UNIFIED INTEGRAL TRANSFORMS (UNIT) CODE APPLIED TO HEAT DIFFUSION IN HETEROGENEOUS MEDIA

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Abstract. *The effort to integrate the knowledge on Integral Transforms application into a computational code resulted in a recently developed open source mixed symbolic-numerical computational code called UNIT (UNified Integral Transforms), that provides a development platform for finding solutions of nonlinear partial differential equations by integral transformation. To demonstrate the robustness of the UNIT code, the present work challenged this code in solving three different situations of heat diffusion dealing with spatially variable coefficients. The selected variations of the thermophysical properties illustrate: a large scale variation such as in Functionally Graded Materials (FGM), abrupt variations such as in layered composites and random variations due to local concentration fluctuations in dispersed phase systems such as composites. The results obtained with the UNIT code show a very good agreement with a dedicated computational implementation of the integral trnasform method, even for severe variations of the thermophysical properties, illustrating its robustness and flexibility.*

Keywords*: Integral Transforms, Heterogeneous media, Heat diffusion, Hybrid methods, UNIT code*

1. INTRODUCTION

The numerical solution of partial differential diffusion models by discrete approaches has been a crucial analysis tool in practice, development and research in engineering sciences, either as user-developed routines, general purpose subroutines from mathematical packages, or object oriented commercial codes. Such solution paths have been co-existing with classical analytical approaches for some classes of problems that allow for exact treatment, and with hybrid numerical-analytical methods for more general, even nonlinear, formulations not a priori tractable by the classical analytical methodologies. This essential synergy of numerical and more analytically oriented approaches is related with benchmarking and covalidation needs, with cost reduction and/or robustness incorporation in certain applications, and most especially with the continuous development of novel hybrid methods. While discrete numerical approaches are progressively and more readily available as automatic routines for general purpose use, even nowadays merged within multiphysics frameworks, analytical and hybrid-type approaches still require a considerable amount of effort in the implementation of the computational algorithms, even though they may involve, in principle, simpler and more cost-effective algorithms. On the other hand, the more recent spreading of the symbolic computation culture, has been allowing for the generalization and systematization of algebraic manipulations that are inherent to such analytic-based methods, and offering an impulse to the establishment of automatic codes based on analytical methods for PDE´s.

Analytical solutions of linear diffusion problems have been systematically solved for seven different classes of heat and mass diffusion problems with the Classical Integral Transform Technique (CITT) (Mikhailov & Ozisik, 1984). Later on, the classical integral transform approach gained a hybrid numerical-analytical implementation, referred to as the Generalized Integral Transform Technique (GITT) (Cotta, 1990; Cotta, 1993; Cotta, 1994; Cotta & Mikhailov, 1997, Cotta, 1998; Cotta & Mikhailov, 2006). This hybrid approach was progressively advanced to overcome barriers posed by different classes of problems such as nonlinear physical properties, moving boundaries, irregular geometries and nonlinear convective terms. The effort to integrate the knowledge on the GITT application into an automatic and unified computational tool resulted in a recently developed open source mixed symbolical-numerical computational code called UNIT, which stands for **UN**ified **I**ntegral **T**ransforms (Sphaier et al., 2009; Cotta et al., 2010), that provides a development platform for finding solutions of partial differential equations by means of integral transforms.

Diffusion problems defined in heterogeneous media involve spatially variable coefficients in different forms, depending on the type of heterogeneity involved, such as large scale variations in functionally graded materials (FGM), abrupt variations in layered composites and random variations due to local concentration fluctuations in dispersed phase systems such as nano-composites and nanofluids (Lin, 1992; Divo & Kassab, 1998; Fudym et al., 2002; Sutradhar & Paulino, 2004; Kumlutas & Tavman, 2006; Naveira-Cotta et al., 2009; Naveira-Cotta et al., 2010a). In the present work we challenge the UNIT code in solving heat diffusion problems in heterogeneous media. The simplest possible auxiliary eigenvalue problem is adopted so as to test the UNIT code solver in the most adverse case, and thus the terms that are responsible for the information on the heterogeneity of the medium are grouped into the source term. This is in fact the main difference of the present approach in comparison with the dedicated solution provided by (Naveira-Cotta, 2009; Naveira-Cotta et al., 2009), where the most appropriate and general eigenvalue problem, with no simplification, was

tackled with the GITT itself. The aim is to demonstrate the flexibility and applicability of the recently advanced automatic symbolic-numerical implementation, by employing representative test problems that provide a number of different and stiff functional forms for the partial differential formulation coefficients.

