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Linear tetrahedral finite elements for thermal shock problems

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Received January 2005
Revised September 2005
Accepted November 2005

Abstract

Purpose – The paper seeks to present an original method for the numerical treatment of thermal shocks in non-linear heat transfer finite element analysis.

Design/methodology/approach – The 3D finite element thermal analysis using linear standard tetrahedral elements may be affected by spurious local extrema in the regions affected by thermal shocks, in such a severe ways to directly discourage the use of these elements. This is especially true in the case of solidification problems, in which melted alloys at very high temperature contact low diffusive mould materials. The present work proposes a slight modification to the discrete heat equation in order to obtain a system matrix in M-matrix form, which ensures an oscillation-free solution.

Findings – The proposed “diffusion-split” method consists basically of using a modified conductivity matrix. It allows for solutions based on linear tetrahedral elements. The performance of the method is evaluated by means of a test case with analytical solution, as well as an industrial application, for which a well-behaved numerical solution is available.

Originality/value – The proposed method should be helpful for computational engineers and software developers in the field of heat transfer analysis. It can be implemented in most existing finite element codes with minimal effort.

Keywords Thermal testing, Heat transfer, Finite element analysis, Linear programming

Paper type Research paper

1. Introduction

The solution of diffusion problems using the standard finite-element method (FEM) is often affected by severe numerical instabilities. These instabilities take for instance the form of unphysical local maxima and minima in solutions expected to be monotonic. Such a spurious behaviour evidences a violation of the maximum principle. In fact, when we discretize the diffusion operator using standard (Galerkin) finite elements, the maximum principle is not always satisfied, as discussed by several authors (Putti and Cordes, 1998; Cordes and Putti, 2001; Kosik *et al.*, 2000). The principle satisfied,

The support of Arcelor and Ascometal companies, and of the french Ministère de l'Economie, des Finances et de l'Industrie in the frame of the OSC-Continuous Casting project, is acknowledged.



a maximum/minimum can only occur either initially or at the boundary, in the latter case a flow from/to the outside must exist (Kosik *et al.*, 2000).

The constraints imposed by this principle on numerical modelling are critical in the regions where the solution exhibits steep gradients. In thermal analysis, with the temperature field as solution, we call thermal shocks these steep variations. They usually appear in the boundary vicinity in a domain initially hot (or cold) that is suddenly cooled (resp. heated) through such boundary.

Zienkiewicz and Taylor (2000) make the mathematical model responsible of the numerical instabilities associated to thermal shocks. In fact, thermal shocks arise due to the jump between initial and boundary conditions, considered to be physically unrealistic by those authors. They propose then to apply gradually the initial conditions, avoiding in such a way the problems caused by thermal shocks on numerical modelling. Unfortunately, in many important processes such as hot forming and casting, some boundary regions suffer very high cooling or heating rates, in a period of time that is very small with respect to the discretization time step, so that the initial jump in boundary conditions really exists and must be modelled. Numerous concrete examples can be given, for instance the contact between a hot metal workpiece and forming tools at a much lower temperature, or between the flow of molten metal and the components of a casting mould.

The proper modelling of thermal shocks at a given time instant is achieved provided the layer currently affected by the thermal shock be at least one-element wide (Hogge and Gerrekens, 1982; Gerrekens, 1988; Wagoner and Chenot, 2001). This is the so-called penetration depth condition. For a mesh of uniform element size Δx , the time increment Δt_{ts} required to satisfy this condition is given by:

$$\Delta t_{ts} = \alpha \frac{\rho c_p}{k} \Delta x^2 \quad (1)$$

where α is a constant of order 1 (Hogge and Gerrekens, 1982; Gerrekens, 1988; Wagoner and Chenot, 2001).

In a purely thermal analysis, thermal shocks have a relatively short-term effect, since the solution is no longer affected once the thermal shock layer is developed enough. However, in a coupled analysis, e.g. a thermo-mechanical analysis, the instabilities in the early stages may invalidate the whole solution, as it is the case for inelastic (history-dependent) materials with thermo-dependent mechanical properties.

We can also satisfy the penetration depth condition by refining the mesh in the concerned regions, as done by Sheu *et al.* (1999) for convection-diffusion and convection-diffusion-reaction problems (Sheu and Chen, 2002), with satisfactory results in terms of accuracy. The adaptive refinement technique proposed by Sheu *et al.* (1999), based on the bisection of rectangular finite elements, allows to restrict the refined grid only to the regions of large gradients, leaving the grid outside unaltered. Unfortunately, the implementation of such technique for general unstructured meshes is not as simple. Further, only 2D problems were considered in those works.

