative numerical procedure is used to solve the direct, adjoint and sensitivity problem.

DIRECT PROBLEM EQUATIONS

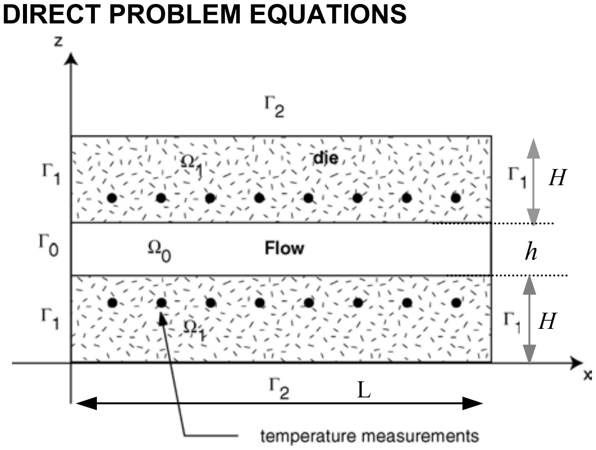

Figure 1 : The extrusion die.

The steady laminar flow of an incompressible fluid is considered through an extrusion die, see Fig 1. The velocity and the temperature fields are governed by the coupled equations of mass, momentum and energy, i.e.

$\vec{\nabla}.\vec{U}=\vec{0}$ in Ω_0	(1)
$\rho_f(\vec{U}.\vec{\nabla}\vec{U})=-\vec{\nabla}p+2\vec{\nabla}(\eta_a\dot{\gamma}D)$ in Ω_0	(2)
$\begin{cases}\rho C_{pf}\vec{U}.\vec{\nabla}T=\vec{\nabla}\left(\lambda_f.\vec{\nabla}T\right)+F\left(T\right)\\ \vec{\nabla}\left(\lambda_w\vec{\nabla}T\right)=0\end{cases}$	(3a) (3b)

Where :

$$D=\frac{1}{2}\left(\vec{\nabla}\vec{U}+\vec{\nabla}\vec{U}^T\right), F\left(T\right)=\sigma : D \qquad (4a\text{-}b)$$

$$\dot{\gamma}=\sqrt{2D:D}\ ;\ \eta_a=\mathbf{inf}\left(\eta_{ref}\ ,K\left(\dot{\gamma}\right)^{n-1}\right) \qquad (5a\text{-}b)$$

and n is the Power Law index .

The following boundary conditions are considered for the velocity field :

At the inlet of the channel :

$$p=P_0\ ;\ \frac{\partial u}{\partial x}=0\ ,\ \ w=0 \text{ on } \Gamma_1 \qquad (6\text{-}a)$$

At the outlet : $p=P_L\ ,\frac{\partial u}{\partial x}=0\ ,\ \frac{\partial w}{\partial x}=0\ ,$ (6-b)

At the internal surface, the usual no-slip boundary condition is used : $\vec{U}=\vec{0}$ (6-c)

For the temperature field, the boundary conditions are taken as follows

At the entrance : $T=T_0\left(z\right)$ (7-a)

$$\lambda_f\frac{\partial T}{\partial \mathrm{n}}=0 \text{ and } \lambda_w\frac{\partial T}{\partial \mathrm{n}}=0 \text{ on } \Gamma_1 \qquad (7\text{-}b)$$

The outer surface temperature of the wall is fixed: $T=T_p\left(x\right)$ on Γ_2 (7-c)

The solution $\left(T,u,w,p\right)$ of equations (1-7) is denoted as the Direct Problem Solution. When the pressure drop is fixed, and the temperature profiles $T_0\left(z\right)$ and $T_p\left(x\right)$ are known, the Direct Problem Solution determines the temperature field within the extrusion die and the velocity field in the channel.

INVERSE PROBLEM

For the Inverse Problem the inlet temperature profile $T_0\left(z\right)$ is regarded as being unknown and is to be estimated. Additional data are required for the solution They consist in temperature measurements $\tilde{Y}_{m,p}$ given by Ns sensors located at appropriate positions $\left(x_m\ ,\ z_p\right)$, $m=1,\ldots Ns$, $p=1,2$ inside the extrusion die. Such measurements may contain random errors, but all the other quantities appearing in the direct problem equations (1-7) are considered to be known with sufficient degree of accuracy.

