Hybrid BEM for the early stage of a 3D unsteady heat diffusion process

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Abstract

This article presents a hybrid three dimensional dual reciprocity boundary element method (BEM) for solving the early stage of a 3D time dependent convective heat transfer equation in non-homogeneous media. The method addresses the problem in which the initial distribution of temperature presents a discontinuous jump at the interface between two regions of very dissimilar diffusion coefficients. The goal of this hybrid formulation is to sort out the numerical inconvenience of different time scales and apparent large flux during early time by combining the 3D BEM with a series of 1D semi-analytical profiles of the time dependent heat diffusion equation, employing a two-level finite difference time integration scheme. This article presents the theoretical background, and one 3D test example. The formulation provided offers convenient advantages for relatively large scale models and complex 3D geometries.

1 Introduction

The problem of transient heat transport through 3D non-homogeneous media represents a real challenge for any standard numerical approach. A particular difficult situation is when the initial distribution of temperature presents a discontinuous jump, and this discontinuity is located at the interface between two regions A and B, as shown in Fig. 1(a), of very dissimilar diffusion coefficients, ie. differing in few to many orders of magnitude. Suppose that A is a region of very low conductivity with initially high temperature and characteristic size L_A, embedded in region B, highly conductive, which is initially at lower temperature. As time passes by, there is a faint energy release from the high temperature region and thermal energy is quickly conveyed by convection and diffusion throughout region B. In view of the different diffusivities a boundary layer-type profile of

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characteristic thickness $d_s(t)$ will develop close to the interface Γ in region A. This scenario presents two different problems. First, the high contrast between the transport properties at both sides of the interface, which introduces time and length scales of very different orders of magnitude; and second, the discontinuous jump of temperature, which introduces a "nearly infinite" thermal flux at early stage of the process. Most time marching integration schemes combined with the conventional finite element method, boundary elements methods (BEMs), finite volume methods, or mesh-less methods are likely to fail when dealing with these kind of problems, being a common symptom large first-time step errors, numerical instabilities, excessive numerical dispersion or diffusion results.

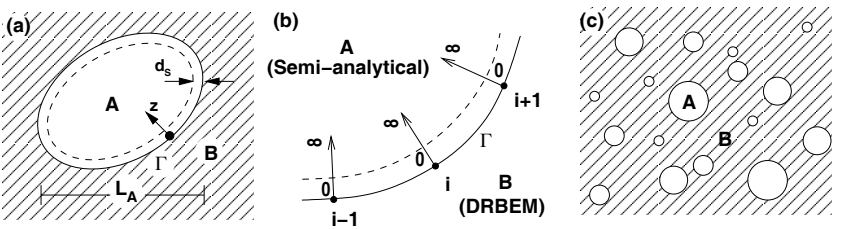

Figure 1: (a) Region of low diffusivity A embedded in a region of high diffusivity B. (b) Each degree of freedom $i = 1, \ldots, N$ at the interface Γ is associated with a semi-analytical profile given by (3).

Numerical modelling with BEM [1, 2] is very attractive in the sense that it avoids volume discretisation and at the same time it uses the fundamental solution of the leading differential operator in the equation to solve. BEM applied to the C-DHT equation has been widely developed in the last decades [3, 4], and a large variety of efficient formulations were established. An interesting approach for improving the accuracy at early time stage has been proposed by Grigoriev and Dargush in [5], where a high-order BEM has been established in terms of a singular flux formulation. Other approaches involve the use of time or space scaling in order to zoom into the boundary layer developed close to the interface and perform asymptotic matching with the far field solution. But the computational implementation of these sub-scaling techniques for arbitrary 3D problems might become too complex. The aim of this work is to propose another approach to solve the time dependent convective-diffusive heat transfer (C-DHT) equation in relatively complex 3D situations with a hybrid Dual Reciprocity BEM (DRBEM) employing a simple finite difference two-time-levels time marching scheme. In the proposed hybrid approach, a standard DRBEM strategy for region B, is coupled at the interface Γ with several independent semi-analytical profiles defined in region A. These profiles should be capable of capturing the solution close to Γ thus avoiding the use of high order time integration schemes, or boundary layer scaling techniques. In addition, the method should employ a minimum amount of adjusting parameters, so that to reduce the computational burden as much as possible. The