In fact, the option of mesh refinement is usually unaffordable in real 3D applications, for which the finite element grids are now frequently non-structured and composed of tetrahedral elements. Let consider for instance a metal casting problem, where an initially extremely rapid cooling process takes place at the interface between the melt and the chilled mould, requiring a highly refined mesh on both domains.

Regarding this constraint, and assuming finite element meshes not especially refined at their boundaries, let us outline then the different approaches developed to deal with thermal shocks using tetrahedral elements.

The first one arises naturally from the penetration depth condition: if the mesh must keep unchanged, a high enough time step, that is Δt_{ts} as determined by equation (1), is needed in the early stage of the simulation. Then, by using an implicit time-stepping scheme, the heat equation can be solved taking Δt_{ts} as time step without stability concerns. Unfortunately, Δt_{ts} is frequently too large for an accurate integration of the heat equation and all the other conservation equations that may be coupled with it, e.g. the momentum and chemical species balances. Jaouen (1998) has proposed to adopt Δt_{ts} as time step, and then to linearly interpolate the computed thermal solution to an adequate time step $\Delta t < \Delta t_{ts}$. This strategy, called asynchronous thermal analysis, gives satisfactory results for linear or slightly non-linear problems, which is not the case in solidification processes.

The second approach is based on the M-matrix theory (Ortega and Rheinboldt, 1970): the satisfaction of the maximum principle requires the system matrix obtained after discretization be an M-matrix (a real, non-singular $n \times n$ -matrix \mathbf{A} is an M-matrix if $\mathbf{A}^{-1} \geq 0$ and all its out-diagonal components are non-positive). Putti and Cordes (1998) and Cordes and putti (2001) proposed an orthogonal subdomain collocation (OSC) technique that produces a diffusion matrix in M-matrix-form when applied to tetrahedral finite elements in a 3D Delaunay triangulation satisfying suitable conditions on the elements geometry adjacent to the boundary affected by thermal shocks. If the capacitance matrix is lumped, it becomes an M-matrix. In such a way, the system matrix for a transient diffusion problem, being the sum of two symmetric M-matrices, is also an M-matrix. It is not longer the case when the system matrix contains an advection (non-symmetric) term, and therefore this approach cannot be generalized to advection-diffusion problems. In addition, the geometrical constraints on the mesh prevent from using general meshing codes, that generally use tetrahedral elements. This leads several authors (Letniowski, 1992; Kosik *et al.*, 2000) to directly discourage the use of linear tetrahedral finite elements; Kosik *et al.* (2000) promote to use the finite volume method (FVM) instead. However, we cannot ignore the wide diffusion of FEM in the existing codes, as well as its versatility compared to FVM.

Not only FVM but also some FEM models are free of oscillations under thermal shocks. This is the case of discontinuous Galerkin (DG) models. Pichelin and Coupez (1999) and Batkam (2002) have developed explicit and implicit DG models, respectively, to solve thermal problems on general 3D triangulations. They used P0 elements, i.e. tetrahedra with constant temperature inside. Therefore, the use of these techniques implies no more nodal but elemental unknowns. Let us remark that in a typical 3D triangulation, the number of elements is about five times greater than the number of vertex nodes. In other words, DG-P0 elements are not only less convenient than P1 elements in terms of the order of the discretization error, but also regarding the computational cost. In addition, the coupling with the resolution of complementary conservation equations, such as momentum or chemical species, for which a nodal solution may be obtained, yields to difficulties regarding the consistency of the different fields of variables.

The present work aims to retain the advantages of using P1 finite elements, making possible at the same time to model thermal shocks when small enough time increments

are used. The diffusion-split method presented here has common items with that of Jaouen (1998) regarding the idea of satisfying the penetration depth condition, as well as with those inspired by the M-matrix theory (Putti and Cordes, 1998; Cordes and Putti, 2001) that focus on the form of the system matrix. The resulting formulation, representing just a slight modification to the standard Galerkin one, can be easily implemented into existing FEM codes.