2. PROBLEM FORMULATION AND SOLUTION METHODOLOGY

We consider the one-dimensional version of the general formulation on transient diffusion presented and solved in (Sphaier et al., 2009; Cotta et al., 2010), for the potential $T(x,t)$, dependent on position x and time t and defined in region $x \in [0,L]$. The formulation includes the transient term, the diffusion operator, a linear dissipation term, nonlinear source terms, and the space variable thermal conductivity and heat capacity, for a heat transfer application, as shown in problem (1) below. The nonlinear equation and boundary source terms may collect nonlinear terms from the different portions of the problem formulation. The coefficients $w(x)$ and $k(x)$, are thus responsible for the information related to the heterogeneity of the medium. The diffusion equation and initial and boundary conditions are given by:

$$w(x)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[k(x)\frac{\partial T(x,t)}{\partial x}\right] - d(x)T(x,t) + P(x,t,T), \quad 0 < x < L,\ t > 0 \tag{1a}$$

$$T(x,0) = f(x), \quad 0 \le x \le L \tag{1b}$$

$$\alpha_0 T(x,t) - \beta_0 k(x)\frac{\partial T(x,t)}{\partial x} = \phi_0(x,t,T), \quad x = 0,\ t > 0 \tag{1c}$$

$$\alpha_1 T(x,t) + \beta_1 k(x)\frac{\partial T(x,t)}{\partial x} = \phi_1(x,t,T), \quad x = L,\ t > 0 \tag{1d}$$

Problem (1) covers a fairly wide range of physical conditions for a typical one-dimensional transient thermal conductivity experimental setup, including the various types of boundary conditions and independent heating, or, for instance, based on an initial space variable thermal excitation throughout the domain, and subsequent temperature measurements acquisition via infrared thermography (Fudym et al., 2008; Naveira-Cotta et al., 2010a; Naveira-Cotta et al., 2010b).

We first recall the analytical solution path adopted in (Naveira-Cotta, 2009; Naveira-Cotta et al., 2009a), where the exact formal solution for the linear version of problem (1) is obtained through the Classical Integral Transform Method (Mikhailov & Ozisik, 1984), based on the eigenvalue problem that incorporates all the space variable coefficients, allowing for the analysis of different classes of heterogeneous media by considering specific functional forms and parameter values for the related space variable coefficients. The Generalized Integral Transform Technique (GITT) is then employed essentially to offer a hybrid numerical-analytical solution of the eigenvalue problem, and this detailed analysis can be found in the cited references.

Here, we seek the formal solution of problem (1), in a more general sense, not accounting for the exact integral transformation that is achievable when the specific eigenvalue problem with all the space variable coefficients is chosen. This alternative more flexible solution path, which forms the basis of the UNIT code (Sphaier et al., 2009; Cotta et al., 2010) is then based on direct application of the Generalized Integral Transform Technique (Cotta, 1990; Cotta, 1993), starting with the inverse formula below:

$$T(x,t) = T_f(x;t) + \sum_{i=1}^{\infty} \tilde{\psi}_i(x)\bar{T}_i(t) \tag{2a}$$

where $T_f(x;t)$ is a filtering solution to be proposed, and the transformed potentials are defined with the integral transformation operation given by

$$\bar{T}_i(t) = \int_0^L w^*(x)\tilde{\psi}_i(x)T^*(x,t)dx \tag{2b}$$

The eigenvalues μ_i and eigenfunctions $\psi_i(x)$, are obtained from the chosen eigenvalue problem below:

$$\frac{d}{dx}\left[k^*(x)\frac{d\psi_i(x)}{dx}\right] + \left[\mu_i^2 w^*(x) - d^*(x)\right]\psi_i(x) = 0, \quad x \in [0,L] \tag{3a}$$

with boundary conditions

$$\alpha_0\psi_i(x)-\gamma_0 k^*(x)\frac{d\psi_i(x)}{dx}=0,\quad x=0 \tag{3b}$$

$$\alpha_1\psi_i(x)+\gamma_1 k^*(x)\frac{d\psi_i(x)}{dx}=0,\quad x=L \tag{3c}$$

where the coefficients $k^*(x)$, $w^*(x)$, and $d^*(x)$ are simpler coefficients chosen so as to construct an eigenvalue problem of known analytical solution to offer the basis for the eigenfunction expansion. For convenience, we also require that eqs.(3b,c) match the homogenous version of the boundary conditions, eqs.(1.c,d), by letting $\gamma_0 = \beta_0 k(0)/ k^*(0)$ and $\gamma_1 = \beta_1 k(L)/ k^*(L)$. The other quantities that appear in the inverse formula (2a) are computed after solving problem (3), such as:

$$\tilde{\psi}_i(x)=\frac{\psi_i(x)}{\sqrt{N_i}},\ \text{normalized eigenfunctions} \tag{4a}$$

$$N_i=\int_0^L w^*(x)\psi_i^2(x)dx,\ \text{normalization integrals} \tag{4b}$$

The UNIT code allows for different choices of filtering solutions, either user provided or automatically determined from the symbolic computation feature of the *Mathematica* system. The simplest possible filtering solution is written as a linear function in the space variable that simultaneously satisfies both boundary conditions (1c,d),

$$T_f(x;t)=a(t)x+b(t) \tag{5}$$

This straightforward linear filter is the default option in the UNIT code and essentially homogenizes the boundary conditions in the filtered partial differential problem to be integral transformed. A more complete analytical filter may be preferred, that further eliminates the source terms in the original equation, eq.(1a), but the above choice was already quite effective in the present situation. The filtered temperature problem formulation is then given by:

$$w(x)\frac{\partial T^*(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[k(x)\frac{\partial T^*(x,t)}{\partial x}\right]-d(x)T^*(x,t)+P^*(x,t,T),\quad 0<x<L,\ t>0 \tag{6a}$$

$$T^*(x,0)=f^*(x)\equiv f(x)-T_f(x;0),\quad 0\le x\le L \tag{6b}$$

$$\alpha_0 T^*(x,t)-\beta_0 k(x)\frac{\partial T^*(x,t)}{\partial x}=0,\quad x=0,\quad t>0 \tag{6c}$$

$$\alpha_1 T^*(x,t)+\beta_1 k(x)\frac{\partial T^*(x,t)}{\partial x}=0,\quad x=L,\quad t>0 \tag{6d}$$

where the filtered source term is written as

$$P^*(x,t,T)=P(x,t,T)-w(x)\frac{\partial T_f(x,t)}{\partial t}+\frac{\partial}{\partial x}\left[k(x)\frac{\partial T_f(x,t)}{\partial x}\right]-d(x)T_f(x,t) \tag{6e}$$

