Proceedings of the World Congress on Engineering 2008 Vol II
WCE 2008, July 2 - 4, 2008, London, U.K.

Inverse Modelling for Estimation of Average Grain Size and Material Constants - An Optimization Approach

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Abstract—**The goal is to build up an inverse model capable of finding the average grain size history during an extrusion process and other material constants by using simulated strain and temperature values. This problem of finding the parameter values is based on linear and nonlinear least-squares regressions, coupled with microstructure control models and the solution of a finite element extrusion model. The problem is ill posed and we use the Tikhonov's regularisation to stabilise the solution process. Further some of the parameters in the model are linear and some are nonlinear. We determine the linear parameters using simple linear algebra and for the computation of non-linear parameters we use MATLAB's routine *lsqnonlin*.**

Keywords: Extrusion; Inverse problem; Parameter estimation; Optimization.

1 Introduction

Numerical modelling of extrusion may be used during a design process to assess the extruded material properties. The extrusion simulation describes the material flow through the die. An extrusion model, which is capable of describing the behaviour of material flow, requires the following input data: (a) material data such as Young's modulus, coefficient of expansion, Poisson's ratio, inelastic heat fraction, specific heat, density, conductivity, flow stress-strain relationship, (b) die design variables and (c) process variables such as ram speed, initial temperature and friction factors.

In reality, material data can be measured using available measuring instruments, but the optimal values of die design variables and process variables are often unknown. In a previous paper[3], we formulated a non-linear least squares inverse model in which the optimal values of die design variables and process variables were estimated to achieve a certain grain size. In the approach the following average grain size equation [7],[8]

$$d = \alpha \left(\frac{d\varepsilon}{dt} \exp\left(\frac{Q}{RT} \right) \right)^{\beta} \tag{1}$$

was used as optimizing criteria to terminate the problem. In equation (1), Q is an activation energy, d is the average recrystallized grain size, T is the temperature, $\frac{d\varepsilon}{dt}$ is the strain rate and R is the universal gas constant.

The values of constants α and β are based on experimental observations and therefore the uncertainty of the constants is very high. Small changes in these values can cause variation in the grain size estimation. The successful application of equation (1) depends on the accuracy of the parameters. Methods to identify the optimal values of α and β are therefore an important part of modelling extrusion processes to increase the reliability of the numerical simulation.

In the present work an alternative method is proposed. The idea is to develop an inverse model for estimating grain size history, using inverse modelling techniques available in the literature. Inverse modelling avoids the use of α and β for the grain size history estimation. To do so we consider the problem in which the material properties of the billet as well as process and die design parameters are known but the material constants α, β and grain size d are not known. The accuracy of the model is examined by using simulated temperature and strain data (generated by the forward model) to which normally-distributed relative noise has been added. We design the inverse model as a least squares minimisation problem associated with an ABAQUS finite element solution of an extrusion process. This is an ill-posed problem and we solve it using regularisation methods.

2 Forward Problem

The thermo-mechanical behaviour of the extrusion process can be described mathematically using conservation of mass, momentum and energy as follows [4], [5], [6]:
The mass conservation is

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{V} = 0 \tag{2}$$

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where ρ is the density of the material and $\mathbf{V}$ is the velocity vector.
The momentum conservation is

$$\rho\frac{D\mathbf{V}}{Dt} = \nabla\cdot\sigma + \rho\mathbf{f} \tag{3}$$

where $\mathbf{f}$ is the body force per unit mass, and σ is Cauchy stress tensor.
The energy conservation is

$$\rho c\left(\frac{\partial\mathbf{T}}{\partial t} + \mathbf{V}\cdot\nabla\mathbf{T}\right) = -\nabla\cdot(-\mathbf{k}\cdot\nabla\mathbf{T}) + \dot{Q} \tag{4}$$

where T is the temperature, c is the specific heat, $\mathbf{k} = k\mathbf{I}$, k denotes thermal conductivity, $\mathbf{T}$ is the temperature and $\dot{Q}$ is the rate of heat generated per unit volume.

Equations (2),(3) and (4) can be solved using finite element methods. We have implemented a solution procedure using ABAQUS to obtain temperature and strain histories during the deformation process. Once the temperature and strain values are obtained, the average grain size at a nodal point can be calculated using equation (1).