2. The heat equation

The well-known local form of the heat equation is:

$$\rho c_p \frac{dT}{dt} - \nabla(k\nabla T) = Q \quad \text{in } \Omega \quad (2)$$

where Ω is the analyzed domain, t the time variable, T the temperature, ρc_p the specific heat, k the thermal conductivity, and Q an internal heat source. First, we consider here the energy equation without possible phase change. This aspect will be discussed in Section 4.2. Equation (2) is subject to the initial condition:

$$T = T^0 \quad \text{at } t = 0 \quad (3)$$

and the following boundary conditions:

$$T = T_w \quad \text{on } \Gamma_T \quad (4)$$

$$-(k\nabla T)\mathbf{n} = q_w \quad \text{on } \Gamma_q \quad (5)$$

$$-(k\nabla T)\mathbf{n} = h(T - T_{\text{ext}}) \quad \text{on } \Gamma_c \quad (6)$$

prescribing the temperature T_w on Γ_T , the heat flux q_w through Γ_q , and the heat exchange through Γ_c due to convection to the environment at temperature T_{ext} with h as the convection coefficient; Γ_T , Γ_q , and Γ_c are non-overlapping portions of the boundary Γ of Ω being \mathbf{n} the unit normal vector pointing outwards to Γ .

3. Standard finite element formulation

The Galerkin FEM applied to the initial and boundary value problem defined by equations (2)-(6) yields the system of first-order differential equations (see the classical FEM literature, e.g. Zienkiewicz and Taylor, 2000, for details):

$$\mathbf{C} \frac{d\mathbf{T}}{dt} + \mathbf{K}\mathbf{T} - \mathbf{F} = \mathbf{0} \quad (7)$$

where \mathbf{T} is the vector of nodal unknown temperatures, \mathbf{C} is the capacitance matrix, \mathbf{K} the conductivity matrix, and \mathbf{F} is the internal source and external flux vector, defined as:

$$\mathbf{C}_{ij} = \int_{\Omega} \rho c_p N_i N_j dV \quad (8)$$

$$\mathbf{K}_{ij} = \int_{\Omega} k \nabla N_i \cdot \nabla N_j \, dV + \int_{\Gamma_c} h N_i N_j \, dS \quad (9)$$

$$\mathbf{F}_i = \int_{\Omega} Q N_i \, dV + \int_{\Gamma_c} q_w N_i \, dS + \int_{\Gamma_c} h T_{\text{ext}} N_i \, dS \quad (10)$$

being N_i the interpolation function associated with node i . The fully-implicit Euler-backward scheme is used to integrate equation (7) in time. Then, once the temperature at time t , say T^t , is known, the temperature T at time $t + \Delta t$ can be obtained by solving the discrete equation:

$$\mathbf{C} \frac{\mathbf{T} - \mathbf{T}^t}{\Delta t} + \mathbf{K}\mathbf{T} - \mathbf{F} = \mathbf{0} \quad (11)$$

4. The diffusion-split method

As mentioned earlier, it is known that the spurious solutions observed in case of thermal shocks are associated with the form of the system matrix (Putti and Cordes, 1998; Cordes and Putti, 2001; Kosik *et al.*, 2000). Then, let us rewrite the governing discrete equation (11) by splitting the diffusion term as follows:

$$\mathbf{C} \frac{\mathbf{T} - \mathbf{T}^t}{\Delta t} + \mathbf{K}^* \mathbf{T} - \mathbf{F} = \mathbf{S} \quad (12)$$

where:

$$\mathbf{S} = (\mathbf{K}^* - \mathbf{K})\mathbf{T} \quad (13)$$

with:

$$\mathbf{K}_{ij}^* = \int_{\Omega} k^* \nabla N_i \cdot \nabla N_j \, dV + \int_{\Gamma_c} h N_i N_j \, dS \quad (14)$$

Now, assuming \mathbf{S} to be an explicit source term, an augmented conductivity k^* can be defined to satisfy the penetration depth condition for Δt as the first time step:

$$k^* = \begin{cases} k & \text{if } \Delta t_{\text{ts}} \leq \Delta t \\ k \frac{\Delta t_{\text{ts}}}{\Delta t} & \text{if } \Delta t_{\text{ts}} > \Delta t \end{cases} \quad (15)$$

The value of k^* decreases with time from the value given by equation (15) at $t = 0$ to the real conductivity k when $t + \Delta t \geq \Delta t_{\text{ts}}$. Therefore, in the latter case, equations (11) and (12) are identical. Regarding the source term \mathbf{S} , an explicit approximation is built by taking a known value of \mathbf{T} in equation (13), \mathbf{T}^t being the best choice since any approximation to \mathbf{T} obtained using an explicit time-stepping scheme may be affected by instabilities. Thus:

$$\mathbf{S} \approx (\mathbf{K}^* - \mathbf{K})\mathbf{T}^t \quad (16)$$

It is interesting to note that during the early stages of the simulation, there is no sensible variation of the temperature outside those regions under thermal shocks, and hence the approximation implied by equation (16) is local and temporary.