Before proceeding to the integral transformation process itself, it is of interest to avoid an implicit transformed system, and thus Eq.(6a) can be rewritten in terms of the chosen weighting function $w^*(x)$, as follows:

$$w^*(x)\frac{\partial T^*(x,t)}{\partial t}=\frac{w^*(x)}{w(x)}\left\{\frac{\partial}{\partial x}\left[k(x)\frac{\partial T^*(x,t)}{\partial x}\right]-d(x)T^*(x,t)+P^*(x,t,T)\right\},\quad 0<x<L,\ t>0 \tag{7a}$$

or simply,

$$w^*(x)\frac{\partial T^*(x,t)}{\partial t}=G(x,t,T),\quad 0<x<L,\quad t>0 \tag{7b}$$

with,

$$G(x,t,T)=\frac{w^*(x)}{w(x)}\left\{\frac{\partial}{\partial x}\left[k(x)\frac{\partial T^*(x,t)}{\partial x}\right]-d(x)T^*(x,t)+P^*(x,t,T)\right\} \tag{7c}$$

The integral transformation is now performed by operating eq.(7b) on with $\int_0^L \tilde{\psi}_i(x) - dx$, to yield the following transformed ordinary differential system:

$$\frac{d\bar{T}_i(t)}{dt} = \bar{g}_i(t,\bar{T}_j), \quad t>0, \quad i,j=1,2,... \tag{8a}$$

with the transformed source terms given by

$$\bar{g}_i(t,\bar{T}_j) = \int_0^L G(x,t,T)\tilde{\psi}_i(x)dx \tag{8b}$$

and the transformed initial conditions

$$\bar{f}_i = \int_0^L w^*(x)\, f^*(x)\overline{\psi_i}(x)dx \tag{8c}$$

The ODE system (8) can be numerically solved to provide results for the transformed temperatures, upon truncation to a sufficiently large finite order *N*. The *Mathematica* platform (Wolfram, 2005) provides the routine *NDSolve* for solving stiff ODE systems such as the one here considered, under automatic absolute and relative error control. Once the transformed potentials have been numerically computed, the *Mathematica* routine automatically provides an interpolating function object that approximates the t variable behavior of the solution in a continuous form. Then, the inversion formula can be recalled to yield the potential field representation at any desired position *x* and time t.

The constructed UNIT code in the *Mathematica* 7.0 platform encompasses all of the symbolic derivations that are required in the above GITT formal solution, besides the numerical computations that are required in the solution of the chosen eigenvalue problem and the transformed ODE system. The user essentially needs to specify the problem formulation, according to Eqs.(1), and then choose how to present results according to the specific needs. In order to computationally solve the problem defined by Eqs. (1), a quite straightforward general algorithm can be described as follows:

- The user provides the input and problem formulation module, which includes the equation and boundary condition coefficients in eqs.(1), besides the corresponding source terms. There is an implicit choice of eigenvalue problem when the coefficients $k^*(x)$, $w^*(x)$, and $d^*(x)$ are specified so as to form the auxiliary problem to be solved for.
- The automatic filtering module is then activated, which is either the simplest possible choice of functions that essentially satisfy the boundary conditions, to make them homogeneous as here discussed, or the filter is provided as a problem formulation by the user, to be handled via symbolic or numerical computation. The option of not providing a filtering solution is also allowed, either because it might not be actually necessary or as a solution strategy to be complemented by an integral balance acceleration *a posteriori* (Cotta, 1993).
- The auxiliary eigenvalue problem of Eqs. (3) is solved for the eigenvalues and related normalized eigenfunctions, either in analytic explicit form, when applicable, as obtained by the symbolic routine DSolve, or through the GITT itself (Naveira-Cotta et al., 2009).
- The transformed initial condition is computed, either analytically (function Integrate) or with a general-purpose procedure through adaptive numerical integration (function NIntegrate). Two additional options are provided to the user, namely, a semi-analytical evaluation where the analytical integration of the eigenfunction oscillatory behavior is preserved, and a simplified and cost-effective numerical integration with Gaussian quadrature, automatically exploiting the frequency of oscillation of the eigenfunctions in the choice of nodes. Similarly, the coefficients on the transformed O.D.E. system of Eq. (8a), once they are not dependent on the transformed potentials, can be evaluated in advance. For the more general situation of nonlinear coefficients, there are some computational savings in grouping them into a single integrand, as represented in Eq.(8b). The coefficients in the transformed system can be obtained by analytical integration, if feasible, or again by the automatic Gaussian quadrature scheme that accounts for the knowledge on the eigenfunctions oscillatory behavior. The alternative semi-analytical integration procedure is also implemented, which is particularly convenient in nonlinear formulations that might require costly numerical integration. For instance, the integral transformation of the equation source term for homogeneous filtered boundary conditions would then be evaluated as:

$$\bar{g}_i(t,\bar{T}_j) = \int_v \tilde{\psi}_i(\mathbf{x})G(x,t,\mathrm{T})dv = \sum_{m=1}^{M}\int_{v_m} \tilde{\psi}_i(x)\hat{G}_m(x,t,\mathrm{T})dv \tag{9}$$

where $\hat{G}_m(x,t,\mathrm{T})$ are simpler representations of the source term, defined in M sub-regions V_m, for which analytical integration of the eigenfunctions is still obtainable. The simplest choice would be the adoption of uniform values of the source terms within the subdomains (zeroth order approximation), but linear and quadratic representations of the source terms behavior are also implemented.

- The truncated O.D.E. system of Eqs. (8a) and (8c) is then numerically solved through function NDSolve of the *Mathematica* system. In general, such initial value problem solvers should work under the automatic selection of a stiff system situation, such as with the BDF (Gear's) method, since the resulting system is likely to become stiff, especially for increasing truncation orders. This subroutine offers an interesting combination of accuracy control, simplicity in use, and reliability.

- Once all the intermediate numerical tasks are accomplished within user-prescribed accuracy, one is left with the need of reaching convergence in the eigenfunction expansions and controlling the truncation order N for the requested accuracy in the final solution. The analytic nature of the inversion formula allows for a direct testing procedure at each specified position within the medium where a solution is desired, and the truncation order N can be decreased (or eventually increased), to fit the user global error requirements over the entire solution domain. The simple tolerance testing formula employed is written as

$$\varepsilon(t) = \max \left| \frac{\sum_{i=N^*+1}^{N} \tilde{\psi}_i(x)\overline{T}_i(t)}{T_f(x;t) + \sum_{i=1}^{N} \tilde{\psi}_i(x)\overline{T}_i(t)} \right| \tag{10}$$

The numerator in Eq. (10) represents those terms that in principle might be abandoned in the evaluation of the inverse formula, without disturbing the final result to within the user-requested accuracy target. Therefore, this testing can be implemented by choosing the value of N^* in the numerator sum, then offering error estimations at any of the selected test positions within the domain.

The open source UNIT code is a development platform for researchers and engineers interested on hybrid integral transform solutions of convection-diffusion problems, readily available for download from the site http:\\2009unit.vndv.com.

3. RESULTS & DISCUSSION

3.1.Functionally Graded Materials (FGM)

As the first example we consider the case of variable coefficients with large scale variations within the domain, such as related to the heat transfer analysis of functionally graded materials (FGM) (Sutradhar and Paulino, 2004). The related dimensionless energy equation, initial and boundary conditions for the FGM example are written as:

$$w(x)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[k(x)\frac{\partial T(x,t)}{\partial x}\right], \quad 0 < x < 1, \quad t > 0 \tag{11a}$$

$$T(x,0) = f(x) = \frac{1-e^{2\beta(1-x)}}{1-e^{2\beta}}, \quad 0 < x < 1 \tag{11b}$$

$$T(0,t) = 0, \quad T(1,t) = 0, \quad t > 0 \tag{11c,d}$$

where the thermophysical properties vary exponentially in the form

$$k(x) = k_0 e^{2\beta x}, \quad w(x) = w_0 e^{2\beta x}, \quad \alpha_0 = \frac{k_0}{w_0} = const. \tag{12a-c}$$

This particular functional form was chosen on purpose as it leads to a problem formulation with exact solution via the classical integral transform method (Ozisik & Mikhailov, 1984), yielding a benchmark solution for this case. The effect of the parameter β on the behavior of the thermophysical properties is illustrated in Fig. 1. Note that for the case of $\beta = 3$, a ratio of approximately 400 times is achieved between the thermal conductivity values at the two edges of the domain. This same problem was handled in (Naveira-Cotta et al., 2009) through a dedicated implementation of the formal exact solution, in conjunction with the GITT hybrid solution of the related eigenvalue problem. Here, the UNIT code solution was pursued for the simplest possible choice of eigenvalue problem throughout, namely, $w^*(x)=1$, $k^*(x)=1$, and $d^*(x)=0$, so as to further challenge the automatic symbolic-numerical routine.