3 Inverse Problem

The goal of inverse modelling is the extraction of model parameter information from data. It is a subject, which supplies tools for the proficient use of data in the estimation of constants appearing in the models. In this inverse problem, the structure of the equation is known; outputs, temperature (T) and strain (ε) values are available. Average grain size history and parameters α and β are the unknowns.

In this section a model is formulated to obtain the best or optimal estimate of grain size history, α and β appearing in equation (1) from temperature and strain estimations made at some nodes in the material inside the forming zone. The microstructural model given equation (1) can be rewritten to solve for strain rate as follows.

$$\frac{d\varepsilon}{dt} = \left(\frac{d}{\alpha}\right)^{1/\beta}\exp\left(\frac{-Q}{RT}\right) \tag{5}$$

Therefore the strain is

$$\begin{aligned}\varepsilon(t) &= \int_0^t\left(\frac{d(\tau)}{\alpha}\right)^{1/\beta}\exp\left(\frac{-Q}{RT(\tau)}\right)d\tau\\ &= \int_0^t K(t,\tau)D(\tau)d\tau \end{aligned}\tag{6}$$

where the kernel $K(t,\tau)$ is:

$$K(t,\tau) = \exp\left(\frac{-Q}{RT(\tau)}\right) \tag{7}$$

and

$$D(\tau) = \left(\frac{d(\tau)}{\alpha}\right)^{\frac{1}{\beta}} \tag{8}$$

If n temperature and strain values are available at the node (X_1, Y_1, Z_1) between 0 and t_f and suppose that we wish to determine $D(\tau)$ at times $\tau_0 = 0, \ldots, t_f$, then discretising (6) by the trapezoidal rule gives a system of linear equations

$$\mathbf{e} = \mathrm{A}(\mathbf{p})\mathbf{q} \tag{9}$$

where $\mathbf{e} = [\varepsilon(\mathbf{0}), \ldots, \varepsilon(\mathbf{t_f})]^{\mathbf{T}}$, $A_{ij} = K(t_i, \tau_j)\beta_{ij}$, $\mathbf{q} = [D(\tau_0), \ldots, D(\tau_f)]^T$ and $\mathbf{p} = [\mathbf{Q}]$, and β_{ij} is a quadrature weight. Generally, minimising an objective function solves inverse problems. The objective function Z that provides minimum variance estimates is the ordinary least squares function

$$minimize \quad Z(\mathbf{p},\ \mathbf{q}) = \|A(\mathbf{p})\mathbf{q} - \mathbf{e}\|_2^2 \tag{10}$$

If the value of activation energy Q is known then the problem becomes a linear least square problem and can be solved easily. But the coefficient matrix of problem (10) always has a very large condition number and is ill posed. Therefore well posedness must be restored by restricting the class of admissible solutions. This can be achieved using regularisation methods [1]. With Tikhonov's regularisation, we introduce the regularised objective function

$$Z(\mathbf{q}) \quad = \quad \|A\mathbf{q} - \mathbf{e}\|_2^2 + \lambda^2\|L\mathbf{q}\|_2^2 \tag{11}$$

where $\|A\mathbf{q} - \mathbf{e}\|_2^2$ is the residual norm (or data misfit function), and $\|L\mathbf{q}\|_2^2$ is the solution norm. We will be interested in the minimisation of the function $Z(\mathbf{q})$ for different values of λ. Note that the objective function Z is the 2-norm of the following system of equations

$$\begin{bmatrix} A \\ \lambda L\end{bmatrix}\mathbf{q} = \begin{bmatrix}\mathbf{e}\\ 0\end{bmatrix},$$

where L is the regularisation operator and λ is the regularisation parameter.

If the value of Q is not known then the problem becomes a nonlinear least square problem as follows.

$$Z(\mathbf{q},\ \mathbf{p}) = \|A(\mathbf{p})\mathbf{q} - \mathbf{e}\|_2^2 + \lambda^2\|L\mathbf{q}\|_2^2. \tag{12}$$

Since the equation (12) has a combination of linear parameters $\mathbf{q}$ and non-linear parameters $\mathbf{p}$, we separate the solution process into two steps. We find the nonlinear parameter $\mathbf{p}$ by constructing an iterative procedure, where at each iteration a linear sub-problem is solved to estimate the linear parameter $\mathbf{q}$ corresponding to that particular value of $\mathbf{p}$.