4.1 The penetration depth condition on unstructured meshes

For non-uniform unstructured meshes, the computation of Δt_{ts} using equation (1) complicates due to the uncertain definition of the mesh size Δx . Jaouen (1998) explores all the non-adiabatic boundaries of the analysed domain, determining the minimum, the maximum, and the average value of Δx , the choice of the adequate value left to the user's expertise. Being the square value of Δx involved in equation (1), the influence of this choice on the proper modeling of thermal shocks is crucial. According to our practical experience, Δt_{ts} is underestimated when computed with the minimum Δx , and hence the penetration depth condition is clearly not satisfied in some regions. On the other hand, the use of the maximum Δx , leading to an overestimation of Δt_{ts} , has a detrimental effect on the accuracy of the diffusion-split method, producing an excessively large k^* . Using the average mesh size, the result is uncertain.

If it were possible to identify a priori those regions under thermal shocks, and the mesh within each region were quite uniform, then we could define a local Δt_{ts} (and hence a local k^*). Anyway, for the sake of simplicity, we prefer to determine a global Δt_{ts} . It is worth noting that in the case of monotonic cooling, Δt_{ts} can be easily determined by solving equation (12) for increasing Δt_{ts} until the computed temperature not exceed the previous one at each node of the mesh. This should not take more than a few iterations to obtain an accurate enough value of Δt_{ts} . Normally, this is made only once at the beginning of the simulation, so the additional computational cost is negligible in practice.

4.2 The diffusion-split method for solidification problems

In the case of liquid-solid phase change, we introduce the enthalpy function:

$$H(T) = \int_0^T \rho c_p(T) dT + g_l \rho L \quad (17)$$

where g_l is the volumetric fraction of liquid ($0 \leq g_l \leq 1$, $g_l = 0$ in the solid, $g_l = 1$ in the liquid), assumed to be a given function of the temperature, and L the specific latent heat of solidification. From the enthalpy function, we can derive an effective heat capacity ρc_{eff} , which accounts for phase change effects. Assuming that g_l is a function of the temperature only, for the sake of simplicity, it is defined as:

$$\rho c_{eff} = \frac{\partial H}{\partial T} = \rho c_p + \rho L \frac{dg_l}{dT} \quad (18)$$

subject to the initial condition (3) and the boundary conditions (4)-(6). In general, equation (18) is only valid in a weak sense, since the first term resembles the Dirac's delta function for eutectic or isothermal transformations. The direct evaluation of ρc_{eff} as done in the early solidification models (Bonacina *et al.*, 1973) yields highly inaccurate results in problems with a narrow solidification range unless in a huge number of sampling points be placed in each element affected by phase change. For this reason, ρc_{eff} is usually regularized as proposed for instance by Lemmon (1979, 1981):

$$\rho c_{\text{eff}} = \frac{\|\nabla H\|}{\|\nabla T\|} \quad (19)$$

where $\|(\ast)\|$ is the norm of vector (\ast) , and spatial regularization is obtained by assuming H interpolated in the same way as T . Formula (18) yields an element-wise constant effective heat capacity for linear tetrahedral and triangular elements. Now the discrete heat equation involving phase change can be written as:

$$\mathbf{C}_{\text{eff}} \frac{\mathbf{T} - \mathbf{T}^t}{\Delta t} + \mathbf{K}\mathbf{T} - \mathbf{F} = \mathbf{0} \quad (20)$$

whose form is identical to that of the original equation, only requiring to replace ρc_p by ρc_{eff} in the definition of the heat capacitance matrix \mathbf{C} , equation (7).

In consequence, the implementation of the diffusion-split method in this case is essentially the same as described above, except for determining Δt_{ts} , which cannot in general be estimated a priori. In the elements undergoing phase change, ρc_{eff} is considerably greater than ρc_p . Also, it is highly variable with time. In this case, Δt_{ts} should be determined at each time step until thermal shocks effects completely disappear. Actually, a general and efficient procedure to determine Δt_{ts} for non-linear problems and unstructured meshes remains a research item.

