Computer Applications in Metallurgical Research

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ABSTRACT

This paper outlines the current efforts in computer applications in metallurgical research at the Defence Metallurgical Research Laboratory, Hyderabad. Work being done on armour penetration studies, optimization of armour profiles for fighting vehicles, computer control of multifunction 2000 tonne forge press, drawing of processing mechanism maps, process modelling of titanium sponge production and methods of curve fitting to experimental data, is described and briefly discussed.

1. INTRODUCTION

Metallurgical research is largely based on experiments. It derives support from thermodynamics, kinetics, and composition-microstructure-property correlations. It is also dependent on many qualitative and semi-quantitative analyses and ideas based on similarities and similitudes. Metallurgical research usually defies analytical approaches. Nevertheless, computers are now becoming extremely useful in many ways. They are being used to control equipment and processes, to record and analyze data. We are now able to generate nearly quantitative solutions through careful computer simulations thereby substituting costly experiments. Computer simulation promises to save enormous time, effort, and money, thereby accelerating the pace of metallurgical research.

In this paper we discuss a few recent examples of computer applications in metallurgical research at Defence Metallurgical Research Laboratory (DMRL), Hyderabad.

2. MODELLING OF THE RESPONSE OF ARMOUR MATERIALS

Penetration of metal targets by projectiles is influenced by many parameters such as material properties, impact velocities, projectile shape, target support, relative dimensions of target and projectile. For a thorough understanding of penetration process, it is necessary to identify the important material properties and to know how they relate to the failure of the target. Computer codes are useful in such investigations.

2.1 Numerical Model

At DMRL, a computer code named PRHD, has been successfully employed to model the penetration process. This code is a 2-dimensional, multimaterial, Lagrangian code for solving material flow problems in the hydrodynamic and elastic-plastic regimes. The material model employed in PRHD includes an equation of state, such as Tillotson equation of state, a deviatoric constitutive relation for elastic and plastic deformation, and a failure criterion such as the Von Mises yield criterion.

If \( v_i \) is the impact velocity and \( v_s \) is velocity of sound in material, then for \( v_i < v_s \) the Tillotson\(^1\) equation of state has the form

\[
P = A.\mu + B.\mu^2
\]

and for \( v_i > v_s \)

\[
P = A.\mu + B.\mu^2 + [A.\mu e^{\delta_i}(\sigma + 1)].e^{\alpha_i(\sigma + 1)^2}
\]

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where, \( \mu = 1/V-1 \) and \( V = \) relative volume.

In Eqns (1) and (2), \( A,B,\mu,\beta,a,n \) are constants for the particular material. The Von Mises yield criterion can be written as

\[
\sigma_{eq} = \sqrt{3/2} \cdot \sqrt{2J}
\]  

(3)

where \( 2J = \varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2 + 2\tau_{xy}^2 \)

A variable yield strength \( (Y) \) in shear can be of the form

\[ Y = Y^0 (1 + \varepsilon_{eq})^n \]

(5)

with

\[ \varepsilon_{eq} = \varepsilon_{eq0} + \varepsilon_{eq1} \cdot X + \varepsilon_{eq2} \cdot X^2 + \varepsilon_{eq3} \cdot X^3 + \varepsilon_{eq4} \cdot X^4 \]

(6)

where \( X = 1-V \)

Table 1 indicates the typical values of the constants used in the model.