Now taking natural logarithms of both sides of the equation (8) and rearranging gives

$$\ln(D) = m\ln(d) + C \tag{13}$$

where $m = \dfrac{1}{\beta}$ and $C = \dfrac{1}{\beta}\ln\left(\dfrac{1}{\alpha}\right)$. Now suppose $n+1$ D values are available and we wish to determine the corresponding d values. This gives

$$K\mathbf{y} = \mathbf{f}, \tag{14}$$

ISBN:978-988-17012-3-7

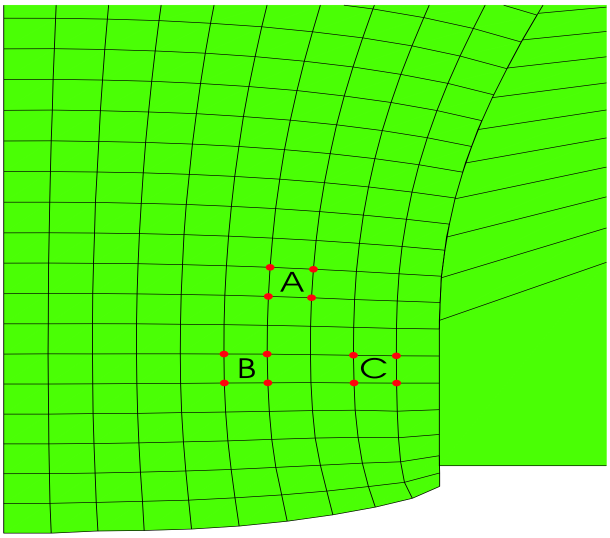

Figure 1: Three considered nodes on deformed mesh

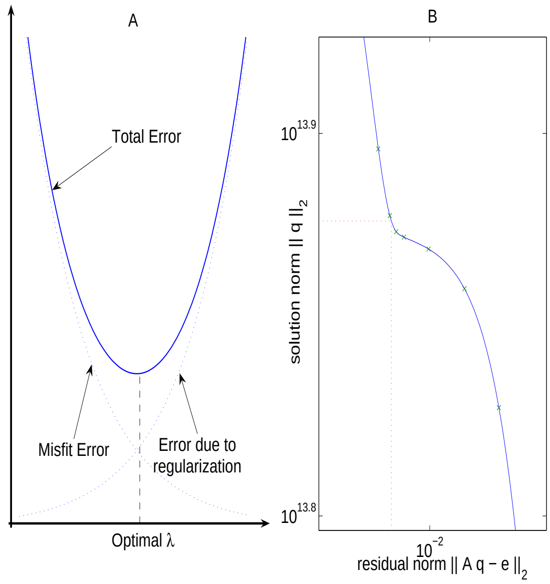

Figure 2: (A):Total error, (B) L-curve.

where

$$\mathbf{K} = \begin{pmatrix} m & 0 & \dots & 0 & 0 \\ 0 & m & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & m & 0 \\ 0 & 0 & \dots & 0 & m \end{pmatrix}$$

$$\mathbf{y} = \begin{pmatrix} \ln\left(\frac{d_1}{d_0}\right) \\ \ln\left(\frac{d_2}{d_0}\right) \\ \vdots \\ \ln\left(\frac{d_{n-1}}{d_0}\right) \\ \ln\left(\frac{d_n}{d_0}\right) \end{pmatrix}, \ \mathbf{f} = \begin{pmatrix} \ln\left(\frac{D_1}{D_0}\right) \\ \ln\left(\frac{D_2}{D_0}\right) \\ \vdots \\ \ln\left(\frac{D_{n-1}}{D_0}\right) \\ \ln\left(\frac{D_n}{D_0}\right) \end{pmatrix}$$

Now the minimisation problem for estimating $\mathbf{y}$ is formulated as

$$\min_{\mathbf{y}} \|K\mathbf{y} - \mathbf{f}\|_2^2. \tag{15}$$

It is a linear problem and therefore the grain size history $d_1, d_2, \dots, d_n$ can be calculated with reasonable accuracy provided the initial grain size is known.

