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Eigenfunction Expansions for Coupled Nonlinear Convection-Diffusion Problems in Complex Physical Domains

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Abstract. This lecture offers an updated review on the Generalized Integral Transform Technique (GITT), with focus on handling complex geometries, coupled problems, and nonlinear convection-diffusion, so as to illustrate some new application paradigms. Special emphasis is given to demonstrating novel developments, such as a single domain reformulation strategy that simplifies the treatment of complex geometries, an integral balance scheme in handling multiscale problems, the adoption of convective eigenvalue problems in dealing with strongly convective formulations, and the direct integral transformation of nonlinear convection-diffusion problems based on nonlinear eigenvalue problems. Representative application examples are then provided that employ recent extensions on the Generalized Integral Transform Technique (GITT), and a few numerical results are reported to illustrate the convergence characteristics of the proposed eigenfunction expansions.

1. Introduction

Integral transforms are classical analytical tools in providing exact solutions for certain classes of linear partial differential equations, which have been extensively employed in engineering and physical sciences, including thermal sciences and engineering, for more than a century [1-4]. With the concurrent development of computers and numerical methods for PDE´s, such class of analytical approach has to some extent lost relevance in the realm of applications, and only retained a complementary role in the verification of numerical codes and in the solution of sufficiently simple linear problems. Nevertheless, the integral transforms method was progressively extended and generalized along the last three decades, leading to the establishment of a hybrid numerical-analytical methodology, known as the Generalized Integral Transform Technique (GITT) [5-11]. The generalized approach consists of choosing an eigenvalue problem, that retains part of the information on the operators of the original problem, and proposing an eigenfunction expansion, which leads to a coupled linear or nonlinear infinite transformed system, usually to be numerically solved upon truncation to a sufficiently large order. Therefore, the numerical task is undertaken essentially in one single independent variable, usually time, and the solution is analytically recovered in all the other space variables. This hybrid numerical-analytical method holds the relative merits on robustness and accuracy of an analytical technique, while gaining the applicability and flexibility of a purely numerical approach. Various classes of problems that could not in principle be handled by the classical

approach were then progressively dealt with via the generalized concept. The list of extensions achieved through the GITT includes solving equations with time variable coefficients, moving boundary problems, nonlinear formulations in general, irregular domains, eigenvalue problems, boundary layer and Navier-Stokes equations, etc, as reviewed in different sources [5-11].

In recent years, there has been an effort to consolidate this knowledge on the GITT into a general purpose open source algorithm, known as the UNIT (UNified Integral Transforms) algorithm [11-14]. Such a demand, together with fairly recent application challenges [15-24], have induced the proposition of novel computational schemes and theoretical extensions, that have not yet been presented in a systematic form, as here attempted. Among such recent advancements, one may point out the proposition of progressive filtering for multidimensional problems [13-14], the implementation of reordering schemes via multiple criteria [13-14], the single domain reformulation strategy for complex geometries [15-19], the solution of coupled nonlinear reactive flow systems [20], the integral balance approach for convergence enhancement of multiscale problems [21-22], the proposition of convective eigenvalue problems for highly convective formulations [23], and the direct use of nonlinear eigenvalue problems in the integral transformation process of nonlinear PDEs [24]. Before incorporating such developments into a general purpose algorithm, it is of interest to compile and link these ideas, so as to permit a continuous unification effort, as here discussed. A couple of selected examples are also presented to illustrate the recent application challenges posed to the integral transforms approach, involving transient conjugated heat transfer in microsystems and on the analysis of mass transfer with multiple nonlinear reactions in biodiesel synthesis within micro-reactors.

2. Formal Solution

So as to provide a basis for the comprehension of the proposed extensions, the formal GITT solution to a general nonlinear convection-diffusion problem is first presented. A transient convection-diffusion problem of n coupled potentials is thus considered, defined in region V, with boundary surface S [14]:

$$w_k(\mathbf{x})L_{k,t}T_k(\mathbf{x},t) = LT_k(\mathbf{x},t) - \mathbf{u}(\mathbf{x},t,\mathbf{T}).\nabla T_k(\mathbf{x},t) + g_k(\mathbf{x},t,\mathbf{T}), \quad \mathbf{x} \in V, \ t > 0, \ k = 1,2,...,n \qquad (1a)$$

where the t variable operator, $L_{k,t}$, for a parabolic or parabolic-hyperbolic formulation may be given by,

$$L_{k,t} \equiv \frac{\partial}{\partial t} \qquad (1b)$$

while for an elliptic or hyperbolic formulation it is written as

$$L_{k,t} \equiv -a_k(t)\frac{\partial}{\partial t}\left[b_k(t)\frac{\partial}{\partial t}\right] \qquad (1c)$$

and the remaining space coordinates operator, with diffusion and linear dissipation, is given as

$$L_k \equiv \nabla \cdot \left(K_k(\mathbf{x})\nabla\right) - d_k(\mathbf{x}) \qquad (1d)$$