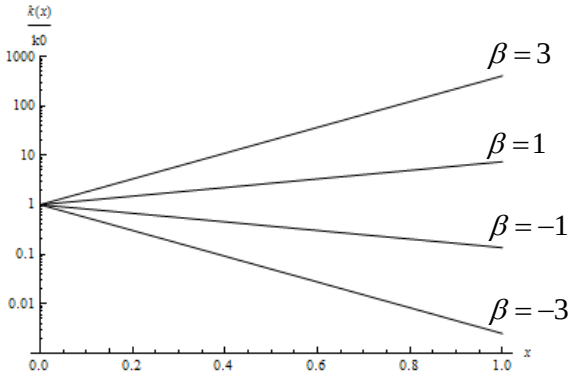
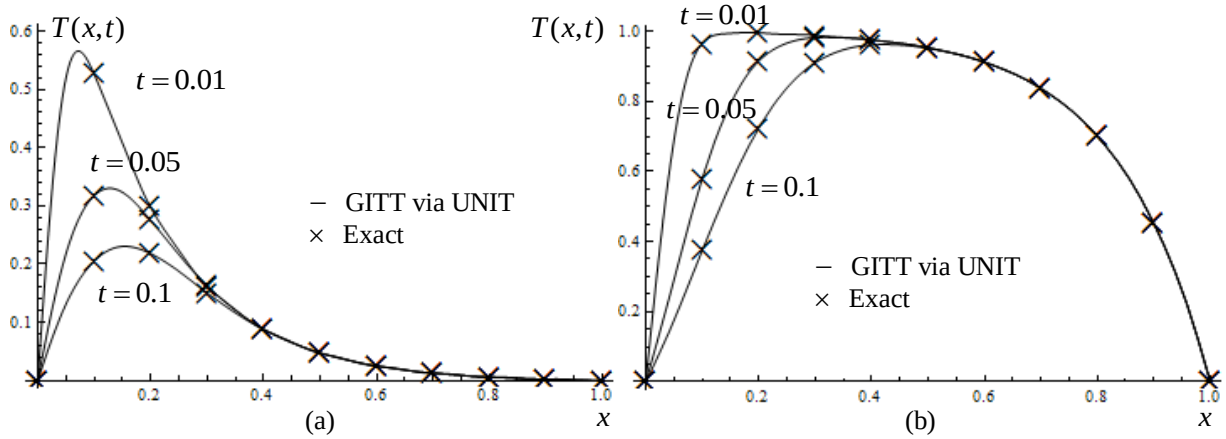


Figure 1 - Behavior of the variable diffusion coefficient $k(x)$ for the FGM example, with β = -3, -1, 1 and 3.

In Figs. 2a. and 2b the transient behavior of the temperature profiles is shown for three time values, $t = 0.01$, 0.05 and 0.1, with $\beta = 3$ and $\beta = -3$, respectively, as solved with the GITT via UNIT code and compared against the exact solution (Naveira-Cotta et al., 2009). The excellent convergence behavior of the expansion is illustrated in Table 1.



Figures 2 – Physical behavior and validation (GITT via UNIT *vs* Exact) of temperature distributions for the FGM with (a) $\beta = 3$ and (b) $\beta = -3$.

Table 1 – Convergence of temperature eigenfunction expansion for the FGM problem.

Method	$t = 0.01$ $\beta = 3$				$t = 0.01$ $\beta = -3$			
	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$
UNIT $N = 40$	0.299159	0.0883170	0.0248731	0.0057496	0.994489	0.975184	0.911569	0.700450
UNIT $N = 50$	0.299412	0.0884360	0.0249094	0.0057654	0.994283	0.975107	0.911546	0.700520
UNIT $N = 60$	0.299433	0.0884460	0.0249048	0.0057643	0.994261	0.975101	0.911544	0.700530
UNIT $N = 70$	0.299442	0.0884510	0.0249048	0.0057642	0.994249	0.975098	0.911543	0.700530
UNIT $N = 80$	0.299450	0.0884550	0.0249062	0.0057648	0.994243	0.975096	0.911542	0.700537
Exact	0.299454	0.0884585	0.0249067	0.0057652	0.994221	0.975093	0.911542	0.700542

3.2. Properties with abrupt variations

We now consider the analysis of problems with abrupt variations on the thermophysical properties (Orlande et al., 2008; Naveira-Cotta, 2010a). The analyzed problem formulation is:

$$w(x)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[k(x)\frac{\partial T(x,t)}{\partial x}\right], \quad 0 < x < 1, \quad t > 0 \tag{13a}$$

$$T(x,0) = f(x), \quad 0 < x < 1 \tag{13b}$$

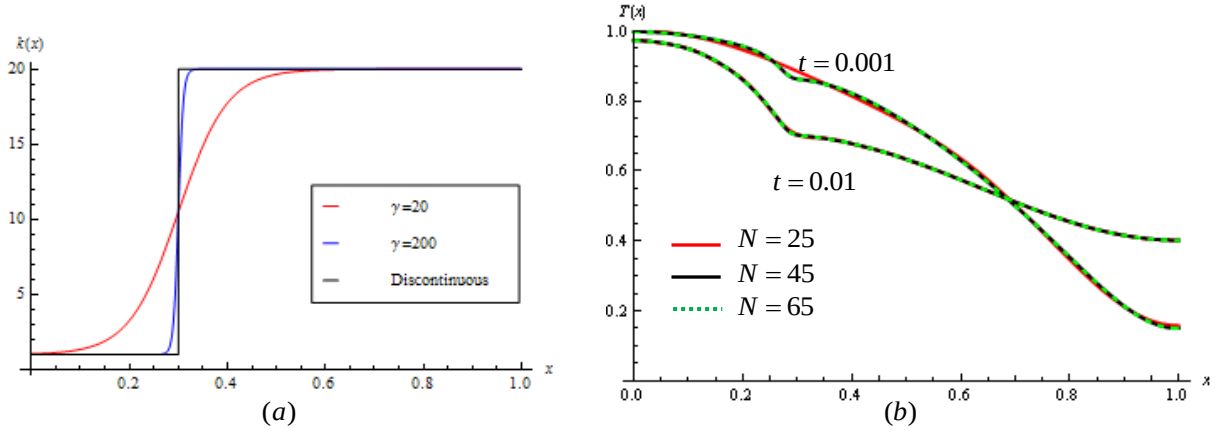
$$\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = 0, \quad \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=1} = 0, \quad t > 0 \tag{13c,d}$$