4 Applications

In this section, we present numerical simulations to demonstrate the solution process and evaluate the accuracy of the model. To do so, we consider an input of temperature and strain values data generated at three elements A, B, C as shown in Figure 1 from a FE-simulation of extrusion using ABAQUS. The data values used in the simulation of extrusion are: initial temperature of work piece and die respectively are $T = 500^oC$ and $T = 450^oC$, work piece's Young's modulus $E = 7 \times 10^{10}\ Pa$, coefficient of expansion $8.4 \times 10^{-5}\ ^oC^{-1}$ at $T = 20\ ^oC$, Poisson's ratio 0.35, inelastic heat fraction 0.9, specific heat 910 $Jkg^{-1}K^{-1}$, density= 2750 kgm^{-3}, conductivity 204 $Wm^{-1}K^{-1}$ when $T = 0\ ^oC$, 225 $Wm^{-1}K^{-1}$ when $T = 300\ ^oC$, die material's Young's modulus $E = 20 \times 10^{10}\ Pa$, coefficient of expansion $8.4 \times 10^{-5}\ ^oC^{-1}$ at $T = 20\ ^oC$, Poisson's ratio 0.30, inelastic heat fraction 0.9, specific heat 450 $Jkg^{-1}K^{-1}$, density 7200 kgm^{-3}, conductivity 204 $Wm^{-1}K^{-1}$ when $T = 0\ ^oC$, 225 $Wm^{-1}K^{-1}$ when $T = 300\ ^oC$.

4.1 Estimation of $d(t)$ for known value of activation energy Q

If the value of Q is known, we will have to solve equation (11) to estimate the grain size. The minimization problem given by equation (11) depends on the optimal value of the regularization parameter λ. A number of techniques have been discussed in the literature[2] for estimating an optimal value of a regularization parameter. Here we use the L-curve criteria to estimate the parameter values. It is based on minimizing the total error equation (11) as shown in Figure 2. A good regularization parameter λ should provide a fair balance between data misfit error and regularization error. The L-curve method shown in figure 2B is based on minimizing total error as shown in Figure 2A.

Once the optimal value of λ is known, we estimate $\mathbf{q} = [D(\tau_0), \dots, D(\tau_f)]^T$ easily and then using equation (15) values $\mathbf{y} = \left[\frac{D_1}{D_0}, \dots, \frac{D_n}{D_0}\right]^T$ are calculated. Figure 3 shows the graph of equation (13) for the initial grain size $d_0 = 200\ \mu m$ and the activation energy $Q = 100\ KJm^{-1}$.

ISBN:978-988-17012-3-7

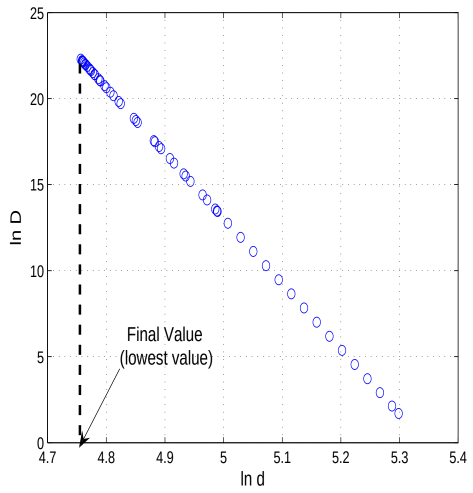

Figure 3: Graph of Equation (13)