integration domain is discretised with a mixed unstructured mesh, where some regions may be decomposed into many sub-domains and some others may be discretised only in their boundary. The former is known as multi-domain region while the latter is identified with single domain region. The assembly of multi and single-domain regions into the same problem provides a suitable pre-processing flexibility which allows the treatment of complicated 3D geometries. Usually, the DRBEM yields a system of equations whose condition number grows with a certain power law of the number of degrees of freedom [6], thus imposing an upper practical limit to the size of the model to solve, this problem for DRBEM has not been completely sorted out so far. We define the *local transient time scale* (τ_L) of a region of the domain of characteristic size L by taking the maximum between the convective (τ_A), the diffusive (τ_D), and the reaction time scales ($1/k_r$), according to $\tau_L = \max(\tau_A, \tau_D, 1/k_r)$, where $\tau_A := L/v$ and $\tau_D = 4L^2/\alpha$, where, $v = |\mathbf{v}|$ is the average absolute value of the velocity in the region, and α is the average local diffusivity. A "slow-transport region" (STR) is defined as the part of the FPM with very low diffusivity such that τ_L is much higher than the local transient time scales defined for any other region in the integration domain or to the time scale of practical interest in the problem (t_h). We define a "fast-transport region" (FTR) as that part of the FPM characterised by high values of conductivity such that $\tau_L(FPM) \ll \tau_L(STR)$. STR's can also be regarded as inclusions embedded in a larger FTR region, as illustrated in Figure 1(c). When STRs are in close contact to FTRs the solution in the former can be expressed in terms of an assembly of one dimensional asymptotic semi-analytical test profiles of the diffusion equation, as sketched in Fig. 1(b). In this approach, the smaller the ratio t_h/τ_L the more accurate the approximation.

2 Governing equations

The heat transfer equation considered for FTR (B-type) regions is given by:

$$\frac{\partial T_f}{\partial t} + \nabla \cdot \mathbf{q} = -k_r T_f + \nabla \cdot \mathbf{q}_m, \tag{1}$$

where k_r is a reaction constant, t is time, T is temperature, the subscript f stands for the FTR, and the heat flux is given by: $\mathbf{q} = \mathbf{v}T_f - \alpha \nabla T_f$. The source term $\mathbf{q}_m$ on the right hand side of (1) represents the flux exchanged with the STR in close contact to the present FTR, and α is the thermal diffusivity of the region. The temperature in the STR is also described by the 3D C-DHT equation. However, in view of the large difference between diffusivities [7], it is enough to solve a 1D local profile of (1) given by:

$$\frac{\partial T_s}{\partial t} - \alpha_s \frac{\partial^2 T_s}{\partial z^2} = -k_r T_s, \tag{2}$$

where subscript s stands for variables in STR (Region A in Fig. 1) and z is the normal distance from the interface to the STR (see Fig. 1a). This approximation

is valid as long as $t_h \ll \tau_L$ or $L_A \gg d_s(t_h)$ in the STR, meaning that the characteristic length of the STR (L_A), see Fig. 1, is several orders of magnitude larger than the penetration depth $d_s(t) = \sqrt{\alpha_s t}/2$ at time t_h into the STR. The STR equation is solved by means of a Semi-Analytical Method (SAM), originally presented by Vinsome and Westerveld [8], later adapted by Birkholzer et al [9] to solute transport problems and recently applied by Peratta and Popov for arbitrary fractured porous media [7]. The idea is to represent the temperature profile along z by means of a reasonably flexible function containing few adjusting parameters to be determined by imposing suitable conservation equations at the interface. The main advantage of this approach is that it can be evaluated in a simple and fast way, thus lowering computational burden. The trial function is defined as follows:

$$T_s(z,t) - T_i = \left(T_f - T_i + p_1 z + p_2 z^2\right) \exp\left[-\frac{z}{d_s}\right], \tag{3}$$

where T_i is temperature in STR at initial time (assumed to be uniform), T_f is the time varying temperature at the interface STR-FTR, and p_1 and p_2 are two time varying best fit parameters to be adjusted by imposing the conservation of energy and continuity of T throughout the interface (Γ). This surface is discretised into N_e Boundary Elements (BEs), each one containing a certain number of collocation points (i), as represented in Fig 1, depending on the interpolation degree of the BEM. Thus, parameters p_1 and p_2 will be different for each collocation point and they must be recalculated at each time step for every grid point according to local conditions at Γ. Hence, p_1 and p_2 can be regarded as new degrees of freedom and their values define a unique local temperature profile for the adjacent STR associated to each freedom node at Γ.

