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Application of Diffuse Approximate Method in Convective-Diffusive Solidification Problems

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Abstract: The steady-state convective-diffusive solid-liquid phase change problem associated with temperature fields in direct-chill, semi-continuously cast billets and slabs from aluminum alloys has been solved by the Diffuse Approximate Method (DAM). The solution is based on formulation, which incorporates the mixture continuum physical model, nine-noded support, second order polynomial trial functions, and Gaussian window weighting functions. Realistic boundary conditions and temperature variation of material properties are included. Two-dimensional test case solution is shown, verified by comparison with the Finite Volume Method (FVM) results for coarse and fine grid arrangement.

1 Introduction

Direct-chill (DC) casting is currently the most common [Altenpohl (1998)] semi-continuous casting practice in production of aluminum alloys. The process involves molten metal being feed through a bottomless water-cooled mould where it is sufficiently solidified around the outer surface that it takes the shape of the mould and acquires sufficient mechanical strength to contain the molten core at the center. As the strand emerges from the mould, water impinges directly from the mould onto the surface (direct-chill), falls over the cast surface and completes the solidification. Related transport, solid-mechanics, and phase change kinetics phenomena are extensively studied [Beckermann (2002)] and many different numerical methods have been used in the past to solve the transport phenomena in the casting. The proper prediction of the temperature, velocity, species, and phase fields in the product is one of the prerequisites for automation of the process and related optimization with respect to its quality and productivity. The FVM represents one of the most widely used techniques [Versteeg and Malalasekera (1995), Atluri, Han, and Rajendran (2004)] for solving the discussed problem. Even when using this classical numerical method in involved coupled transport phenomena context, i.e. prediction of the macrosegregation, several not sufficiently understood iteration scheme issues [Venneker and Katgerman (2002)] surprisingly appear. Several mesh-reduction techniques such as the Boundary Element Method (BEM) have been used in the past to solve the heat transfer in respective DC casting model. The use of classical BEM in the two-domain context of solidification has been developed in [Fic, Nowak, and Bialecki (2000)]. The use of Dual Reciprocity Boundary Element Method (DRBEM) in the framework of the one-domain context has been developed in [Šarler and Mencinger (1999)]. The use of Radial Basis Function Collocation Method (RBFCM) in present context has been pioneered in [Šarler, Kovačević and Chen (2003)]. In this paper, the DAM [Nayroles, Touzot, and Villon (1991); Sadat and Prax (1996)] is upgraded to nonlinear convective-diffusive transport phenomena problems with nonlinear material properties and phase change, and applied to the posed industrial problem. The present research has been incited by the need for straightforward numerical resolution refinement in areas with high gradients and difficulties in application of the FVM in macrosegregation problems.

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2 Governing Equations

The heat transfer in DC casting can be reasonably represented in the framework of the mixture continuum formulation [Bennon and Incropera (1987)] which assumes local thermodynamic equilibrium between the phases. This formulation can in solidification context involve quite complicated constitutive relations. This paper focuses on convective-diffusive heat transport. Consider a connected fixed domain Ω with boundary Γ occupied by a phase change material described with the temperature dependent density $\rho_{\wp}$ of the phase $\wp$, temperature dependent specific heat at constant pressure $c_{\wp}$, effective thermal conductivity k, and the specific latent heat of the solid-liquid phase change h_m. The mixture continuum formulation of the enthalpy conservation for the assumed system is

$$\frac{\partial}{\partial t}(\rho h)+\nabla\cdot(\rho\vec{v}h)=\nabla\cdot(k\nabla T)$$
$$+\nabla\cdot\left(\rho\vec{v}h-f_S^V\rho_S\vec{v}_S h_S-f_L^V\rho_L\vec{v}_L h_L\right) \quad (1)$$