The velocity field can be considered to be established from the entrance of the channel, hence only the energy equation has to be inversed. The inverse problem is formulated by introducing the following least square functional:

$$J(T_0)=\frac{1}{2}\sum_{p=1}^{2}\sum_{m=1}^{\frac{Ns}{2}}\left|T(x_m,z_p,T_0)-\tilde{Y}_{m,p}\right|^2 \qquad (8)$$

where $T(x_m,z_p,T_0)$ are the temperature computed from the Direct Problem Solution at the measurement locations, by using an estimated inlet temperature profile $T_0(z)$.

Minimisation of the functional (8) is achieved according to the **C**onjugate ***G***radient **M**ethod (**C.G.M**) such that

$$T_0^{n+1}=T_0^n-\gamma^n p^n \text{ for } n=0,1,2... \qquad (9)$$

$$p^{n+1}=\vec{\nabla}J^n(T_0)+\beta^n p^n \qquad (10)$$

where γ^n is the descent length and p^n the descent direction, at iteration *n*.
To perform the iterations according to Eq.(9-10), the gradient of the functional $\vec{\nabla}J(T_0)$ is needed.

SENSITIVITY PROBLEM

In order to develop the sensitivity problem equations, a variation $\varepsilon\delta T_0$ of the inlet temperature profile is considered, and the resulting temperature is denoted $T^+=T(x,z,T_0+\varepsilon\delta T_0)$. The sensitivity is then defined by : $\theta=\lim_{\varepsilon\to 0}\left(\frac{T^+-T(T_0)}{\varepsilon}\right)$ (11)

Developing the direct problem equations for $T(x,z,T_0)$ and $T(x,z,T_0+\varepsilon\delta T_0)$ and then subtracting the resulting expressions, leads to

$$\begin{aligned}
&\rho C_{Pf}\vec{U}.\vec{\nabla}\theta=\lambda_f\Delta(\theta) && \text{in } \Omega\\
&\lambda_w\frac{\partial\theta}{\partial n}=0 && \text{on } \Gamma_1\\
&\lambda_f\frac{\partial\theta}{\partial n}=0 && \text{on } \Gamma_3\\
&\lambda_w\frac{\partial\theta}{\partial n}+h(x)\theta=0 && \text{on } \Gamma_2\\
&\theta=\delta T_0 && \text{on } \Gamma_0\\
&\vec{\nabla}(\lambda_w\vec{\nabla}\theta)=0 && \text{in } \Omega_1
\end{aligned}$$

where $\vec{U}$ is the direct problem velocity profile in the extrusion die.

ADJOINT PROBLEM

The variation $\delta J(T_0)$ due to the variation δT_0 of the inlet temperature profile is developed according to the definition:

$$\delta J=\lim_{\varepsilon\to 0}\frac{J(T_0+\varepsilon\delta T_0)-J(T_0)}{\varepsilon} \qquad (12a)$$

From equation (8), we have :

$$\delta J(T_0)=\int_\Omega\sum_{p=1}^{2}\sum_{m=1}^{\frac{Ns}{2}}e_{m,p}.\theta(x_m,z_p)\delta(x-x_m)\delta(z-z_p)d\Omega$$

where : $e_{m,p}=\left|T(x_m,z_p,T_0)-\tilde{Y}_{m,p}\right|$

In order to get the gradient $\nabla J(T_0)$ which, by definition, satisfies:

$$\delta J(T_0)=\int_{\Gamma_0}\nabla J(T_0).\delta T_0.d\Gamma_0 \qquad (12b)$$

the above expression of $\delta J(T_0)$ is transformed under this new form, by introducing an adjoint variable Ψ. This is usually done by considering a Lagrangian *L* and by taking the multiplier Ψ such that

$$\frac{\partial L}{\partial T}\delta T=0 \quad \forall\,\delta T \qquad (13)$$

According to this stationary condition, the following adjoint problem equations are obtained

$$\rho C_{Pf}\vec{U}.\vec{\nabla}\Psi-\lambda_f\Delta\Psi=-\frac{\partial F(T)}{\partial T}\Psi+\sum_{p=1}^{2}\sum_{m=1}^{\frac{Ns}{2}}e_{m,p}\delta(x-x_m)\delta(z-z_p) \quad \text{in } \Omega$$

