Modelling of Convective-Conductive Heat Transfer with Phase Change in an Electrically Heated UO_2 Pool

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Abstract

This paper describes an explicit finite element solution to transient conductive-convective heat transfer problems with phase change within an electrically heated region. The basic governing equations include the incompressible Navier-Stokes equations and the thermal energy equation. The phase change is modelled by a variant of the enthalpy method. Heat is generated by Joule effect due to the passage of an electric current for which a steady situation is assumed. An explicit scheme is used for the time integration, based on a fractional step method. A second-order Taylor-Galerkin method is introduced in the convection phase. The equations are discretized successively in space using the standard Galerkin finite element method. A reduced integration has been introduced as an option. In addition, a group representation is used for the non-linear velocity terms. To illustrate the proposed methodology, an application related to experimental tests is described.

1. Introduction

One of the critical issues of Post Accident Heat Removal (PAHR) following a hypothetical meltdown of a fast-reactor core is the problem of molten pool cooling. Out-of-pile experimental studies are in progress at the JRC Ispra and are intended to produce a molten pool of UO_2 by means of direct electrical heating. The numerical simulation of such experiments requires modelling of the transient conductive-convective heat transfer in a molten region and the corresponding behaviour of the enclosing structure. The numerical technique developed at the JRC to simulate this problem is summarized in this paper.

Section 2 of this report introduces the basic governing equations including modelling of the phase change. Section 3 presents the time discretization procedure distinguishing between the convection phase, the diffusion phase and the incompressibility phase. In section 4, the space discretization is introduced and the general solution procedure is described. Finally, section 5 is devoted to the description of a typical application related to the PAHR experimental tests.

2. Basic Equations

The basic equations governing the velocity field are the incompressible Navier-Stokes equations, and are given as

$$\rho\left(\frac{\partial \underline{u}}{\partial t} + \underline{u}\cdot\underline{\nabla u}\right) = -\underline{\nabla}p + \underline{\nabla}\cdot(2\mu\underline{\underline{D}}(\underline{u})) - \rho\underline{g}\alpha(T-T_r) \tag{1}$$

with $\underline{\nabla}\cdot\underline{u} = 0$ (2)

The transport of thermal energy is described by

$$\rho c_p\left(\frac{\partial T}{\partial t} + \underline{u}\cdot\underline{\nabla T}\right) = \underline{\nabla}\cdot(k\underline{\nabla}T) + Q. \tag{3}$$

To determine the heat sources generated by the electric current, a steady situation is assumed in which case the electrical potential satisfies the Laplace equation:

$$\underline{\nabla}\cdot(\sigma\underline{\nabla}V) = 0 \tag{4}$$

and the associated heat source is given by Joule's law:

$$Q = \sigma(\underline{\nabla}V\cdot\underline{\nabla}V). \tag{5}$$

In the above equations, t is the time, $\underline{u}$ is the velocity field, p the pressure, T the temperature, ρ the density, $\underline{\underline{D}}$ the deformation tensor, μ the dynamic viscosity, α the linear coefficient of thermal expansion, $\underline{g}$ the acceleration of gravity, T_r a reference temperature, c_p the heat capacity, k the thermal conductivity, Q the volumetric heat source, σ the electrical conductivity and V the electrical potential. The material properties are temperature dependent.

The velocity components or the total surface stress are specified on the boundary. The thermal equation requires that a temperature, a heat flux, a convective or radiative heat transfer condition be specified on the boundary. For the electrical part, the potential or its normal gradient must be imposed along the boundary. Initial conditions are given for the velocity and the temperature.

The solid to liquid phase change is modelled by a variant of the enthalpy method and is assumed to occur over a finite temperature range [1]

$$\Delta T = T_\ell - T_s \tag{6}$$

where T_ℓ is a liquidus and T_s a solidus temperature. Over this interval, the specific heat is evaluated as

$$\overset{\Delta}{c_p} = c_p + L/\Delta T \tag{7}$$

where L is the latent heat. The Navier-Stokes equations are solved in the whole region at each time interval and the velocity is simply reduced to zero in the solid zone.