Table 1. Constants of the numerical model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Al</th>
<th>Mild steel</th>
<th>Cu</th>
<th>W</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Mbar</td>
<td>0.7520</td>
<td>1.2800</td>
<td>1.3900</td>
<td>3.0800</td>
</tr>
<tr>
<td>B</td>
<td>Mbar</td>
<td>0.6500</td>
<td>1.0500</td>
<td>1.1000</td>
<td>2.5000</td>
</tr>
<tr>
<td>( \beta )</td>
<td>5.0000</td>
<td>5.0000</td>
<td>5.0000</td>
<td>5.0000</td>
<td>10.0000</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>5.0000</td>
<td>5.0000</td>
<td>5.0000</td>
<td>5.0000</td>
<td>10.0000</td>
</tr>
<tr>
<td>( Y^0 )</td>
<td>Mbar</td>
<td>0.0029</td>
<td>0.0034</td>
<td>0.0012</td>
<td>0.0220</td>
</tr>
<tr>
<td>( \rho )</td>
<td>g/cc</td>
<td>2.7000</td>
<td>7.8600</td>
<td>8.9000</td>
<td>19.1700</td>
</tr>
<tr>
<td>( T )</td>
<td>Mbar</td>
<td>125.0000</td>
<td>40.0000</td>
<td>36.0000</td>
<td>77.0000</td>
</tr>
<tr>
<td>( \eta )</td>
<td>0.1000</td>
<td>0.3500</td>
<td>0.4500</td>
<td>0.1300</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{00} )</td>
<td>0.0028</td>
<td>-0.0013</td>
<td>-0.0012</td>
<td>-0.0004</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{01} )</td>
<td>-0.0056</td>
<td>-0.0029</td>
<td>-0.0023</td>
<td>-0.0006</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{02} )</td>
<td>0.1364</td>
<td>0.1012</td>
<td>0.0753</td>
<td>0.0306</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{03} )</td>
<td>0.2495</td>
<td>0.2051</td>
<td>0.1526</td>
<td>0.1336</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{04} )</td>
<td>0.3160</td>
<td>0.2901</td>
<td>0.2190</td>
<td>0.1604</td>
<td></td>
</tr>
</tbody>
</table>

2.2 Example

Figure 1 shows the projectile-target configurations at various times for a 6 mm diameter steel conical...
projectile of \( L/D \) ratio of 4.5 impacting a 20 mm thick mild steel plate at a velocity of 800 m/s. The complete perforation takes place in 90 \( \mu \)s.

The weight and location of centre of gravity of each plate are computed next. These data are then combined with the other data of the tank to determine the overall weight and out of balance moment. Different profiles are analyzed to select the one which offers the best possible protection with the least weight and dimensional penalties.

The graphics phase of the software facilitates the viewing of the designed turret profile. It also permits turret rotation and allows us to check the design flaws, interferences and constraints.

Figure 3 shows an example of optimized turret profile at two different positions. The limitations at the driver’s hatch in some positions can be seen clearly.

4. COMPUTER CONTROL OF MULTIFUNCTION FORGE PRESS

Forging is one of the oldest methods of hot metal forming. Essentially it consists of applying a controlled amount of force on a hot metal. Though the principle of forging operation is simple, there are a number of variations in modern forging operations: open die forging, closed die forging, isothermal forging and liquid metal forging. In industrial practice, separate equipment are used to carry out each of the above mentioned forging operations.

The advent of microprocessor technology in the seventies has made it possible to integrate the above functions into a single equipment, thus substantially reducing the capital investment.

At DMRL, hot metal forming technologies are being developed for aluminium, titanium and other materials for defence applications on a 2000 tonne multifunction forge press. This press is unique in that it incorporates all the modes of forging. It also provides a capability for metal extrusion.

The forge press is hydraulically operated and controlled by a state-of-the-art electronic control system. The block diagram of the system is shown in Figs 4 and 5. The control system is built around 8-bit, Z-80 microprocessors in a modular fashion. The motor-control-centre (MCC) which controls the different electric motors driving the hydraulic pumps is monitored and controlled by the ‘Electric Control Processing Unit (CPU)’. A number of digital input/output channels are
One of the major features of this press is the provision for data collection. Temperatures, positions, speed and strains at different locations are monitored throughout the operation of the press. Computer control is used to advantage in recording these data continuously on the PC. The data can be later recalled for detailed analysis.

Using the computer interfacing and data acquisition facility of the forge press, parameters for open die forging of titanium alloys and extrusion of advanced aluminium alloys have been established. As an illustration, a plot of forging force versus displacement during the near isothermal forging of IMI-685 material is shown in Fig. 6. Such data are useful for detailed studies on processing of various materials.

5. PROCESSING MAPS

Deformation processing of materials requires the selection of the correct process parameters, viz. temperature and strain rate, so as to increase the yield and improve the quality of the product. Trial and error methods generally employed for optimizing these
Figure 4. Block diagram of 2000 T forge press.

Figure 5. Block diagram of forge press control system.
has been interpreted to show regimes where processes such as dynamic recovery, dynamic recrystallization, void formation and wedge cracking dominate.

These maps can be easily constructed with the help of a computer software\(^6\) mentioned above. The data input for the software is obtained from simple hot compression tests on laboratory scale specimens of the material. We thus have a simple and powerful tool for optimizing the processing conditions of all materials.