5. Applications

5.1 Test case: one-dimensional cooling

Let us consider first the 1D case of a semi-infinite domain, initially at the uniform temperature $T^0 = 800^\circ\text{C}$, whose surface temperature suddenly falls to a value $T_w = 25^\circ\text{C}$, kept constant. Table I lists the material properties. This problem illustrates some typical features of thermal analysis in steel hot forming. We use a 3D structured triangulation with uniform element size $\Delta x = 2\text{ mm}$ in the flux direction. A constant time step $\Delta t = 0.1\text{ s}$ is adopted.

In this case, the original Galerkin solution is affected by thermal shocks, as evidenced by the spurious temperature increment of 13.2°C at the first time step for a node located 4 mm-far from the cooled wall (Figure 1).

For linear tetrahedral finite elements and consistent (not-lumped) capacitance matrix, the constant α in equation (1) is taken equal to unity (Jaouen, 1998), obtaining then $\Delta t_{\text{ts}} = 0.748\text{ s}$. However, using the procedure described in the preceding section, every nodal point is already free of unphysical heating for $\Delta t_{\text{ts}} = 0.544\text{ s}$. And, by tolerating a small temperature overshoot of 0.1°C for instance, this value reduces to 0.287 s . The augmented conductivity k^* is computed using equation (15) for the first time step, and decreases linearly with time until reach the original value k for $t \geq \Delta t_{\text{ts}}$. Let us remind that the closer the values of Δt and Δt_{ts} , the lesser the artificial increment of the conductivity in the thermal regions when the diffusion-split method is used. This is clearly evident in Figure 1 where the temperature rate at the first time step increases as k^* does, which is an unphysical but numerical effect of the diffusion-split method.

Table I.
Material properties for
the 1D cooling problem

Density (ρ)	7,800 kg/m ³
Heat capacity (c_p)	360 J/(kg°C)
Thermal conductivity (k)	15 W/(m°C)

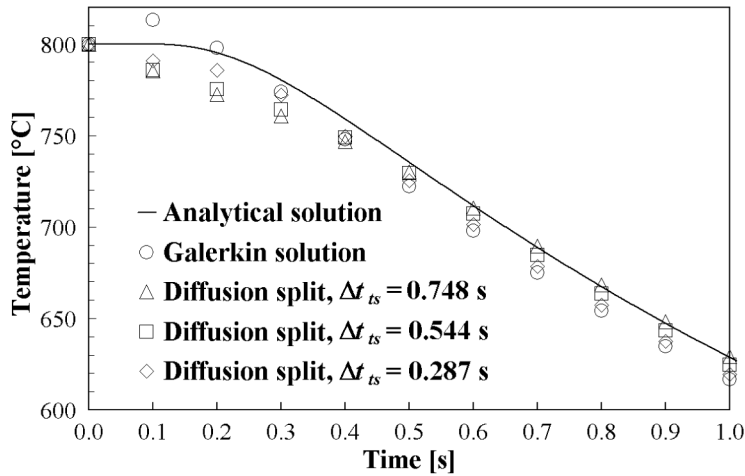


Figure 1. One-dimensional academic test for thermal shock. Early evolution of the temperature at a node situated 4 mm-far from the chilled wall

5.2 Ingot solidification

We consider now the ingot casting model shown in Figure 2. The material properties of each component and other model parameters are listed in Table II. For the sake of simplicity, the solid fraction is supposed to be linear between the liquidus and solidus temperature. The model is axisymmetric, and a small sector of 12° is considered for 3D simulation. The ingot has a radius of 0.433 m at the top, and its total height is 2.58 m. This is a typical simulation illustrating the problems posed by thermal shocks in current 3D applications.

First, due to the very different diffusion properties of the different components, an excessively large time step is needed in order to satisfy the penetration depth condition. Taking into account the average element size (since the mesh density is quite uniform in each subdomain), equation (1) yields the values of Δt_{ts} listed in Table II.

For $\Delta t = 0.1$ s (an adequate value of the time increment for the early stages of the simulation), the obtained solution using standard Galerkin FEM with P1 elements is completely useless, exhibiting nodal temperatures that are 94°C above the initial temperature in the ingot. The solution is even worse in the domain of smallest diffusivity: in the casting powder, this spurious overheating attains 320°C , while negative temperatures are observed in the insulator.