where the space variable coefficients with abrupt variation are governed by the parameter γ in the function below

$$k(x) = k_1 + (k_2 - k_1)\delta(x), \quad w(x) = w_1 + (w_2 - w_1)\delta(x) \tag{14a,b}$$

$$\delta(x) = \frac{1}{1 + e^{-\gamma(x - xc)}} \tag{14c}$$

with x_c being the interface position. The initial condition is arbitrarily chosen as $f(x) = 1 - x^2$. Fig. 3a. illustrates the behavior of the variable coefficient $k(x)$ with $k_1 = 1$, $k_2 = 20$, $w_1 = 1$, $w_2 = 4$, $x_c = 0.3$ and for the parameter $\gamma = 20,\ 200$ and the discontinuous situation. In Fig. 3b. are shown the results obtained through the UNIT code for $\gamma = 200$ at $t = 0.001$ and $t = 0.01$ considering different truncation orders $N = 25$, 45 and 65. Table 2 below more closely illustrates the convergence behavior of the temperature eigenfunction expansion for this case, which is fully converged to four significant digits and agrees with the dedicated computation in (Naveira-Cotta et al., 2009).



Figures 3 – (a) Abruptly variable thermal conductivity. (b) Results for linear heat diffusion in heterogeneous media.

Table 2 – Convergence of temperature eigenfunction expansion for the abrupt variation problem ($\gamma = 200$).

Method	$t = 0.001$				$t = 0.01$			
	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$
UNIT $N = 25$	0.946641	0.814250	0.636081	0.346372	0.838215	0.670491	0.578623	0.452474
UNIT $N = 35$	0.952572	0.819150	0.628030	0.351627	0.852720	0.675334	0.572659	0.452789
UNIT $N = 45$	0.956912	0.822098	0.629902	0.353351	0.860751	0.678245	0.574727	0.454811
UNIT $N = 55$	0.956568	0.822366	0.630013	0.353433	0.860426	0.678560	0.574867	0.454918
UNIT $N = 65$	0.956603	0.822250	0.629957	0.353386	0.860423	0.678437	0.574803	0.454865
GITT[1]	0.956536	0.822182	0.629859	0.353286	0.860514	0.678413	0.574732	0.454773

[1]Temperature expansion truncation order: 100; Coefficient expansion truncation order: 110. (Naveira-Cotta et al., 2009)