with subscripts S and L denoting the solid and the liquid phase, respectively. The mixture density is defined as $\rho=f_S^V\rho_S+f_L^V\rho_L$, the mixture velocity is defined as $\rho\vec{v}=f_S^V\rho_S\vec{v}_S+f_L^V\rho_L\vec{v}_L$, and the mixture enthalpy is defined as $h=f_S^V h_S+f_L^V h_L$. The constitutive mixture temperature - mixture enthalpy relationships are

$$h_S=\int_{T_{ref}}^{T}c_S dT \quad h_L=h_S(T)+\int_{T_S}^{T}(c_L-c_S)dT+h_m \quad (2)$$

with T_{ref} and T_S standing for the reference temperature and solidus temperature, respectively. Thermal conductivity and specific heat of the phases can arbitrarily depend on temperature. The liquid volume fraction f_L^V is assumed to vary from 0 to 1 between solidus T_S and liquidus temperature T_L. We seek for mixture temperature at time $t_0+\Delta t$ by assuming known temperature and velocity fields at time t_0, and boundary conditions.

3 Solution Procedure

The solution of the problem is demonstrated on the general transport equation defined on a fixed domain Ω with boundary Γ, standing for a reasonably broad spectra of mass, energy, momentum and species transfer problems (and includes also equation (1) as a special case).

$$\frac{\partial}{\partial t}[\rho C(\Phi)]+\nabla\cdot[\rho\vec{v}C(\Phi)]=-\nabla\cdot(-\mathbf{D}\nabla\Phi)+S \quad (3)$$

with $\rho,\Phi,t,\vec{v},\mathbf{D}$, and S standing for density, transport variable, time, velocity, diffusion matrix and source, respectively. Scalar function C stands for possible more involved constitutive relations between conserved and diffused quantities. The solution of the governing equation for the transport variable at the final time $t_0+\Delta t$ is sought, where t_0 represents the initial time and Δt the positive time increment. The solution is constructed by the initial and boundary conditions that follow. The initial value of the transport variable $\Phi(\vec{p},t)$ at point with position vector $\vec{p}$ and time t_0 is defined through the known function Φ_0

$$\Phi(\vec{p},t)=\Phi_0(\vec{p});\ p\in\Omega+\Gamma \quad (4)$$

The boundary Γ is divided into not necessarily connected parts $\Gamma=\Gamma_D\cup\Gamma_N\cup\Gamma_R$ with Dirichlet, Neumann and Robin type boundary conditions, respectively. These boundary conditions are at the boundary point $\vec{p}$ with normal $\vec{n}_\Gamma$ and time $t_0<t\le t_0+\Delta t$ defined through known functions Φ_Γ^D, Φ_Γ^R, $\Phi_{\Gamma ref}^R$

$$\Phi=\Phi_\Gamma^D;\ \vec{p}\in\Gamma_D$$
$$\frac{\partial}{\partial n_\Gamma}\Phi=\Phi_\Gamma^N;\ p\in\Gamma_N$$
$$\frac{\partial}{\partial n_\Gamma}\Phi=\Phi_\Gamma^R\left(\Phi-\Phi_{\Gamma ref}^R\right);\ p\in\Gamma_R \quad (5)$$

The involved parameters of the governing equation and boundary conditions are assumed to depend on the transport variable, space and time. The solution procedure is in this paper based on the combined explicit-implicit scheme. The discretisation in time can be written as

$$\frac{\partial}{\partial t}(\rho C(\Phi))\approx\frac{\rho C-\rho_0 C_0}{\Delta t}$$
$$\approx\frac{\overline{\rho}\overline{C}+\overline{\rho}\frac{d\overline{C}}{d\Phi}\left(\Phi-\overline{\Phi}\right)-\rho_0 C_0}{\Delta t} \quad (6)$$

by using the two-level time discretisation and Taylor expansion of the function $C(\Phi)$. The known quantities are denoted with overbar. The source term can be expanded as

$$S(\Phi)\approx\overline{S}+\frac{d\overline{S}}{d\Phi}\left(\Phi-\overline{\Phi}\right) \quad (7)$$