In order to apply the diffusion-split solution, we choose to admit an overheating of 0.5°C in the ingot at the first time step. In such a way, the value of Δt_{ts} falls to 11 s, and considerably less artificial diffusion is added. A reference solution is obtained using the above mentioned explicit Taylor DG (TDG) method with P0 triangular elements (Pichelin and Coupez, 1999), proved to be free of instabilities caused by thermal shocks.

Figure 3 shows the temperature through a cross section of the ingot, situated 1.60 m far from the bottom, at the beginning of simulation ($t = 1.1$ s). A good agreement between diffusion-split and TDG solutions is observed. The points in the plot correspond to the centre of the TDG elements, while they are nodal values for the 3D triangulation, letting us note that the 2D TDG mesh is about 2.5-times denser than the 3D mesh in this region.

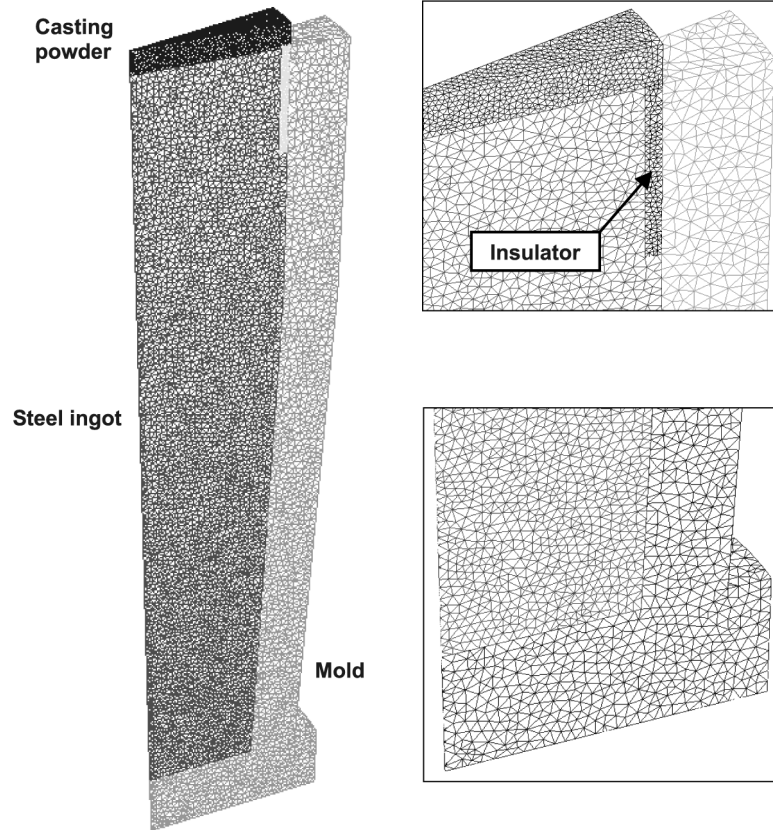


Figure 2.
Industrial application test.
FEM model of an ingot
casting process

Once the solidification has progressed in the ingot, the agreement between both models remains satisfactory, as shown in Figure 4 for the temperature field at time $t = 20$ min and $t = 2$ h. The slight differences can be attributed to the effects of nodal smoothing, which is a necessary post-treatment in the case of TDG calculations, and to the differences in mesh densities.

6. Conclusions

The diffusion-split method makes possible to solve problems involving thermal shocks using the FEM with linear tetrahedral elements. Compared to the previous models using P1 elements, the diffusion-split method works for general meshes, contrary to the OSC-FEM method (Putti and Cordes, 1998; Cordes and Putti, 2001), and the heat equation is solved for an adequate time step (i.e. not excessively large), contrary to the so-called asynchronous analysis (Jaouen, 1998). Compared to the DG methods using P0 elements (Pichelin and Coupez, 1999; Batkam, 2002), the present model has not only a better accuracy order, but also a smaller computational cost. The present model can be implemented in most existing FEM codes with a minimal effort.