$$\Psi=0 \quad \text{on } \Gamma_0$$

$$\lambda_w\frac{\partial\Psi}{\partial n}=0 \quad \text{on } \Gamma_1$$

$$\lambda_w\frac{\partial T}{\partial n}+h(x)\Psi=0 \quad \text{on } \Gamma_2$$

$$\lambda_f\frac{\partial\Psi}{\partial n}+\rho C_{Pf}\vec{U}.\vec{n}\,\Psi=0 \quad \text{on } \Gamma_3$$

together with the gradient equation

$$\vec{\nabla}J(T_0)=\lambda_f\frac{\partial\Psi}{\partial n_0} \qquad (14)$$

CONJUGATE GRADIENT ALGORITHM

The conjugate gradient algorithm involves the resolution of three set of coupled equations at each step of the iterative process. The overall CGM algorithm may be summarized as follows:

1. choose an initial guess $T_0(z)$.,
2. solve the direct problem given by Eqs, (1-7), to obtain $T(x,\, z,\, T_0)$.
3. knowing the computed $T(x_m,\, z_p,\, T_0)$ and the measured temperatures $\widetilde{Y}_{m,p}$, at the sensor location compute the least square functional $J(T_0)$, eq. (8)
4. solve the adjoint problem, eq (13)
5. compute the gradient $\vec{\nabla} J(T_0)$, eq. (14)
6. compute the direction of descent p^n,

   if $n = 0$, $p^n = \vec{\nabla} J^n(T_0)$

   otherwise $p^{n+1} = \vec{\nabla} J^n(T_0) + \beta^n p^n$ with

$$\beta^n = \frac{\left\| \vec{\nabla} J(T_0)^{n+1} \right\|^2}{\left\| \vec{\nabla} J(T_0)^n \right\|^2}.$$

7. solve the sensitivity problem with $\delta T_0 = p^n$
8. compute the step size

$$\gamma^n = \frac{\sum_{p=1}^{2} \sum_{m=1}^{\frac{Ns}{2}} \theta^n(x_m, z_p, T_0)\left(T^n(x_m, z_p, T_0) - \widetilde{Y}_{m,p}\right)}{\sum_{p=1}^{2} \sum_{m=1}^{\frac{Ns}{2}} \theta^n(x_m, z_p)^2}$$

9. correct the inlet temperature profile.
$T_0^{n+1}(z) = T_0^n(z) - \gamma^n p^n$;
10. terminate the iteration when the convergence criterion is satisfied. Otherwise, go to step 2.

RESULTS AND DISCUSSION

In order to examine the feasibility and then the accuracy of the inverse analysis for estimating the unknown inlet distribution temperature, by using the Conjugate Gradient Method (C.G.M), several test conditions including a constant function and a smooth function are studied. The effects of measurement errors are also analysed. The computational technique used here is based on a Finite Volume Method (FVM) discretization of the governing mass, momentum and energy equations. The system of the governing equations is discretized by employing the staggered grid for Marker and Cell (MAC) method. An augmented lagrangian method is used to compute the solution of the coupling velocity-pressure equations (1-7). The grids are non uniformly spaced in z direction. The **mesh** spacing is taken smaller **near** the **wall**. The grids in the principal direction of flow are uniformly spaced (200×160). This distribution was dictated by the desire to capture the details of the viscous dissipation, because the temperature rise occurs in the region very near the wall, the temperature rise remains very low in the centre of the channel die.

The problem is solved for a die geometry illustrated in figure 1. The flow of a Newtonian polymer is studied in a parallelipedic channel. The height, the length and the width of the channel are respectively $h = 2.10^{-3}\, m$ $L = 0.2\, m$ and $l = 2.10^{-2}\, m$, and the solid wall thickness is $H = 15.10^{-3}\, m$. The coordinate system is considered such that *Ox* is the principal direction of the flow, *z* is the thickness coordinate, and *y* the width coordinate. It is assumed that the channel ratio l/h is sufficiently large such that a two-dimensional solution $T(x, z)$ is valid at *y = 0*.

The properties of the polymer melt are taken as $\rho_f = 10^3 kg/m^3$, $\lambda_f = 0.2 W/mK$, $\eta = 10^3 Pa.s$ and $C_{pf} = 2.10^3\, J/kg\, K$. The pressure drop in the channel die is taken as $\Delta p = 300.bar$ and the specified temperature at the outer wall of the die is $T_p(x) = 473\, K$. The principal wall material considered in this study is carbon steel, where the thermal conductivity is taken as $\lambda_w = 10 W/mK$, $C_{pw} = 400\ \ J/kgK$ and the density $\rho_w = 7800\, kg/m^3$.