The unknown Φ can be calculated from the equation

$$\Phi=[\frac{\rho_0}{\Delta t}C_0-\frac{\overline{\rho}}{\Delta t}\overline{C}+\frac{\overline{\rho}}{\Delta t}\frac{d\overline{C}}{d\Phi}\overline{\Phi}+\nabla\cdot(\mathbf{D}_0\nabla\Phi_0)$$
$$-\nabla\cdot(\rho_0\vec{v}_0 C_0)+\overline{S}-\frac{d\overline{S}}{d\Phi}\overline{\Phi}]/[\frac{\overline{\rho}}{\Delta t}\frac{d\overline{C}}{d\Phi}-\frac{d\overline{S}}{d\Phi}] \quad (8)$$

The value of the transport variable Φ_n is solved in a set of nodes $\vec{p}_n; n = 1, 2, ..., N$ of which N_Ω belong to the domain and N_Γ to the boundary. The iterations over one timestep are completed when the equation (9) left is satisfied, and the steady-state is achieved when the equation (9) right is achieved

$$\max\left|\Phi_n - \overline{\Phi}_n\right| \leq \Phi_{itr} \quad \max\left|\Phi_n - \Phi_0\right| \leq \Phi_{ste} \tag{9}$$

The value of the unknown derivatives of the variable Φ_n in point $\vec{p}_n$ is approximated by the moving least squares method which uses the values of Φ_i at I points $\vec{p}_i;\ i = 1, 2, ..., I$, situated in the vicinity of and including $\vec{p}_n$. One can write the following approximation of the function and its first and second order partial derivatives

$$\Phi(\vec{p}) \approx \textstyle\sum_{k=1}^{K} {}_n\alpha_k \psi_k(\vec{p} - \vec{p}_n) \tag{10}$$

$$\frac{\partial}{\partial p_\varsigma}\Phi(\vec{p}) \approx \textstyle\sum_{k=1}^{K} {}_n\alpha_k \frac{\partial}{\partial p_\varsigma}\psi_k(\vec{p} - \vec{p}_n) \tag{11}$$

$$\frac{\partial^2}{\partial p_{\varsigma\xi}}\Phi(\vec{p}) \approx \textstyle\sum_{k=1}^{K} {}_n\alpha_k \frac{\partial^2}{\partial p_{\varsigma\xi}}\psi_k(\vec{p} - \vec{p}_n); \quad \varsigma, \xi = x, y; \tag{12}$$

Functions ψ_k have been chosen as polynomials $\psi_1 = 1$, $\psi_2(\vec{p}) = p_x$, $\psi_3 = p_y$, $\psi_4(\vec{p}) = p_x p_y$, $\psi_5(\vec{p}) = p_x^2$, $\psi_6 = p_y^2$, i.e. $K = 6$. The initial conditions are assumed to be known in all nodes $\vec{p}_n$. The coefficients ${}_n\alpha_k$ can be calculated from the minimization of the following functional

$$\begin{aligned}
&\Im({}_n\vec{\alpha}) = \\
&\sum_{i=1}^{I}\Upsilon_{\Omega i}\omega_n(\vec{p}_i - \vec{p}_n)\left[\Phi_i - \textstyle\sum_{k=1}^{K} {}_n\alpha_k\psi_k(\vec{p}_i - \vec{p}_n)\right]^2 \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{D}\omega_n(\vec{p}_i - \vec{p}_n)\left[\Phi_{\Gamma i}^{D} - \textstyle\sum_{k=1}^{K} {}_n\alpha_k\psi_k(\vec{p}_i - \vec{p}_n)\right]^2 \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{N}\omega_n(\vec{p}_i - \vec{p}_n)\left[\Phi_{\Gamma i}^{N} - \textstyle\sum_{k=1}^{K} {}_n\alpha_k\frac{\partial}{\partial n_\Gamma}\psi_k(\vec{p}_i - \vec{p}_n)\right]^2 \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{R}\omega_n(\vec{p}_i - \vec{p}_n) \\
&[\Phi_{\Gamma i}^{R}\left(\textstyle\sum_{k=1}^{K} {}_n\alpha_k\psi_k(\vec{p}_i - \vec{p}_n) - \Phi_{\Gamma ref i}^{R}\right) \\
&-\textstyle\sum_{k=1}^{K} {}_n\alpha_k\frac{\partial}{\partial n_\Gamma}\psi_k(\vec{p}_i - \vec{p}_n)]^2
\end{aligned} \tag{13}$$