<i>Ingot</i>	
Density (ρ)	7,450 kg/m ³
Heat capacity (c_p)	510 J/(kg°C)
Thermal conductivity (k)	30 W/(m°C)
Latent heat (L)	241,000 J/kg
Solidus temperature	1,432°C
Liquidus temperature	1,454°C
Initial temperature	1,534°C
Time step (Δt_{ts})	20.3 s
<i>Mold</i>	
Density (ρ)	7,200 kg/m ³
Heat capacity (c_p)	600 J/(kg°C)
Thermal conductivity (k)	30 W/(m°C)
Initial temperature	80°C
Time step (Δt_{ts})	36.3 s
<i>Insulator</i>	
Density (ρ)	780 kg/m ³
Heat capacity (c_p)	848.5 J/(kg°C)
Thermal conductivity (k)	0.82 W/(m°C)
Initial temperature	60°C
Time step (Δt_{ts})	41.3 s
<i>Casting powder</i>	
Density (ρ)	500 kg/m ³
Heat capacity (c_p)	1,100 J/(kg°C)
Thermal conductivity (k)	0.35 W/(m°C)
Initial temperature	1,534°C
Time step (Δt_{ts})	70.3 s
<i>Interfaces between materials</i>	
Heat exchange coefficient (h)	1,000 W/(m ² °C)
<i>Interfaces with air</i>	
Heat exchange coefficient (h)	30 W/(m ² °C)
External temperature (T_{ext})	20°C

Table II. Material properties and simulation data for the ingot solidification problem

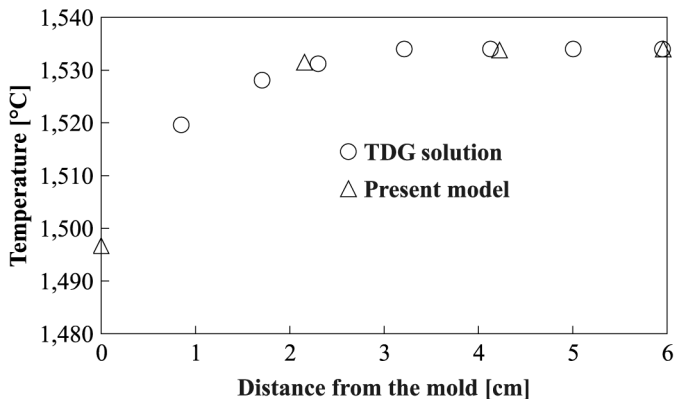


Figure 3. Temperature in the ingot at time 1.1 s in a cross section located 1.6 m-far from the ingot bottom

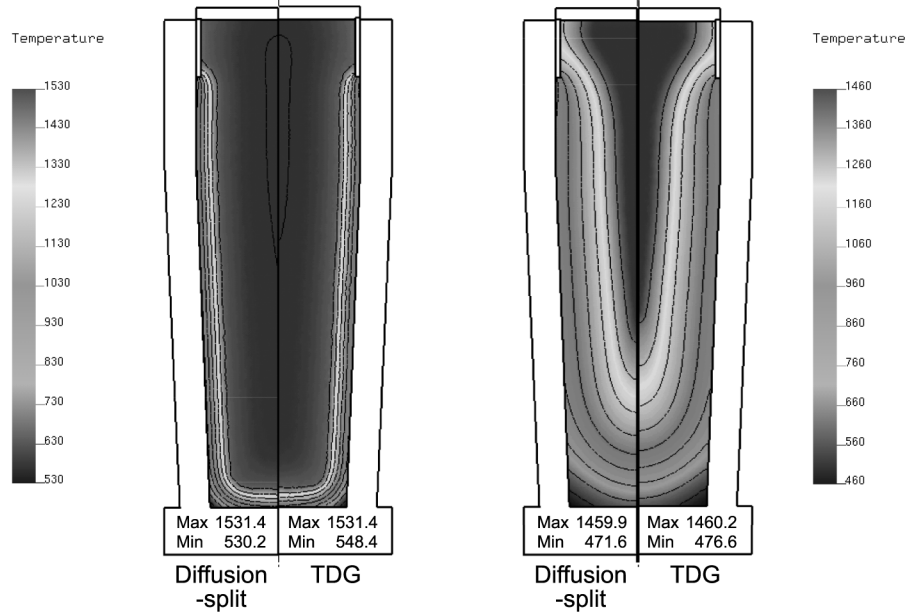


Figure 4. Temperature in the ingot after 20 min (left) and 2 hours (right). On the left side ingot sections, the temperature distribution obtained with the proposed diffusion-split method (3D calculation). On the right side, the same distribution as obtained by the explicit TDG method (2D calculation)

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