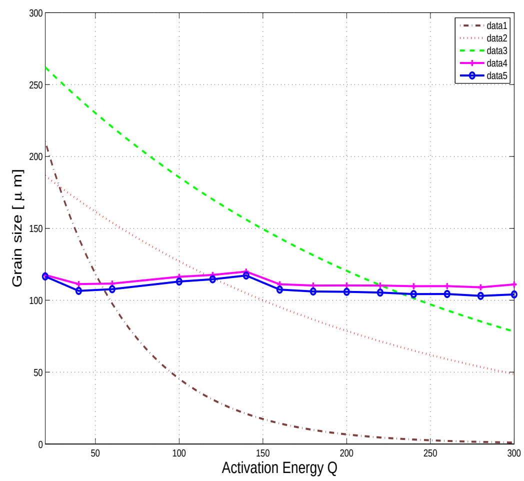

Figure 4: Grain size vs Q for different material constants

The accuracy of value Q we use in equation (1) may or may not be very high since it is based on experimental observations and the accuracy of estimation of d is also subject to error. Therefore it is appropriate to analyze the effect of inaccuracy of the Q value. To investigate we changed the Q values, while all other values are unchanged. Table (1) shows the optimal values of α and β for the respective values of Q obtained using the proposed method. Figure 4 depict the comparison of grain size variation. Data 4 in this graph is the grain size estimation using the proposed method and data 5 is the grain size variation obtained by equation (1)for the respective α and β values given in table (1). Data 1, Data 2 and Data 3 respectively are the grain size values for ($\alpha = 278$ & $\beta = -0.080$), ($\alpha = 200$ & $\beta = -0.020$) and ($\alpha = 279$ & $\beta = -0.018$) by equation (1). When Q is underestimated, the average grain size estimated value using equation (1) is higher than it used to be and increases approximately quadratically with decreasing Q value. When Q is overestimated, the average grain size estimated value is lower than it used to be and decreases approximately quadratically with increasing Q value. The graph of Data 4 and Data 5 are approximately the same. This shows that even if the Q value is wrong, it is possible to estimate d accurately using equation (1) if appropriate α and β values are available. It is not achievable in a real practical environment, but can be only possible through inverse modelling techniques.

4.2 Estimation of $d(t)$ for unknown value of activation energy Q

Here the problem is concerned with the estimation of grain size $d(t)$ values and the activation energy (Q). This estimation process contains a combination of a nonlinear parameter (Q) and linear parameters ($d(t)$). This is different from a linear problem and therefore we cannot only use linear algebra to solve this problem. This problem can be solved by constructing an iterative procedure as mentioned above. Alternatively we can solve the equation (12) for a sequence of Q values to get a best value for Q which minimizes equation (12), since we have only one nonlinear parameter. Figure 5A, 5B respectively shows the variation of Z with Q at the nodes A, B, C for the ram speed 12.5 $mm\ s^{-1}$ and 6.5 $mm\ s^{-1}$. The graphs clearly show that the best value of Q is not same for all cases. In the literature we can find that the activation energy of the material varies with temperature. During the extrusion process the temperature inside the deformation zone is not constant everywhere. Therefore using constant Q value in equation (1) will not give an accurate result unless appropriate values of α and β are used. Again the estimation of α and β which suits the Q value is not achievable in a real practical environment.

Q	β	α
20	-0.044	140
50	-0.080	278
100	-0.026	209
140	-0.020	200
180	-0.019	240
220	-0.018	279
300	-0.019	412

Table 1: % of variation with Q values

5 Summary and conclusion

The objective of the work demonstrated in this paper is to develop an inverse model capable of concurrently estimating the average grain size, activation energy and

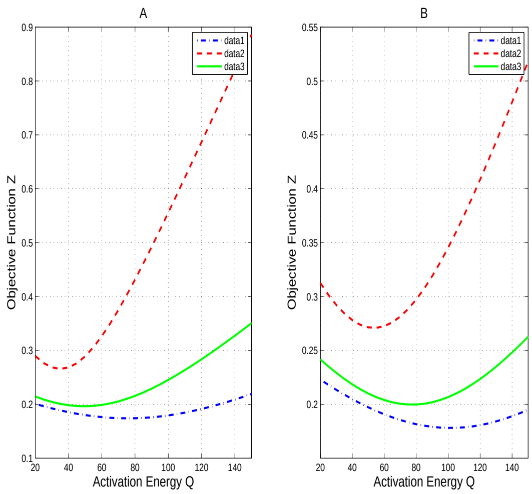

Figure 5: Z vs Q

other material constants appearing in the model. The approach is based on a non-linear least squares estimation using simulated temperature and strain value history inside the deformation zone. Since the problem is ill-posed we apply Tikhonov's regularisation method to stabilise the solution process. Some of the parameters in the problem are linear and some are nonlinear. We determined the linear parameters using simple linear algebra and for the computation of non-linear parameters we used *MATLAB*'s routine *lsqnonlin*. The optimal value of the regularisation parameter is obtained using the linear L-curve for the linear problem.

Firstly, the usefulness of an inverse modeling technique in the grain size estimation process has been demonstrated. The inverse modelling technique has been applied to equation (1) with the situation in which α, β and Q values are unknown. Secondly, it has been shown that the error in traditional d estimation increases quadratically with the error in Q if the α and β values are adjusted accordingly to cater for Q. The appropriate values of α and β can only be found using the above mentioned inverse modelling technique. Thirdly, it has been demonstrated the optimal value of the activation energy inside the deformation region is not constant and varies with the temperature. Therefore the traditional d estimation using equation (1) with constant values of Q, α and β will not give the accurate value if the temperature inside the deformation zone is not constant.

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