This leads to the following system of $K \times K$ equations for calculation of the unknown coefficients ${}_n\alpha_k$ in each of the points $\vec{p}_n$

$$\textstyle\sum_{k=1}^{K} {}_nA_{jkn}\alpha_k = {}_nb_j; \quad j = 1, 2, ..., K \tag{14}$$

$$\begin{aligned}
{}_nA_{jk} &= \sum_{i=1}^{I}\Upsilon_{\Omega i}\psi_j(\vec{p}_i - \vec{p}_n)\omega_n(\vec{p}_i - \vec{p}_n)\psi_k(\vec{p}_i - \vec{p}_n) \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{D}\psi_j(\vec{p}_i - \vec{p}_n)\ \omega_n(\vec{p}_i - \vec{p}_n)\psi_k(\vec{p}_i - \vec{p}_n) \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{N}\frac{\partial}{\partial n_\Gamma}\psi_j(\vec{p}_i - \vec{p}_n)\omega_n(\vec{p}_i - \vec{p}_n)\frac{\partial}{\partial n_\Gamma}\psi_k(\vec{p}_i - \vec{p}_n) \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{R}\left(\Phi_{\Gamma ref i}^{R}\psi_j(\vec{p}_i - \vec{p}_n) + \frac{\partial}{\partial n_\Gamma}\psi_j(\vec{p}_i - \vec{p}_n)\right)\omega_n \\
&\cdot(\vec{p}_i - \vec{p}_n)\left(\Phi_{\Gamma ref i}^{R}\psi_k(\vec{p}_i - \vec{p}_n) + \frac{\partial}{\partial n_\Gamma}\psi_k(\vec{p}_i - \vec{p}_n)\right)
\end{aligned} \tag{15}$$

$$\begin{aligned}
{}_nb_j &= \sum_{i=1}^{I}\Upsilon_{\Omega i}\psi_j(\vec{p}_i - \vec{p}_n)\omega_n(\vec{p}_i - \vec{p}_n)\Phi_i + \\
&\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{D}\psi_j(\vec{p}_i - \vec{p}_n)\ \omega_n(\vec{p}_i - \vec{p}_n)\Phi_{\Gamma i}^{D} \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{N}\frac{\partial}{\partial n_\Gamma}\psi_j(\vec{p}_i - \vec{p}_n)\omega_n(\vec{p}_i - \vec{p}_n)\Phi_{\Gamma i}^{N} \\
&+\sum_{i=1}^{I}\Upsilon_{\Gamma i}^{R}[\left(\Phi_{\Gamma i}^{R}\right)^2\Phi_{\Gamma ref i}^{R}\psi_j(\vec{p}_i - \vec{p}_n) + \\
&\Phi_{\Gamma i}^{R}\Phi_{\Gamma ref i}^{R}\frac{\partial}{\partial n_\Gamma}\psi_j(\vec{p}_i - \vec{p}_n)]\omega_n(\vec{p}_i - \vec{p}_n)
\end{aligned} \tag{16}$$

The following point condition indicators have been used in equations (13,14,15,16)

$$\Upsilon_{\Omega i}^{D} = \begin{cases} 1; \vec{p} \in \Omega \\ 0; \vec{p} \notin \Omega \end{cases} \quad \Upsilon_{\Gamma i}^{D} = \begin{cases} 1; \vec{p} \in \Gamma^D \\ 0; \vec{p} \notin \Gamma^D \end{cases}$$

$$\Upsilon_{\Gamma i}^{N} = \begin{cases} 1; \vec{p} \in \Gamma^N \\ 0; \vec{p} \notin \Gamma^N \end{cases} \quad \Upsilon_{\Gamma i}^{R} = \begin{cases} 1; \vec{p} \in \Gamma^R \\ 0; \vec{p} \notin \Gamma^R \end{cases} \tag{17}$$