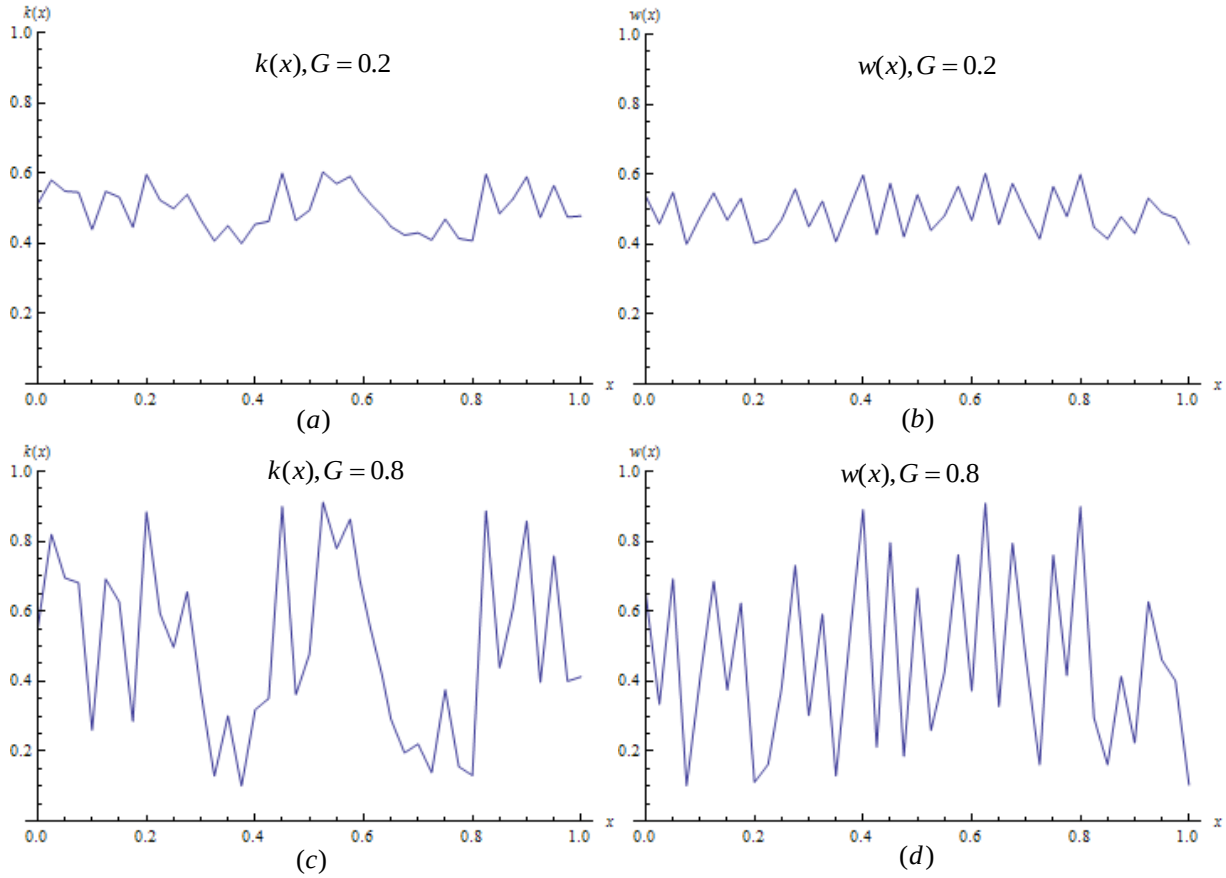
3.3. Properties with random variations

Now we consider the problem formulation with random variations in the properties values, typical of local concentration fluctuations in dispersed phase systems such as composites. The randomly generated coefficients were obtained based on the example of (Lin, 1992), by first generating a number of positions within the medium, and then producing random scaling factors for the properties variations at each position, normalized by their average value. The resulting values are then interpolated to provide continuous functions. The variable coefficients are the given by:

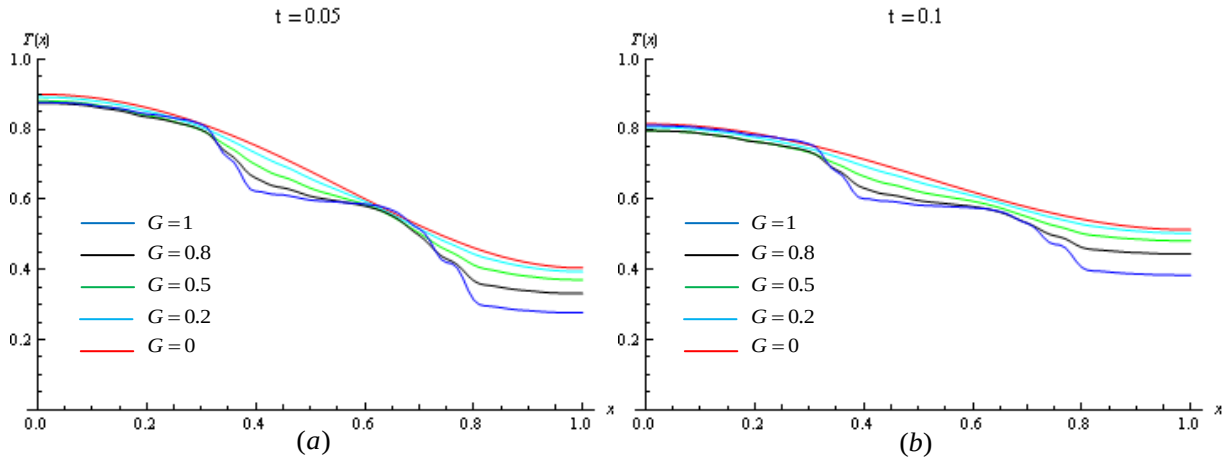
$$k(x) = \left[1 + \left(\frac{g_1(x)}{\overline{g}_1} - 1\right)G\right], \quad w(x) = \left[1 + \left(\frac{g_2(x)}{\overline{g}_2} - 1\right)G\right] \tag{15a,b}$$

where $g_1(x)$ and $g_2(x)$ are linearly interpolated functions within selected positions x and properties values randomly generated in the interval $[0,1]$. Here, just for illustration purposes, the x positions were taken as equally distributed points within the domain. For $G = 1$ one obtains the full random pattern of the generated functions, while $G = 0$ recovers the uniform thermophysical properties situation. Figs. 4a-d below illustrate the employed $k(x)$ and $w(x)$ coefficients by taking $k_0 = w_0 = 0.5$, with $G = 0.2$ and 0.8. A total of 41 equally spaced points were taken along the domain for the random properties generation, while the random numbers at each position were kept unchanged for the

different gains. Figs. 5a. and 5b. illustrate the temperature profile behavior at two different dimensionless times, respectively, for $t = 0.05$ and $t = 0.1$. Table 3 shows the convergence behavior of the solution varying the number of sub-regions (M), with the second order semi-analytical integration, for the same two cases: $G = 0.2$ and 0.8. Clearly, the case with larger variation amplitudes requires a more refined integration scheme. The convergence behavior of the temperature field is also demonstrated while varying the truncation order in the eigenfunction expansion, for different values of G =0.2, 0.5, and 0.8, respectively, in Tables 4 to 6. One may observe that for increasing values of G the convergence of the solution becomes slower, which is expected since higher values of G yield patterns with abrupt random variations of larger amplitudes, much more different from the uniform average values adopted in the very simple chosen eigenvalue problem. Nevertheless, at least three significant digits are converged for the case G=0.5, and at least two digits, in the worst situation, for G=0.8, in the range of truncation orders here analyzed.