The initial or boundary conditions in the t variable are given, respectively, by

$$T_k(\mathbf{x},0) = f_k(\mathbf{x}), \quad \mathbf{x} \in V, \quad \text{for the parabolic formulation} \qquad (1e)$$

$$T_k(\mathbf{x},0) = f_k(\mathbf{x}), \quad \frac{\partial T_k(\mathbf{x},0)}{\partial t} = h_k(\mathbf{x}), \quad \mathbf{x} \in V, \quad \text{for the hyperbolic formulation} \qquad (1f)$$

or

$$\left[\lambda_{k,l}(t) + (-1)^{l+1}\gamma_{k,l}(t)\frac{\partial}{\partial t}\right]T_k(\mathbf{x},t) = f_{k,l}(\mathbf{x}), \text{ at } t=t_l, \ l=0,1, \ \mathbf{x} \in V, \text{ for the elliptic formulation} \qquad (1g)$$

and the boundary conditions in the remaining coordinates is concisely written as

$$B_k T_k(\mathbf{x},t) = \phi_k(\mathbf{x},t,\mathbf{T}), \ \mathbf{x} \in S, \ t > 0 \qquad (1h)$$

with the boundary conditions operator

$$B_k \equiv \left[\alpha_k(\mathbf{x}) + \beta_k(\mathbf{x}) K_k(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \right] \tag{1i}$$

where $\mathbf{n}$ denotes the outward-drawn normal to the surface S, and the coupled potentials vector is given by

$$\mathbf{T} = \{ T_1, T_2, ..., T_k, ..., T_n \} \tag{1j}$$

Equations (1) are fairly general since nonlinear terms may be grouped into the equations and boundary conditions source terms. In the case of decoupled linear source terms, i.e., $g \equiv g(\mathbf{x},t)$, and $\phi \equiv \phi(\mathbf{x},t)$, and in the absence of the convective term ($\mathbf{u} \equiv 0$), this example is reduced to a class I linear diffusion problem for each potential, according to the classification in [4], and exact analytical solutions are readily available via the Classical Integral Transform Technique.

Following the formal solution procedure for nonlinear convection-diffusion problems through integral transforms, one starts with the proposition of eigenfunction expansions for the associated potentials. The preferred eigenvalue problem choice appears from the direct application of the separation of variables methodology to the linear homogeneous purely diffusive version of the proposed problem. Thus, the recommended set of decoupled auxiliary problems is here given by:

$$[L_k + \mu_{ki}^2 w_k(\mathbf{x})]\psi_{ki}(\mathbf{x}) = 0, \quad \mathbf{x} \in V \tag{2a}$$

$$B_k \psi_{ki}(\mathbf{x}) = 0, \quad \mathbf{x} \in S \tag{2b}$$

where the eigenvalues, μ_{ki}, and associated eigenfunctions, $\psi_{ki}(\mathbf{x})$, are assumed to be known from exact analytical expressions, for instance obtained through symbolic computation [25], or application of the GITT itself [6,11]. One should notice that eqs. (1) are presented in such a form which already reflects this choice of eigenvalue problems, given by eqs. (2), with the adoption of linear $\mathbf{x}$-dependent coefficients in both the equations and boundary conditions, and incorporating the remaining terms (coupling, nonlinear and convective terms) into the source terms, without loss of generality.

Making use of the orthogonality properties of the eigenfunctions, it is then possible to define the following integral transform pairs:

$$\bar{T}_{ki}(t) = \int_V w_k(\mathbf{x}) \tilde{\psi}_{ki}(\mathbf{x}) T_k(\mathbf{x},t) dV, \qquad \text{transforms} \tag{3a}$$

$$T_k(\mathbf{x},t) = \sum_{i=1}^{\infty} \tilde{\psi}_{ki}(\mathbf{x}) \bar{T}_{k,i}(t), \qquad \text{inverses} \tag{3b}$$

where the symmetric kernels $\tilde{\psi}_{ki}(\mathbf{x})$ are given by

$$\tilde{\psi}_{ki}(\mathbf{x}) = \frac{\psi_{ki}(\mathbf{x})}{\sqrt{N_{ki}}}; \quad N_{ki} = \int_v w_k(\mathbf{x}) \psi_{ki}^2(\mathbf{x}) dv \tag{3c,d}$$

with N_{ki} being the normalization integral.