The following weighting function has been chosen

$$\begin{aligned}
&\omega_n(\vec{p}) = \exp\left(-c_n\vec{p}\cdot\vec{p}/\sigma_n^2\right); |\vec{p}| \leq \sigma_n; \\
&\omega_n(\vec{p}) = 0; |\vec{p}| > \sigma_n
\end{aligned} \tag{18}$$

according with the recommendations from [Sadat and Prax (1996)] with $c_n = 7$. The size of support σ_n is chosen to contain 9 nodes. The calculation over one timestep involves the following operations: I) coefficients ${}_n\alpha_k$ are calculated from initial conditions in the domain nodes from system (14), II) Equation (8) is used to calculate unknowns in the domain nodes at $t_0+\Delta t$, III) unknowns at the Dirichlet boundary at time $t_0+\Delta t$ are determined from the Dirichlet boundary conditions, IV) ${}_n\alpha_k$ at time $t_0+\Delta t$ are calculated in the domain nodes from system (14), V) finally, the unknowns at time $t_0+\Delta t$ in the Neumann and Robin boundary points are determined from equation (10) by extrapolation from the nearest domain node.

4 Numerical Example

This section elaborates the solution of a simplified model of the DC casting process by the developed DAM in two dimensions. The steady state solution is shown in this paper, approached by a false transient calculation using a fixed timestep of 0.5s for uniform 125×25 node arrangement and 0.1s for uniform 250×50 node arrangement. The temperature iteration error T_{itr} has been set to $0.001K$ and the steady state criterion T_{ste} to $0.01K$. The enthalpy reference temperature T_{ref} has been set to $0K$. The following simplified DC casting case is considered. The computational domain is a rectangle (coordinates $p_x,\ p_y$) $-1.25m \le p_x \le 0m$, $0m \le p_y \le 0.25m$. The boundary conditions on the top at $p_x = 0m$ are of the Dirichlet type with $T_\Gamma^D = 980K$, and the boundary conditions at the bottom at $p_x = -1.25m$ are of the Neumann type with $F_\Gamma^N = 0W/m^2$. The boundary conditions at the outer surface are of the Robin type with $T_{\Gamma ref}^R = 298K$. The heat transfer coefficients between $0m \le p_x \le -0.01m$, $-0.01m < p_x \le -0.06m$, $-0.06m < p_x \le -0.1m$, and $-0.1m < p_x \le -1.25m$, are $T_\Gamma^R = 0W/m^2K$, $T_\Gamma^R = 3000W/m^2K$, $T_\Gamma^R = 150W/m^2K$, and $T_\Gamma^R = 4000W/m^2K$, respectively. Material properties correspond to a simplified Al4.5%Cu alloy [Šarler and Mencinger (1999)]: $\rho_S = \rho_L = 2982kg/m^3$, $k_S = 120.7W/mK$, $k_L = 57.3W/mK$, $k = f_S^V k_S + f_L^V k_L$, $c_S = 1032W/mK$, $c_L = 1179W/mK$, $h_M = 348.2kJ/kgK$, $T_S = 775K$, $T_L = 911K$. The liquid fraction increases linearly between T_S and T_L. The initial temperature grows linearly with the p_x coordinate from $298K$ at the bottom to $980K$at the top of the slab. The uniform casting velocity is $v_{Sx} = v_{Lx} = -0.000633m/s$, $v_{Sy} = v_{Ly} = 0m/s$. The DAM solution has been obtained on equidistant 125×25 and 250×50 node arrangements. The calculated results for 125×25 node arrangement are shown in Figure 1, together with the reference FVM results, calculated in the same nodes. Visual comparison of the results on finer grid arrangement 250×50 shows no difference between the two methods. Absolute difference for the coarse grid are shown in Figure 2 and for the fine grid in Figure 3. The DAM calculation requires approximately five times more CPU time than the FVM calculation. By comparing the difference between the two methods in Figure 2 and Figure 3 one can observe the convergence of both methods towards the same results.