The polymer melt enters the extrusion die at $x = 0$ with a temperature profile $T_0(z)$. To study the estimation of this inlet profile, two specific examples are considered: a non uniform profile in the first example, and a uniform one in the second example. For each case, the direct problem is solved to generate the measured temperature $\widetilde{Y}_{m,p}$ and the velocity profile in the channel, see figures 2, 3. The temperature $\widetilde{Y}_{m,p}$ are then used as “experimental” data and the velocity are then used to solve the adjoint and the sensitivity problems, to reconstruct the inlet temperature profile, according to the conjugate gradient algorithm.

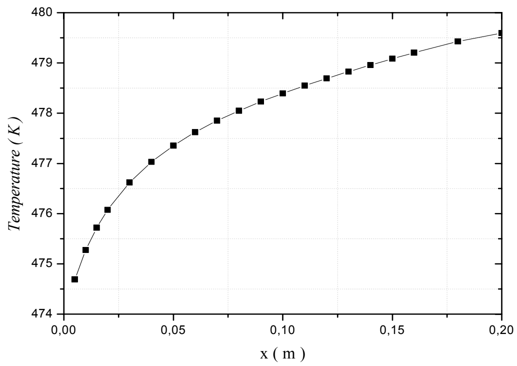

Figure 2 : The measured temperature $\widetilde{Y}_{m,p}$

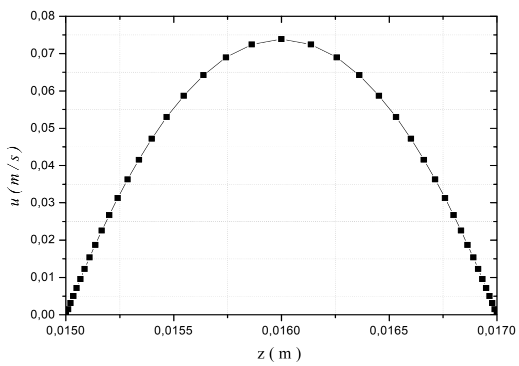

Figure 3 : The x velocity profile $\Delta p = 3.10^7\,Pa$, $T_p(x) = 473\,K$

Example 1

The inlet temperature profile is chosen as the developed solution of a Newtonian fluid between two parallel isothermal walls, it is characterized by a peak between the centreline of the channel and the die wall, due to the high viscous dissipation. By using the conjugate gradient method, the initial guesses of the unknown variable can be chosen arbitrary. Two different temperature profile guesses $T_0^{n=0}(z)$ are studied, a parabolic one and a uniform one.

a) *Uniform guess.* The computation starts from the uniform guess $T_0^{n=0}(z) = 473^\circ K$ and used the temperature measurements given by *2x20 = 40* sensors located at z_p , $p = 1, 2$ in the die wall, see figure 1.

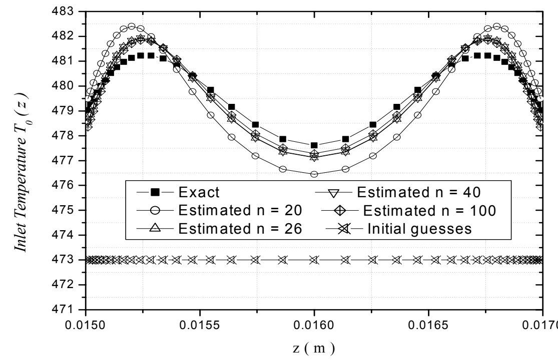

Figure 4 : Exact and Estimated inlet Temperature profiles for different iterations