3. Time Discretization

To arrive at a computationally simple and efficient method for solving the above non-linear equations, it is highly attractive to use a low-order explicit finite difference time integration procedure. However, two major problems must be faced: first, for convection-dominated problems, it is known that low-order explicit time integration schemes give poor results and secondly the incompressibility constraint and the associated pressure term in the Navier-Stokes equations have an implicit nature. In order to deal with these problems, a splitting-up (or fractional step) method is defined in which the different phases - convection, diffusion and incompressibility - are treated separately by an appropriate method [2,3].

3.1 Convection Phase

The application of first-order time integration schemes to spatially centered approximations of hyperbolic equations introduces an implicit negative viscosity which destabilizes the time integration process. To overcome this problem, a Taylor-Galerkin method is used [4]. This method defines higher-order time stepping schemes which compensate for the implicit negative viscosity by incorporating an equal amount of positive viscosity. The method uses a Taylor series expansion in the time step to derive a single step integration algorithm with improved accuracy. A second-order Taylor-Galerkin method for the forward Euler time integration scheme is applied here to the convective terms in the momentum and thermal energy equations.

The convection phase in the momentum equation is discretized as

$$\frac{u_i^* - u_i^{old}}{\Delta t} = -\underline{\nabla}\cdot(u_i\underline{u})^{old} + \frac{\Delta t}{2}\underline{\nabla}\cdot[(\underline{u}\cdot\underline{\nabla}u_i)\underline{u}]^{old} + \frac{\Delta t}{2}\underline{\nabla}\cdot[u_i(\underline{u}\cdot\underline{\nabla u})]^{old} \tag{8}$$

where u_i are the components of the velocity vector $\underline{u}$. Likewise this method is applied to the convection of the temperature field

$$\frac{T^* - T^{old}}{\Delta t} = -\underline{u}^{mean}\cdot\underline{\nabla}T^{old} + \frac{\Delta t}{2}\underline{\nabla}\cdot[(\underline{u}\cdot\underline{\nabla}T)\underline{u}]^{old}, \tag{9}$$

where

$$\underline{u}^{mean} = \frac{1}{2}(\underline{u}^{old} + \underline{u}^{new}) = \underline{u}^{old} + \frac{\Delta t}{2}\left(\frac{\partial \underline{u}}{\partial t}\right)^{old},$$

$$\underline{u}^{mean}\cdot\underline{\nabla}T^{old} = \underline{\nabla}\cdot(T^{old}\underline{u}^{mean}) = \underline{\nabla}\cdot(T\underline{u})^{old} + \frac{\Delta t}{2}\underline{\nabla}\cdot\left(T\frac{\partial \underline{u}}{\partial t}\right)^{old}.$$

The conservative form is used in the first-order time derivatives, while the advective form in the second-order time derivatives. The asterisk denote intermediate values at the end of the advection phase and Δt is the time step.

The boundary conditions of prescribed velocity and of prescribed temperature are applied to equations (8) and (9), respectively.

3.2 Diffusion Phase

This phase includes the viscosity and buoyancy terms of the Navier-Stokes equations and the diffusion and source terms of the energy equation. A simple first-order forward Euler time-integration scheme is used:

$$\rho\,\frac{\underline{u}^{**} - \underline{u}^*}{\Delta t} = \underline{\nabla}\cdot(2\mu\underline{\underline{D}}(\underline{u}^*)) - \rho\underline{g}\alpha(T^{old} - T_r) \tag{10}$$

where superscript ** refers to the intermediate velocity including the convection, viscosity and buoyancy effects and

$$\rho c_p\,\frac{T^{new} - T^*}{\Delta t} = \underline{\nabla}\cdot(k\underline{\nabla}T^*) + \sigma(\underline{\nabla}V^{new}\cdot\underline{\nabla}V^{new}) \tag{11}$$

where the electrical potential V is determined at each time step by

$$\underline{\nabla}\cdot(\sigma\underline{\nabla}V^{new}) = 0\,. \tag{12}$$

The boundary conditions of prescribed velocity or prescribed stress are applied to equation (10) while for the temperature equation (11), the complete set of boundary conditions is applied. Boundary conditions for the electrical potential are included in (12).