5 Conclusions

The present paper demonstrates the successful use of the DAM for numerical evaluation of a physical model that could be previously efficiently solved only by more established numerical methods. It probably represents the first industrial use of this type of mesh-free method for solving convective-diffusive solid-liquid phase change problems with temperature dependent material properties and complex boundary conditions. All types of technically relevant boundary conditions have been introduced in a systematic way. The accuracy of the method is similar to the FVM. When compared with other mesh-free methods used in present context one can conclude: The method can cope with physically more involved situations than the front tracking BEM [Fic, Nowak and Bialecki (2000)], where the calculations are limited to a uniform velocity field, constant material properties of the phases, and isothermal phase-change. When compared with the DRBEM [Šarler and Mencinger (1999)], the method does not need any integrations and boundary polygonisation. The method appears much more efficient as the RBFCM [Šarler, Kovačević and Chen (2003)], because it does not require a solution of the large systems of equations. Instead, small (in our case 6x6) systems of linear equations have to be solved in each timestep for each node. The method is going to be used in coupled transport phenomena context in our future work.

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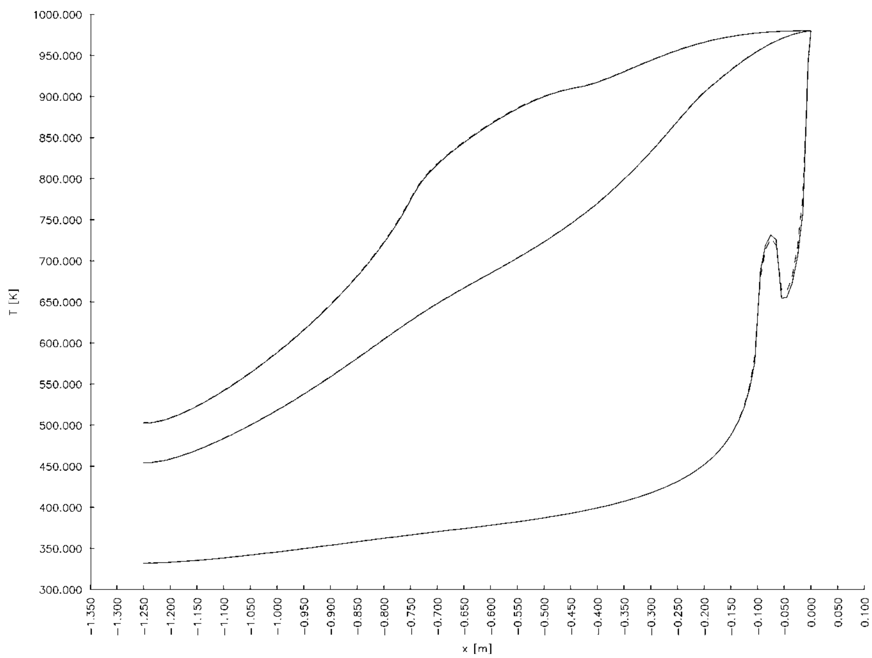

Figure 1 : Calculated temperature distribution in the slab for 125x25 node arrangement. Solid curve: FVM, dashed curve: DAM. Upper curve – centerline, center curve – mid thickness, and lower curve – surface temperature.