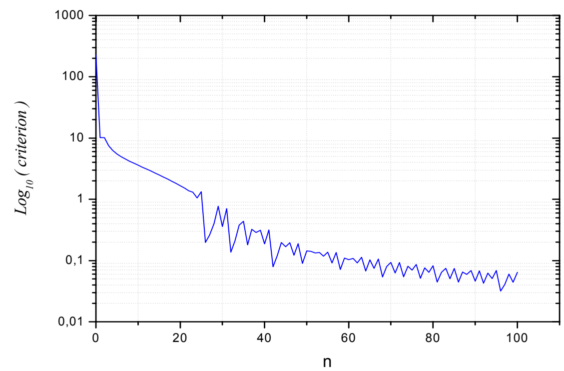

Figure 5 : Least square Criterion $J(T_0(z))$ for different iterations

Figure 4 illustrates the effects of the number of iterations on the accuracy of the estimation. After 26 and 40 iterations it appears satisfactory in comparison to the true profile. It is observed that when the number of iteration increases, the final value of the least square criterion decreases and a reasonably inlet temperature solution is obtained after 100 iterations. Although the optimal number of iterations is difficult to be determined a priori, the plot of the iterative process, figure 5, confirms the efficiency of the Conjugate Gradient Method (C.G.M), and suggests that the optimal number of iterations is between 26 and 40 iterations. The estimated temperature profile is in excellent agreement with the exact solution except near the wall. This is due to diffusive nature of the heat equation and the smoothing effect of the inverse algorithm.

b) *Parabolic guess.* Figure 6 show the comparison between the estimated inlet temperature profile and the exact one. For this case, the solution obtained after 150 iterations appears satisfactory in comparison with the true solution. The temperature inlet profile is represented quite well, as well the peak than near the wall.

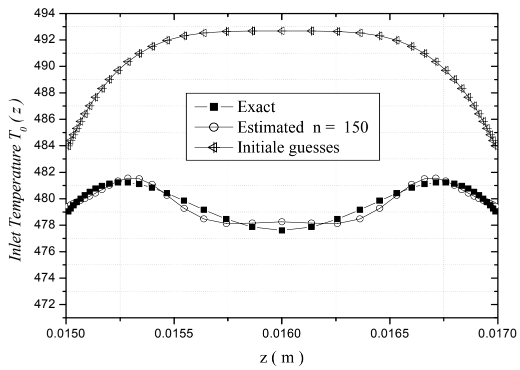

Figure 6 : Exact and the Estimate inlet Temperature profile for 150 iterations

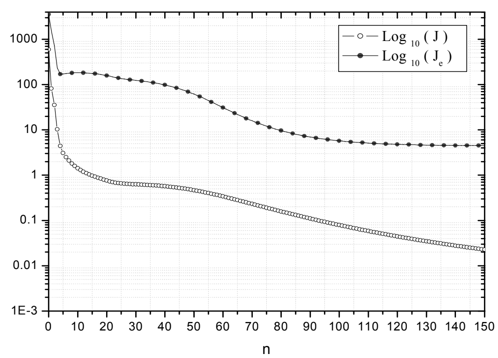

Figure 7 : Criterion $J\left(T_0\left(z\right)\right)$ and J_e for different iterations.

J_e, norm of the deviation between the exact and the computed solution, is computed on the total number $(Ne = 39)$ of grid points $\left(z_e\right)$, $e = 1, 2, ...Ne$, at the inlet boundary of the channel die. The variability of J_e and the criterion of convergence $J\left(T_0\left(z\right)\right)$ with the number of iteration can be seen on figure 7.

Example 2:

In polymer extrusion modelling, the material is usually assumed to have a constant temperature at the entrance of the die and the die is usually controlled at a given temperature. For this reason we consider a uniform inlet temperature profile. Three typical initial guesses are checked :

(i) a uniform initial guesses.

(ii) a fourth order polynomial with a maximum at the centreline

(iii) a non uniform profile characterized by a peak between the centreline and the wall.

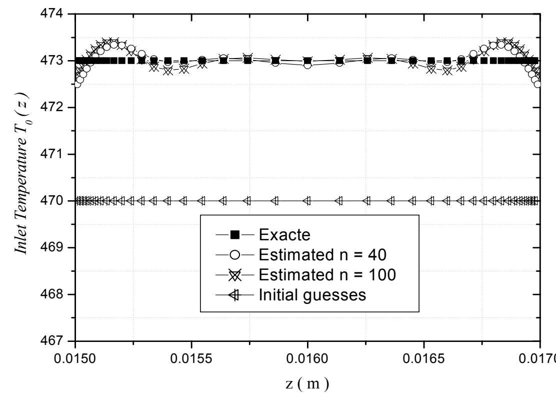

Figure 8 : Exact and Estimated inlet Temperature profiles for different iterations; case (i)