6. PROCESS MODELLING FOR TITANIUM SPONGE PRODUCTION

Titanium metal is industrially produced by reducing TiCl\(_4\) with liquid magnesium or sodium in steel reactors under argon atmosphere. The reduction reaction is exothermic. The process is generally managed by controlling the process parameters like feed rate of TiCl\(_4\), reaction temperature and external cooling of the reactor. Computer-based control for sodium reduction process is adopted. A statistical control strategy is normally adopted for magnesiothermic reduction process because satisfactory models for the reaction mechanisms are not available.

In the present study at DMRL, an attempt has been made to develop a reaction model for its use in the process control. As a first step, computer-based calculations were made for prediction of temperature distribution inside the reactor using finite element method. The temperature data were utilized to calculate the reaction rate constants affecting the rate of the overall reaction.

The reaction kinetics is assumed to be determined by a combination of intrinsic reaction rate-determining factors and also the sponge growth rate kinetics involving the following steps:

(a) convective mass transfer of titanium tetrachloride to the reaction front (\(K_g\))
(b) the surface chemical reaction (\(K_s\))
(c) exchange of reactants through the porous solid barrier (over the liquid magnesium) (\(K_c\)).

6.1 Temperature Profiles

The heat generated in the reduction reactions is transferred to the reactor walls by conduction through the reaction mass. A knowledge of temperature distribution inside the reactor is essential for determining the reaction rate constants.
The governing differential equation for heat conduction in an axisymmetric cylindrical body is

\[ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} = \frac{\partial T}{\partial t} \]  

This was solved by the finite element method with the following initial boundary conditions:

- \( t = 0 \), \( T = 830 \, ^\circ C \) throughout the mass
- \( t > 0 \), \( T = 860 \, ^\circ C \) at the walls

and

\[ K \left[ \frac{\partial T}{\partial r} \frac{\partial}{\partial r} + \frac{\partial T}{\partial z} \frac{\partial}{\partial z} \right] + h (T - T_x) = 0 \]

A program has been developed in FORTRAN to solve the above equation and it was run using DPS-6/850 super mini computer for various TiCl\(_4\) feed rates. Figure 8 shows the surface temperature profiles computed for different TiCl\(_4\) feed rates.

6.2 Kinetics Modelling

The reaction rate constants of the three steps, \( K_g \), \( K_s \) and \( K_e \) were determined using the physicochemical data available in the literature. The temperature data required for these calculations were taken from the results of the program.

The overall reaction rate constant, \( K_0 \), is determined as,
Temperature profiles.

\[
\frac{1}{K_O} = \frac{1}{K_g} + \frac{1}{K_s} + \frac{1}{K_e} \quad (9)
\]

The experimental conversion rate constant \( (K_r) \) is found to be related to the overall reaction rate constant by,

\[K_r = K_e^2/h_o\]

The rate of conversion of magnesium is given as

\[ -\ln(1 - X) = 497.2 \frac{K_r}{h_o} t^2 \quad (10)\]

where \( t \) is time in seconds and \( h_o \) is the height of the initial magnesium column in the reactor. This expression is found to be valid for nearly 70 per cent conversion of magnesium.

7. CURVE FITTING

A simple yet immensely useful area where the digital computer contributes in engineering applications is that of curve fitting. We have developed a package in FORTRAN that can be used for polynomial regression curve fitting as well as adaptive piece-wise curve fitting.

For polynomial regression curve fitting, the well known least-squares method is used. In the program, either the degree of approximating polynomial may be specified or the best-fit polynomial can be obtained.

For adaptive piece-wise curve fitting, two methods called \( f \) sense and \( p \) sense are employed. The \( f \) sense is similar to the simplex method of linear programming and the \( p \) sense employs the Householder transformations. It is best to use the \( f \) sense for data containing noise, especially when the data are large.

The piece-wise curve fitting part of the package is completely adaptive in nature and is different from the traditional curve fitting methods. Whereas the traditional methods require the total number and locations of knots to be specified in advance, the present package calculates by itself the total number and location of knots needed.

The inputs for this package are: \( X-Y \) coordinates, degree of approximating polynomial, number of continuous derivatives, and error tolerance.

At DMRL this package is being used for many curve fitting applications to fit the experimental data.

REFERENCES