Next, we derive the two local equations used to determine p_1 and p_2. The idea is to insert (3) into the C-DHT for the STR (2) and to evaluate it in the interface ($z = 0$). The time derivative of T in either STR or FTR is approximated by the two-time level finite difference scheme defined by:

$$\frac{\partial T}{\partial t} \approx \frac{T^{m+1} - T^m}{\delta t}; \quad \text{and} \quad \begin{pmatrix} T \\ \partial_n T \end{pmatrix} = \theta \begin{pmatrix} T \\ \partial_n T \end{pmatrix}^{m+1} - \bar{\theta} \begin{pmatrix} T \\ \partial_n T \end{pmatrix}^{m} \tag{4}$$

where $\theta \in [0,1]$; $\bar{\theta} := (\theta - 1)$; $\partial_n T := \hat{n} \cdot \nabla T$; and $\hat{n}$ is the normal vector at the interface. The first and second derivatives of T_s at the interface ($z = 0$) are, respectively:

$$\left.\frac{\partial T_m}{\partial z}\right|_{z=0} = p_1 - \frac{T_f - T_i}{d_s}, \quad \text{and} \quad \left.\frac{\partial^2 T_m}{\partial z^2}\right|_{z=0} = 2p_2 - 2\frac{p_1}{d_s} + \frac{T_f - T_i}{d_s^2}. \tag{5}$$

By inserting (4) and (5) for $z = 0$ into (2), we obtain the first equation:

$$\frac{T_f^{m+1} - T_f^m}{\alpha_s \delta t} = \frac{T_f^{m+1} - T_i}{d_s^2} - 2\frac{p_1}{d_s} + 2p_2 - \frac{k}{\alpha_s} T_f^{m+1} \tag{6}$$

The second equation is provided by the energetic balance in a local 3D control volume attached to a freedom node at the interface. It remains valid as long as the

height δz of the control volume is considerable larger than the penetration depth and considerably smaller than the size of the STR, ie. $L_{STR} \gg \delta z \gg d_s$. The time derivative of the energy contained in a differential volume of unitary cross section and height dz in the STR can be written as:

$$\frac{\partial}{\partial t}\int_V (T_s - T_i)\, dV = -\alpha_s \left.\frac{\partial T_s}{\partial z}\right|_{z=0} + k_r \int_V (T_s - T_i)\, dV, \tag{7}$$

where it was considered that $\partial T_s/\partial z = 0$ when $z \gg d_s$. Next, it is convenient to define the following energy integral:

$$I(t) := \int_V (T_f - T_i)\, dV = \int_z (T_s(z,t) - T_i)\, dz, \tag{8}$$

which is proportional to the internal energy in dV, and can be expressed in terms of p_1 and p_2 by means of eq (3) as: $I(t) = (T_f - T_i)\, d_s + d_s^2 p_1 + 2d_s^3 p_2$. Then, the energy balance equation can be written in the following way:

$$I^{m+1} = I^m - \alpha_s \delta t \left(p_1 - \frac{T_f - T_i}{d_s}\right), \tag{9}$$

where $I^m = I(t_m)$ and $I^{m+1} = I(t_m + \delta t)$, are the energy integrals at times t_m and $t_m + \delta t$, respectively. Finally, (6) and (9) form a system of two equations with two unknowns (p_1, p_2) for each degree of freedom at Γ of the form:

$$\begin{bmatrix} 2\frac{\alpha_s}{d_s} & -2\alpha_s \\ \alpha_s + \xi d_s^2 & 2\xi d_s^3 \end{bmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \mathbf{B}\left(T_f^{m+1}, T_f^m, T_i, 1\right)^t \tag{10}$$

and matrix $\mathbf{B} \in R^{2\times 4}$ on the right hand side term is given by:

$$B = \begin{bmatrix} \theta\mu - \frac{1}{\delta t} & -\bar{\theta}\mu + \frac{1}{\delta t} & -\frac{\alpha_s}{d_s^2} & 0 \\ -d_s\xi + \frac{\alpha_s\theta}{d_s} & -\frac{\bar{\theta}\alpha_s}{d_s} & d_s\xi - \frac{\alpha_s}{d_s} & I^m(k_r - \xi) \end{bmatrix} \tag{11}$$

being $\xi := 1/\delta t - k_r\theta$ and $\mu := k_r + \alpha_s/d_s^2$. The temperature profile in the STR, can be obtained by solving the system (10) for the parameters p_1 and p_2. Note that T_s^{m+1} becomes function of the temperature in the interface (T_f) at Γ, at present and previous time levels, the initial temperature in the block T_i and the energy content in the volume I.