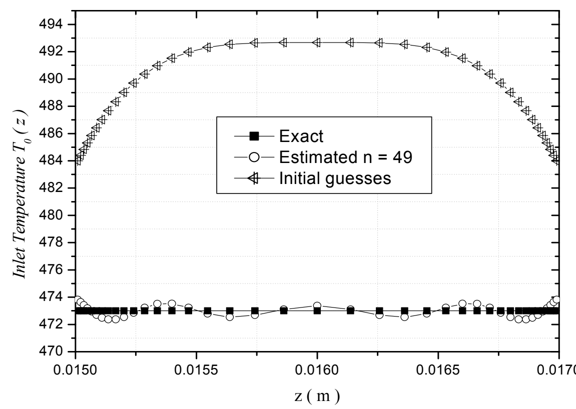

Figure 9 : Exact and Estimated inlet Temperature profile for 49 iterations; case (ii)

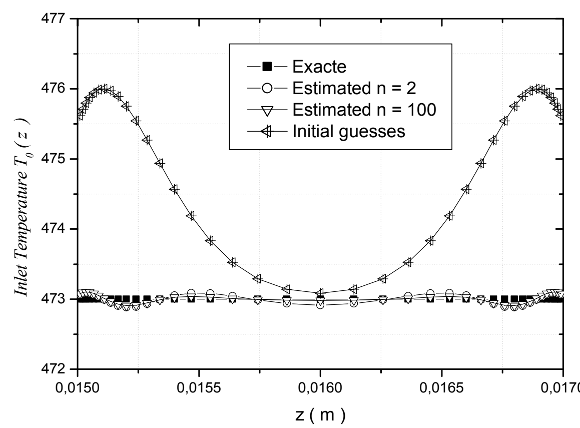

Figure 10 : Exact and Estimated inlet Temperature profile for different iterations; case (iii)

Figures 8, 9, and 10 shows the reconstructed inlet temperature profile. For three cases, there are little differences between the exact and the estimate temperature at the centreline of the extrusion die, expect near the wall, where the viscous dissipation plays a central role. It is interesting to note that, for three cases, the estimated solution oscillates around the exact one.

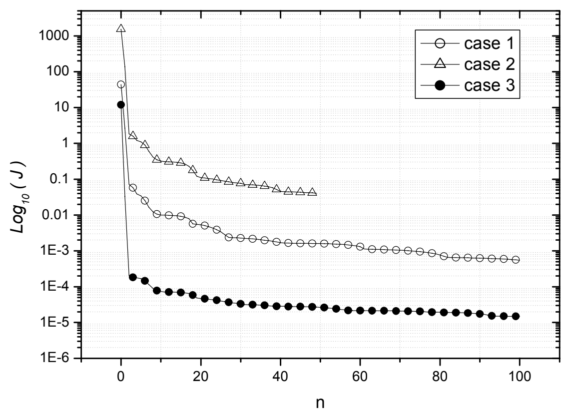

Figure 11 : Criterion $J(T_0(z))$ for different iterations.

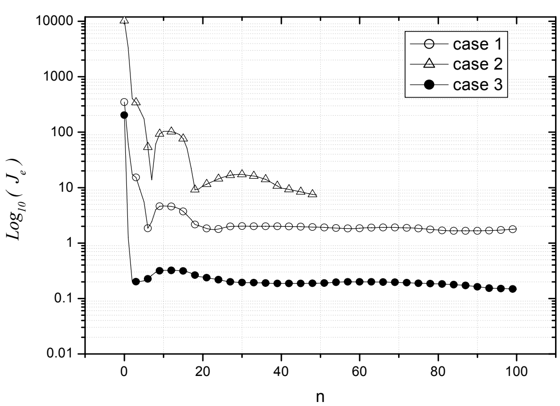

Figure 12 : Criterion J_e for different iterations.

Figure 11 shows the effects of the initial guesses on the convergence rate of the conjugate gradient $J(T_0(z))$. The choice of the iteration number ***n*** for each case is very important. For example in case 3, the inverse solution obtained after one hundred iterations appears satisfactory in comparison. In order to explain the convergence of the iterative process, we present in figure 12 the variability in J_e after ***n*** iteration. As observed in case 2, the amplitude of variability of the J_e tends to decrease towards a constant value after 49 iterations.

Results with noisy data

Since all experimental data are corrupted by noise, the challenge is to develop a stable algorithm, the more less susceptible to noise. To assess the effect of noisy data on the reconstructed inlet temperature profile, random values was added to the exact data at sensor locations. The exact data and those with a zero mean Gaussian noise $(\sigma = 0.1K)$, are shown in figures 13 and 14.