3.3 Incompressibility Phase

This phase calculates the final velocity field $\underline{u}^{new}$ by adding to $\underline{u}^{**}$ the dynamic effect of the pressure p^{new} determined so that the incompressibility condition remains satisfied:

$$\rho \frac{\underline{u}^{new} - \underline{u}^{**}}{\Delta t} = -\underline{\nabla} p^{new} \tag{13}$$

and

$$\underline{\nabla} \cdot \underline{u}^{new} = 0 . \tag{14}$$

Imposed pressure loads on the boundary are applied here. From the prescribed velocity field, only the normal component of the velocity is imposed in this phase [3].

4. Space Discretization

A weak formulation of the non-linear problem given in equations (8) - (14) is obtained by taking the scalar product of each equation with an arbitrary weighting function W belonging to a suitable space and then integrating by parts all the terms with second-order spatial derivatives in equations (8) - (12) and the pressure term in equation (13). The integration by parts in equations (8) and (9) introduces surface terms which account for the outflow of the quantities u_i or T along the streamlines of the convection field $\underline{u}$. The fully discretized equations are subsequently obtained by means of the conventional Galerkin-Bubnov finite element method based on four-noded isoparametric quadrilateral elements. Bilinear shape functions are employed for the velocity, temperature and electrical potential while the pressure is assumed to be elementwise constant.

To represent the convective terms more economically, the group finite element formulation is introduced [5]. A single shape function N_k is used to approximate the product that appears within the convective terms:

$$u_i u_j = \sum_k N_k (u_i u_j)_k . \tag{15}$$

In relation to the group formulation, the integrals involving the convective terms are numerically approximated by a one-point quadrature instead of a two-by-two Gaussian integration. This increases the cost effectiveness of the method with only a small loss in accuracy. The reduced integration procedure is also used for the diffusion terms together with a hourglass control scheme [6].

The Galerkin formulation of the incompressibility phase leads to a projection operation for the velocity. The pressure is given by a linear system of equations which is solved using the Cholesky decomposition method [3].

The electrical potential field is governed by a linear system. However, since the electrical conductivity depends upon the temperature, the governing matrix has to be assembled and factorized at each time step. The Cholesky decomposition method is used.

The general computational procedure to solve the coupled problem starts with the determination of the velocity field, in three distinct phases, followed by the determination of the electrical potential field, and finally the solution of the temperature field in two different phases. Updating the temperature dependent material properties is made at the beginning of each time step.

5. Application

To illustrate the proposed method, a simulation of Joule heating and subsequent melting of UO_2 powder has been made in an axisymmetric cylindrical geometry with a radius $R = 0.36$ m and a height $H = 0.17$ m, as represented in Fig. 1. The boundary conditions and the finite element mesh of 20x16 quadrilaterals are also shown in this figure.

The heat capacity, thermal conductivity and electrical conductivity of the UO_2 powder are modelled as temperature dependent properties and the liquid properties are taken to be constant. The density of the UO_2 is modelled by a constant value equal to that of the liquid at the melting temperature.

As shown in Fig. 2, the initial temperature of the powder is given as a function of the radial direction only, and is axially uniform. The values are such that all the material is initially in the solid phase. Then a potential difference is applied across the horizontal electrodes whose radius is $r = 0.17$ m. The time history of the potential drop is shown in Fig. 3(a). This generates a current passing through the powder and heats it up. The current intensity i can be calculated along a closed surface as:

$$i = - \oint \sigma \, \underline{\nabla} V \cdot \underline{dS} \qquad (16)$$

and is represented in Fig. 3(b) as a function of time. The solid-liquid phase change of the UO_2 is assumed to take place in the temperature range between $T_s = 3098$ K and $T_\ell = 3148$ K with a latent heat $L = 2.554 \cdot 10^5$ J/kg.