3 DRBEM

The time dependent C-DHT in the FTR is solved with the DRBEM [4, 10]. First, the C-DHT is cast into a Poisson-like equation $\alpha_f \nabla^2 T_f(\mathbf{x}) = \rho(\mathbf{x}, t)$; $\mathbf{x} \in \Omega$; with an arbitrary source term $\rho(\mathbf{x}, t)$ and suitable Dirichlet, Neumann or Robin boundary conditions at the boundary $\partial(\Omega)$.

Then, in the context of the BEM, the matrix form of the discretised integral formulation can be expressed in the following way:

$$\alpha_f \left(\mathbf{H}\, \mathbf{T_f} - \mathbf{G}\, \partial_\mathbf{n} \mathbf{T_f} \right) = \mathbf{S}\boldsymbol{\rho}, \tag{12}$$

where $\mathbf{H} \in R^{M\times M}$ and $\mathbf{G} \in R^{M\times N}$ are the standard BEM matrices based on the Green's function of Laplace equation, $\mathbf{S} \in R^{M\times M}$ is the DRM matrix, N is the number of freedom nodes used to discretise Γ, $M = N + L$, and L is the number of DRM nodes in Ω. The column arrays $\mathbf{T_f} \in R^{(M\times 1)}$ and $\partial_\mathbf{n}\mathbf{T_f} \in R^{(N\times 1)}$ specify T_f and $\partial T_f/\partial \hat{n}$ in each freedom node and the DRM matrices are defined as follows [4, 11]:

$$\mathbf{S} := \left(\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}} \right) \mathbf{F}^{-1}, \qquad \mathbf{S} \in R^{M\times M} \tag{13}$$

where $\mathbf{F} = f_{ij}, \in R^{(M+4)\times(M+4)}$ is the 3D augmented thin plate splines radial basis functions matrix defined by the set $\{r_{ij}, 1, x_j, y_j, z_j\}$. Here, r_{ij} is the distance between i and j freedom nodes, whereas $1, x_j, y_j, z_j$ is the augmentation polynomial at point j. Then, $\hat{\mathbf{U}} = \hat{u}_{ij}, \in R^{M\times(M+4)}$ and $\hat{\mathbf{Q}} = \partial \hat{u}_{ij}/\partial \hat{n}_i \in R^{N\times(M+4)}$ are the usual DRM matrices, whose elements obey the following relationship $\nabla^2 \hat{u}_{ij} := f_{ij}$. Next, the generalised right hand side term for the C-DHT ρ is given by:

$$\rho(\mathbf{x}, t) = \frac{\partial T_f}{\partial t} + \mathbf{v} \cdot \nabla T_f + k_r T_f. \tag{14}$$

Finally, the matrix form of the discretised integral formulation can be expressed in the following way:

$$\mathbf{H}\mathbf{T_f} - \mathbf{G}\partial_\mathbf{n}\mathbf{T_f} = \frac{\mathbf{S}}{\alpha_f} \left[\frac{\mathbf{T_f^{m+1}} - \mathbf{T_f^m}}{\delta t} + \sum_{p=1}^{3} \left(\mathbf{V}_p \cdot \mathbf{T}_p \right) T_f + k_r \mathbf{T_f} \right], \tag{15}$$

where the following matrices were employed [6, 11]: $\mathbf{V}_p = \text{diag}\{v_p\}$ and $\mathbf{T}_p = \nabla_p \mathbf{F} \cdot \mathbf{F}^{-1}$; where $\mathbf{V} \in R^{M\times M\times 3}$ and $\mathbf{T} \in R^{M\times M\times 3}$, see ref. [11] for details.

4 Numerical implementation

The linear system established by eq. (10) provides the parameters p_1 and p_2 of each freedom node in Γ. These parameters define a unique 1D profile of temperature in the STR that best matches the required conservation equations. However, in a large scale calculation it might be more useful to deal with temperatures (T_f^{m+1}) and normal fluxes (q_m^{m+1}) rather than with p_1 and p_2. The change of variables: $(p_1, p_2) \rightarrow (T_f, q_m)^{m+1}$ can be done by expressing the normal flux

exchanged between STR and FTR in terms of p_1 as: $q_m = v_n T_f - \alpha_s \frac{\partial T_s}{\partial n} = \alpha_s \left(p_1 - \frac{T_f - T_i}{d_s} \right)$, so that to obtain:

$$p_1 = \frac{q_m}{\alpha_s} + \frac{T_f - T_i}{d_s}. \tag{16}$$

Then, combination of eqs. (2), (5) and (16), yields:

$$p_2 = \frac{q_m}{\alpha_s d_s} + \frac{T_f - T_i}{2d_s^2} + \frac{1}{2\alpha_s}\frac{\partial T_s}{\partial t} - \frac{k_r}{2\alpha_s} T_f, \tag{17}$$

or expressed in a more suitable way:

$$\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \mathbf{E} \begin{pmatrix} T_f^{m+1} \\ q_m^{m+1} \end{pmatrix} + \mathbf{F}, \tag{18}$$

where

$$\mathbf{E} = \frac{1}{\alpha_s} \begin{pmatrix} \frac{\alpha_s}{d_s} & 1 \\ \frac{\alpha_s}{2d_s^2} + \frac{1}{2\delta t} - \frac{k_r}{2} & \frac{1}{d_s} \end{pmatrix} \quad \text{and} \quad \mathbf{F} = -\frac{T_i}{d_s} \begin{pmatrix} 1 \\ \frac{1}{2d_s} + \frac{1 d_s}{2\alpha_s \delta t} \frac{T_f}{T_i} \end{pmatrix}. \tag{19}$$

The use of (18) in (10) provides a more suitable expression that relates temperature with normal flux at the interface:

$$A_1^* T_f^{m+1} + A_2^* q_m^{m+1} = B^* \tag{20}$$

where

$$A_1^* = (1-\theta)\frac{\alpha_s}{d_s} + \left(3 + \frac{d_s^2}{\alpha_s \delta t} - \frac{d_s^2 k_r}{\alpha_s} \right) d_s \xi, \qquad A_2^* = 1 + 3\frac{\xi d_s^2}{\alpha_s},$$

$$B^* = (1-\theta)\frac{\alpha_s}{d_s} T_f^m + 3 d_s \xi T_i + I^m (k_r + \xi) + \frac{d_s^3 \xi}{\alpha_s \delta t}.$$

Thus the semi-analytical part of the method introduces one equation (20) per each freedom node located at Γ. Note that the coefficients $A_{1,2}^*$ and the right hand side term RHS^* involved in (20) depend only on the energy integral I and the field values at the previous time step (m), as well as the material properties and the initial temperature T_i, but they no longer depend on the unknown T_f^{m+1}. Next, assembly of eq. (15) yields the following system of linear equations:

$$\mathbf{M_1 T_f^{m+1}} - \theta \mathbf{G q_f^{m+1}} = \bar{\mathbf{M}}_\mathbf{1} \mathbf{T_f^m} - \bar{\theta} \mathbf{G q_f^m} \tag{21}$$

where

$$\begin{pmatrix} \mathbf{M_1} \\ \bar{\mathbf{M}}_\mathbf{1} \end{pmatrix} := \begin{pmatrix} \theta \\ \bar{\theta} \end{pmatrix} \alpha_f \mathbf{H} - \begin{pmatrix} \theta \\ \bar{\theta} \end{pmatrix} \mathbf{S} \sum_{p=1}^{3} (\mathbf{V}_p \cdot \mathbf{T}_p) - \begin{pmatrix} \xi \\ \bar{\xi} \end{pmatrix} \mathbf{S} \tag{22}$$

and $\bar{\xi} := 1/\delta t - k_r \bar{\theta}$. After applying proper boundary conditions, eq.(21) yields a system of equations of the form $\mathbf{Ux} = \mathbf{b}$, where array $\mathbf{x}$ contains the unknowns

q and T, and b is composed of the right hand side term of eq (21) and the corresponding boundary conditions. Finally, eqs (20) and (21) are solved together, either by assembling all the equations in the same system of equations or by an iterative technique between STR and FTR systems, in order to solve the coupled FTR-STR problem.

5 Results

Some benchmark examples with this approach have already been conducted in our recent paper [7], particularly for problems of flow and solute transport through fractured and non-fractured porous media. This section will present one of those results in the context of a heat transfer problem.