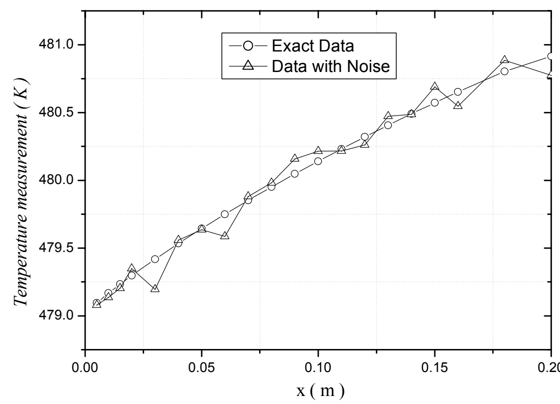

Figure 13 :Temperature profile $T(x, z_1)$ within Inferior wall $z_1 = 0.01495\,m$

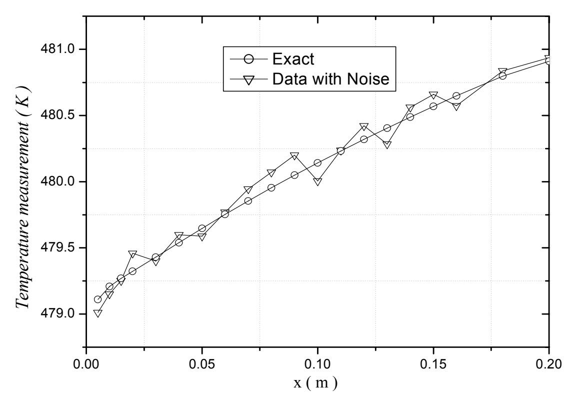

Figure 14 : Temperature profile $T(x, z_2)$ within Superior wall $z_2 = 0.01704\,m$

Figure 15 shows the difference between the reconstructed inlet temperature profile obtained using exact and noisy data. The temperature peak was represented quite well by the inverse solution after 150 iteration. It can be seen that the estimated profile using noisy data is not symmetric. This confirm that the level of the noisy data is not the same in the superior and inferior wall. We remark that, due the existence of noise in data, it is meaningless to proceed the iteration to very small criterion value (figure 16). In fact it is inappropriate because the noise will spoil the estimation. One has to use a stopping criterion such as the stability of the J_e .

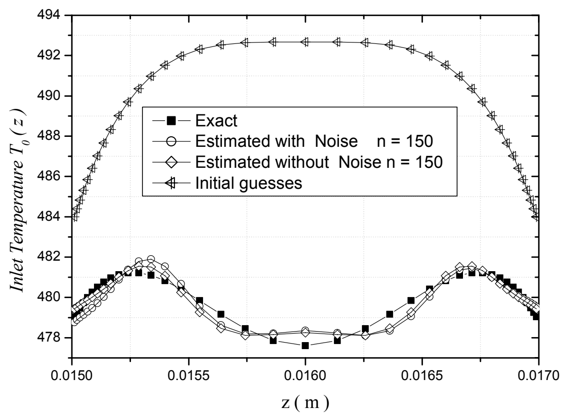

Figure 15 : comparison between the Exact and the reconstructed temperature profiles when the data are exact and when the data contain a noise.

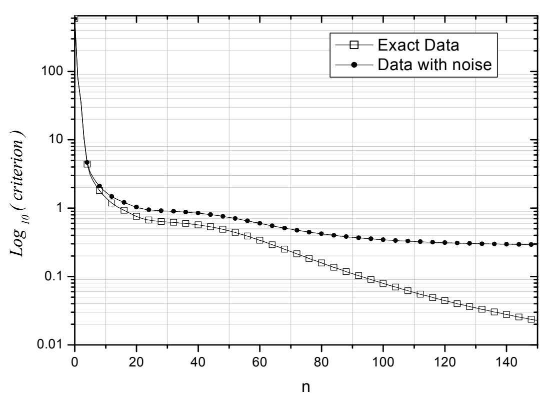

Figure 16 : *Criteria* J_e *and* $J(T_0(z))$ for different iterations.

CONCLUSION

An inverse algorithm was developed to construct the inlet temperature profile of the melted polymer from the temperature data measured in the solid wall of the die. In order to examine the feasibility and then the accuracy of the inverse analysis for estimating the unknown inlet distribution temperature, by using the **C**onjugate **G**radient **M**ethod (**C.G.M**), several test conditions are studied. The effects of measurement errors are also analysed. In a parallel study, the design of an experimental instrumented die is in progress.

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