The integral transformation of eq.(1a) is accomplished by applying the operator $\int_V \tilde{\psi}_{ki}(\mathbf{x})(\cdot) dV$ and making use of the boundary conditions given by eqs. (1g) and (2b), yielding:

$$L_{k,t} \bar{T}_{ki}(t) + \mu_{ki}^2 \bar{T}_{ki}(t) = \bar{g}_{ki}(t,\overline{\mathbf{T}}), \; i=1,2,..., \quad t>0, \quad k=1,2,...,n \tag{4a}$$

where the transformed source term $\bar{g}_{ki}(t,\overline{\mathbf{T}})$ is due to the integral transformation of the equation source terms and of the boundary source terms:

$$\bar{g}_{ki}(t,\overline{\mathbf{T}}) = \int_V \tilde{\psi}_{ki}(\mathbf{x}) \left[-\mathbf{u}(\mathbf{x},t,\mathbf{T}).\nabla T_k(\mathbf{x},t) + g_k(\mathbf{x},t,\mathbf{T}) \right] dV + \int_S \phi_k(\mathbf{x},t,\mathbf{T}) \left[\frac{\tilde{\psi}_{ki}(\mathbf{x}) - K_k(\mathbf{x}) \dfrac{\partial \tilde{\psi}_{ki}(\mathbf{x})}{\partial \mathbf{n}}}{\alpha_k(\mathbf{x}) + \beta_k(\mathbf{x})} \right] ds \tag{4b}$$

The initial or boundary conditions in the t variable given by eqs. (1e-1g) are transformed through the operator $\int_V w_k(\mathbf{x}) \tilde{\psi}_{ki}(\mathbf{x})(\cdot) dV$, to provide:

$$\overline{T}_{ki}(0) = \overline{f}_{ki} \equiv \int_V w_k(\mathbf{x})\tilde{\psi}_{ki}(\mathbf{x})f_k(\mathbf{x})dV \text{ , for the parabolic problem} \tag{4c}$$

$$\overline{T}_{ki}(0) = \overline{f}_{ki} \text{ ; } \frac{d\overline{T}_{ki}}{dt}\bigg|_{t=0} = \overline{h}_{ki} \equiv \int_V w_k(\mathbf{x})\tilde{\psi}_{ki}(\mathbf{x})h_k(\mathbf{x})dV \text{ , for the hyperbolic problem} \tag{4d,e}$$

$$\left[\lambda_{k,l}(t) + (-1)^{l+1}\gamma_{k,l}(t)\frac{d}{dt}\right]\overline{T}_{ki}(t) = \overline{f}_{k,li} \equiv \int_V w_k(\mathbf{x})\tilde{\psi}_{ki}(\mathbf{x})f_{k,l}(\mathbf{x})dV, \text{ at } t=t_l, l=0,1, \text{ for the elliptic}$$

$$\text{problem} \tag{4f}$$

For the solution of the infinite coupled system of nonlinear ordinary differential equations given by eqs. (4), one usually needs to make use of numerical algorithms, after the truncation of the system to a sufficiently large finite order. For instance, the built-in routine of the *Mathematica* system [25], NDSolve, may be employed, which is able to provide reliable solutions under automatic absolute and relative errors control. After 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 $\mathbf{x}$ and t.

The formal solution regarding the standard procedure of the UNIT algorithm is known as the total transformation scheme, described in [11-14], in which all spatial variables are integral transformed. There is also the partial integral transformation scheme option of the UNIT algorithm [11,14], as an alternative solution path to problems with a strong convective direction, which is not eliminated through integral transformation, but kept within the transformed system. This alternative transformation scheme will not be examined in the present review.

3. Recent Developments
A few recent developments are now discussed, which significantly enhance the applicability of the hybrid approach in complex geometric configurations, multiscale variable properties and/or dimensions, and coupled convective and nonlinear formulations.

3.1. Reordering Schemes
In multidimensional applications, the final integral transform solution for the related potential could in principle be expressed as double or triple infinite summations for two or three-dimensional transient problems, respectively. From a computational point of view, only a truncated version of such summations should be actually evaluated. However, if one just truncates each individual summation to a certain prescribed finite order, computations become quite ineffective. Some important information to the final result can be disregarded due to the fixed summations limits, while other terms are accounted for that have practically no contribution to convergence of the potential in the relative accuracy required. Therefore, for an appropriate computation of these expansions, the infinite multiple summations should first be converted to a single sum representation with the appropriate reordering of terms according to their individual contribution to the final numerical result [8]. Then, it becomes possible to evaluate the minimal number of eigenvalues and related derived quantities required to reach the user-prescribed accuracy target. Since the final solution is not, of course, known a priori, the parameter which shall govern this reordering scheme must be chosen with care. The most common choice of reordering strategy is based on arranging in increasing order the sum of the squared eigenvalues in each spatial coordinate, which offers a good compromise between the overall convergence enhancement and simplicity in use. However, individual applications may require more elaborate reordering that accounts for the influence of transformed initial conditions and transformed nonlinear source terms in the ODE system, as discussed in what follows.