The convective movement due to the buoyancy terms started at 850 s. The evaluated quantity of molten material is represented in Fig. 4(c) as a function of time. The isotherms and streamlines, at a time of 1100 s, are shown in Figs. 4 and 5, respectively.

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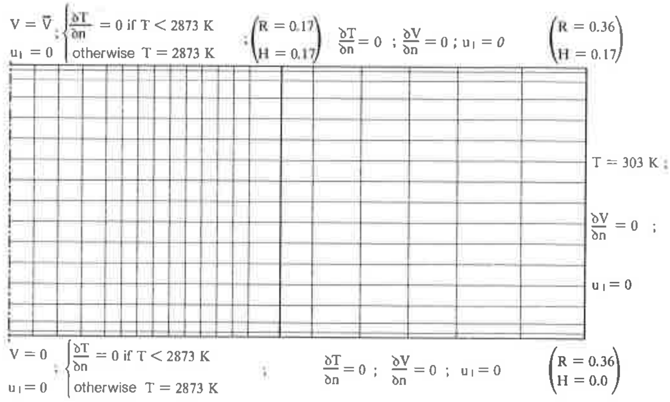

Fig. 1 - Geometry and finite element discretization

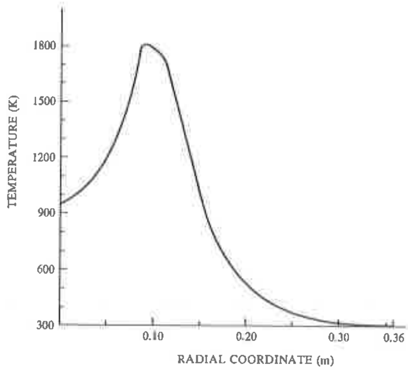

Fig. 2 - Initial temperature distribution

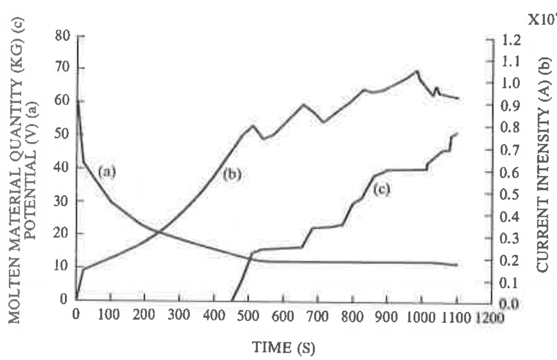

Fig. 3 - Applied potential difference across the electrodes (a), current intensity (b), molten material quantity (c) versus time

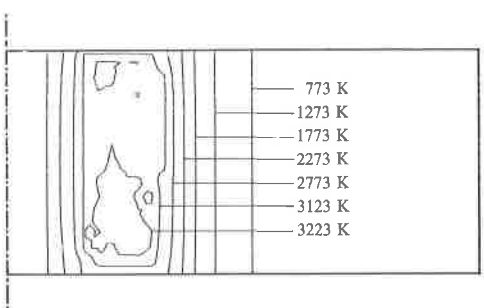

Fig. 4 - Isotherms at t = 1100 s

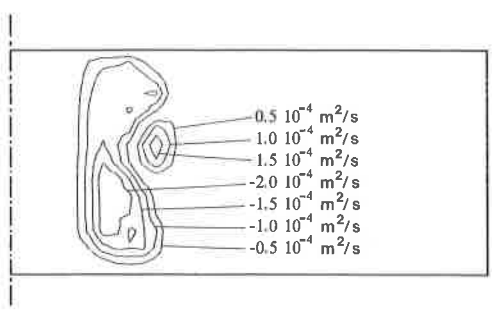

Fig. 5 - Streamlines at t = 1100 s