5.1 Test problem for a slab

The test example consists of a slab of length $L = 21m$ and square cross section of $1m$ by $1m$, constant along L, as shown in Fig. 2. The block is composed of two regions: STR and FTR, corresponding to $\alpha_{STR} = 10^{-10}m^2/s$ and $\alpha_{FTR} = 10^{-6}m^2/s$, respectively. The former extends from $y = 0$ to $y = 1m$ and the latter from $y = 1m$ to $y = L = 21m$. The interface Γ is located at $y = L_s = 1m$. A convective term corresponding to $v = 9.98^{-11}m/s$ in y direction has been switched on. The surface at $y = 0$ is kept at constant temperature $T = 1$, while all the other surfaces are considered as adiabatic. The initial condition is given by: $T(\mathbf{x}, 0) = 1$ if $\mathbf{x} \in$ [STR] and $T(\mathbf{x}, 0) = 0$ anywhere else. Hence an the initial distribution yields an apparent infinite diffusive flux at $y = 1$. The coupled problem STR-FTR is assembled into a unique linear system of equations. The STR has one sub-domain with its boundary discretised into 182 linear discontinuous triangles. The FTR is decomposed into 539 sub-domains, each sub-domain is a linear discontinuous tetrahedron like the ones employed by the FEM. Figure 2(a) shows the meshed slab of the two regions.

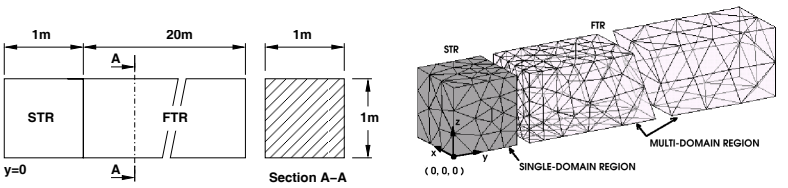

Figure 2: Dimensions of the test example, and 3D mesh of the model.

The volume mesh (involving 282 geometrical nodes was created with a FEM-like mesh generator [12, 13] based on the advance frontal method [14]. The derivatives of the DRM matrix F were used in order to compute the gradient of the temperature for the FTR region: $\partial T(\mathbf{x})/\partial x_p|_{x_i} = \sum_{j=1}^{N+4} \partial f_j(\mathbf{x})/\partial x_p|_{x_i} \alpha_j$

where the summation extends over the total number of RBFs associated to a given sub-domain (see [11] for more details). In the case of linear tetrahedrons there are three discontinuous freedom nodes per element, therefore $N = 12$, and the $\mathbf{F}$ matrix in the DRM has dimensions of 16×16. The solution for the temperature profile has been compared to a one dimensional Eulerian FVM reference code, based on cell-center formulation with MacCormak time integration scheme and constant time step. The convective term is calculated with an upwind discretisation scheme and the diffusive term with centered differences. The temperature profiles obtained with the SAM compared to the reference FVM along y coordinate at time levels $t_A = 0s$, $t_B = 5 \times 10^3 s$ and $t_C = 5 \times 10^4 s$ are shown in Fig. 3. The time step for the SAM $\delta t = 5 \times 10^3 s$ was kept constant along the time iterations. Good agreement is being observed between both results.

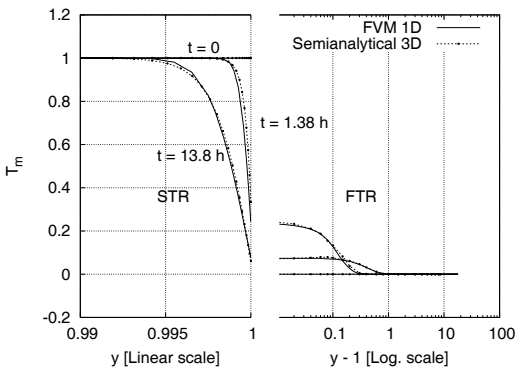

Figure 3: Temperature profile along the test slab in the STR(left) and FTR(right) regions at different time levels.

6 Conclusions

A hybrid semi-analytical approach coupled to the DRBEM for solving the early stage of 3D time dependent heat transport problems in non-homogeneous media has been proposed and tested with a simple 3D example involving a large aspect ratio composite body. The approach is suitable for 3D heat transfer problems dominated by diffusion, and of particular use when the initial distribution of temperature presents a discontinuous jump at the interface between two regions whose diffusivity constants differ in many orders of magnitude. By means of a semi-analytical profile, a linear equation that relates the temperature with its normal flux has been derived. In a block regarded as a sub-domain of low diffusivity in comparison with the surrounding media, this relation leads to two matrices which play the same role as the matrices resulting from the single and double layer integrals in the BEM, but with only one non-zero coefficient per row, respectively. Hence, they can be easily coupled to conventional BEM systems of equations in order to solve more complex geometrical situations.

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