Figures 4 –Behavior of the variable diffusion and thermal capacitance coefficients, $k(x)$ and $w(x)$, for the random properties example, with $G = 0.2$ (a-b) and with $G = 0.8$ (c-d).



Figures 5 – Temperature distributions for the random properties example with $G = 0,\ 0.2,\ 0.5,\ 0.8$ and 1, at two different dimensionless times : $t = 0.05$ (a) and at $t = 0.1$ (b)

Table 3 – Convergence of UNIT code solution ($N = 70$ terms in eigenfunction expansion) with different number of sub-regions in the semi-analytical integration (M), for $G = 0.2$ and $G = 0.8$.

M	$G = 0.2,\ N = 70,\ t = 0.1$				$G = 0.8,\ N = 70,\ t = 0.1$			
	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$
$M = 360$	0.791140	0.712956	0.627982	0.540992	0.837339	0.734938	0.622731	0.500930
$M = 380$	0.790998	0.713604	0.627686	0.541651	0.818277	0.710375	0.643878	0.489622
$M = 400$	0.790401	0.713516	0.627184	0.541168	0.824206	0.712316	0.641536	0.490609
$M = 420$	0.790376	0.713176	0.627243	0.541419	0.823595	0.711918	0.642521	0.492229
GITT[1]	0.790358	0.713431	0.627278	0.541537	0.824474	0.715097	0.644814	0.494964

[1]Temperature expansion truncation order: 130; Coefficient expansion truncation order: 80. (Naveira-Cotta et al., 2009)

Table 4 – Convergence of temperature expansion for the random variations problem for $G = 0.2$, with $M = 420$.

Method	$t = 0.05$				$t = 0.1$			
	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$
UNIT $N = 30$	0.852407	0.762114	0.620424	0.451106	0.791173	0.716865	0.611192	0.543517
UNIT $N = 40$	0.862331	0.752019	0.614121	0.455441	0.790454	0.713221	0.628043	0.540233
UNIT $N = 50$	0.863473	0.751298	0.611906	0.457267	0.790230	0.713290	0.627310	0.541450
UNIT $N = 60$	0.863640	0.751686	0.611970	0.457656	0.790218	0.713136	0.627194	0.541452
UNIT $N = 70$	0.863616	0.751651	0.611988	0.457630	0.790376	0.713176	0.627243	0.541419
GITT[1]	0.863769	0.751067	0.612032	0.457890	0.790358	0.713431	0.627278	0.541537

[1]Temperature expansion truncation order: 130; Coefficient expansion truncation order: 80. (Naveira-Cotta et al., 2009)

Table 5 – Convergence of temperature expansion for the random variations problem for $G = 0.5$, with $M = 420$.

Method	$t = 0.05$				$t = 0.1$			
	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$
UNIT $N = 30$	0.858432	0.744861	0.587726	0.453946	0.795920	0.726467	0.644948	0.522308
UNIT $N = 40$	0.868371	0.747645	0.626972	0.443154	0.816069	0.713212	0.632678	0.532082
UNIT $N = 50$	0.869999	0.747726	0.627575	0.442359	0.800101	0.713405	0.635013	0.529276
UNIT $N = 60$	0.869975	0.747763	0.627610	0.442239	0.800264	0.713516	0.635094	0.529291
UNIT $N = 70$	0.869916	0.747729	0.627693	0.442291	0.800303	0.713570	0.635136	0.529285
GITT[1]	0.870880	0.748470	0.627424	0.442530	0.800430	0.713492	0.635133	0.529107

[1]Temperature expansion truncation order: 130; Coefficient expansion truncation order: 80. (Naveira-Cotta et al., 2009)

Table 6 – Convergence of temperature expansion for the random variations problem for $G = 0.8$, with $M = 420$.

Method	$t = 0.05$				$t = 0.1$			
	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$
UNIT $N = 30$	0.885132	0.737244	0.640958	0.410935	0.828359	0.708773	0.628221	0.511239
UNIT $N = 40$	0.877961	0.743037	0.648139	0.410382	0.825049	0.709996	0.643107	0.506194
UNIT $N = 50$	0.882139	0.744086	0.649718	0.409421	0. 823877	0.711665	0.641057	0.492702
UNIT $N = 60$	0.882340	0.744181	0.649453	0.408935	0.823546	0.711922	0.642301	0.492025
UNIT $N = 70$	0.882339	0.744206	0.649415	0.409018	0.823595	0.711918	0.642521	0.492229
GITT[1]	0.887136	0.745236	0.646225	0.407719	0.824474	0.715097	0.644814	0.494964

[1]Temperature expansion truncation order: 130; Coefficient expansion truncation order: 80. (Naveira-Cotta et al., 2009)

4. CONCLUSIONS

In the present work we have challenged the recently constructed UNIT code in solving heat diffusion problems in heterogeneous media, characterized by spatially variable coefficients. Three different heat diffusion problems were herein studied where the variation of the thermophysical properties were illustrated by (i) large scale variations such as in Functionally Graded Materials (FGM), (ii) abrupt variations such as in layered media and (iii) random variations due to local concentration fluctuations in dispersed phase systems such as composites. The results obtained with the UNIT code show excellent agreement with a dedicated computation also based on integral transforms, even for severe variations of the thermophysical properties, illustrating its robustness and flexibility as a simulation tool in this class of problems.

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