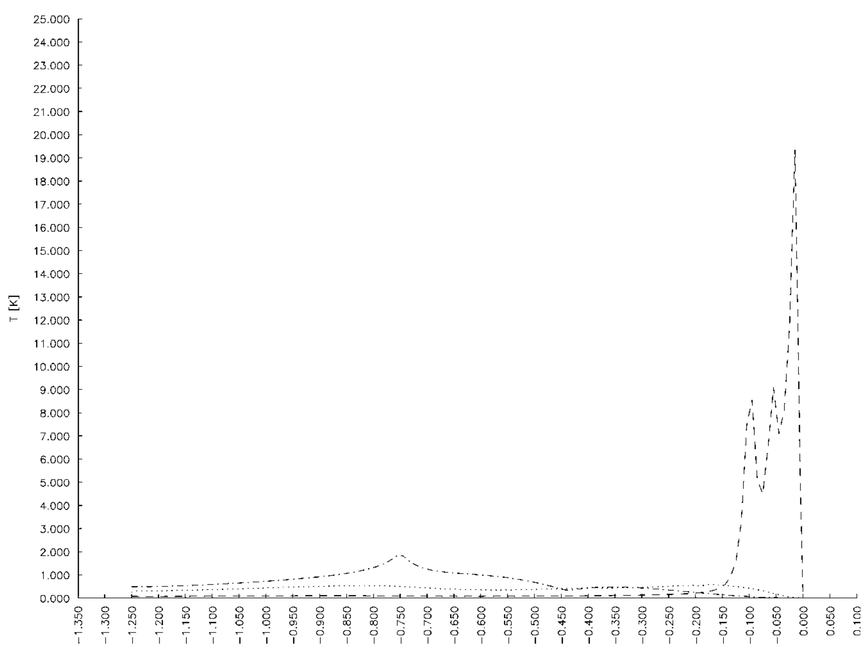

Figure 2 : Absolute difference between the FVM and DAM solutions for 125x25 node arrangement. Dashed curve – surface temperature, dotted curve – mid-thickness temperature, and dot-dashed curve – centerline temperature.

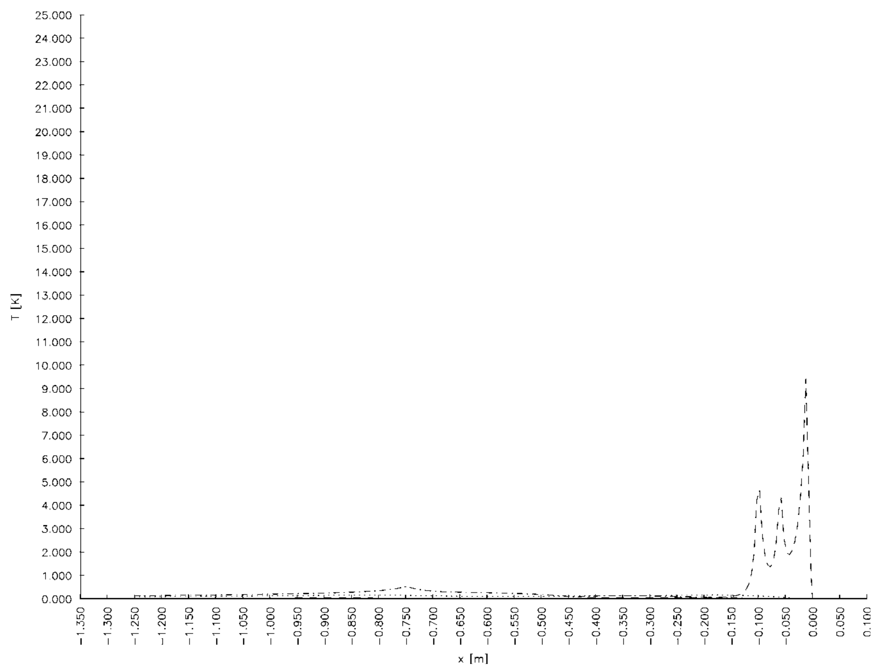

Figure 3 : Absolute difference between the FVM and DAM solutions for 250x50 node arrangement. Dashed curve – surface temperature, dotted curve – mid-thickness temperature, and dot-dashed curve – centerline temperature.

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