To more clearly understand alternative reordering schemes, let us start from the formal solution of the transformed potentials, equations (4), for the parabolic problem case, which is written as:

$$\bar{T}_{ki}(t) = \bar{f}_{ki}\exp\left(-\mu_i^2 t\right) + \int_0^t \bar{g}_{ki}(t',\mathbf{T})\exp\left[-\mu_i^2(t-t')\right]dt' \tag{5}$$

Integration by parts of eq.(5) provides an alternative expression that allows the understanding of the influence of the transformed initial conditions and source terms in the choice of reordering schemes, in rewriting the multiple series as a single one:

$$\bar{T}_{ki}(t) = \bar{f}_{ki}\exp\left(-\mu_i^2 t\right) + \frac{1}{\mu_i^2}\left[\bar{g}_{ki}(t,\mathbf{T}) - \bar{g}_{ki}(0,\mathbf{T})\exp\left(-\mu_i^2 t\right)\right] - \frac{1}{\mu_i^2}\int_0^t \frac{d\bar{g}_{ki}}{dt'}\exp\left[-\mu_i^2(t-t')\right]dt' \tag{6}$$

It is evident that the squared eigenvalues, which involve the combination of the eigenvalues in each spatial coordinate, play the most important role in the decay of the absolute values of the transformed potentials, and thus of the infinite summation parcels, both through the exponential term $\exp\left(-\mu_i^2 t\right)$ and, at lower convergence rates, through the inverse of the squared eigenvalues, $1/\mu_i^2$. Therefore, the traditionally employed reordering scheme based on the ascending order of the squared eigenvalues should be able to account for the most important terms in the adequate reorganization of the expansion. Nevertheless, supposing that the last integral term in eq. (6) plays a less important role in the reordering choice, and in fact it vanishes when the source term is not time dependent, one concludes that the decay of the transformed initial condition and the transformed source term evolution from its initial value, play a complementary role in the selection of terms in the eigenfunction expansion for a fixed truncation order. Thus, a more robust selection can be proposed, based on adding to the initially reordered terms, according to the squared eigenvalues criterion, those extra terms that might be of significant contribution to the final result under the analysis of the initial condition decay and/or the transformed source term behavior. In the first case, for the lowest time value of interest, $t = t_{\min}$, the criterion that reorders the terms based on the decay of the initial conditions is based on sorting in decreasing order from the expression $\bar{f}_{ki}\exp\left(-\mu_i^2 t_{\min}\right)$. In the second case, for the general situation of a nonlinear transformed source term, the estimation of the terms importance is more difficult, since the source terms, in the more general nonlinear situation, are not known *a priori*. One possible approach is to consider the limiting case of an uniform unitary source term, representing for instance its normalized maximum value, and analyzing the reordering of terms in descending absolute value based on the expression $\frac{1}{\mu_i^2}\int_V \tilde{\varphi}_{ki}(\mathbf{x})dV$. Therefore, combining the three criteria, and eliminating the duplicates with respect to the traditional reordering scheme based on the squared eigenvalues, a few extra terms are added to the initially reordered terms that may have still some relevant effect in the final truncated summation.

3.2. Single Domain Formulation

Consider now a general transient convection-diffusion problem, which corresponds to the general parabolic formulation represented in section 2, defined in a complex multidimensional configuration that is represented by n_V different sub-regions with volumes V_l, $l = 1, 2, ..., n_V$, with potential and flux continuity at the interfaces among themselves, as illustrated in Figure 1a [11]. We consider that a certain number of potentials are to be calculated in each sub-region, $T_{k,l}(\mathbf{x},t)$, $k = 1, 2, ..., n$, governed in the corresponding sub-region through this fairly general formulation including the general equation and boundary source terms, respectively, $P_{k,l}(\mathbf{x},t,\mathbf{T})$ and $\phi_{k,l}(\mathbf{x},t,\mathbf{T})$. For conciseness, the nonlinear equation source term already incorporates the nonlinear convective term in eq.(1a). Thus,

$$w_{k,l}(\mathbf{x})\frac{\partial T_{k,l}(\mathbf{x},t)}{\partial t} = \nabla \cdot \left(K_{k,l}(\mathbf{x})\nabla T_{k,l}(\mathbf{x},t)\right) - d_{k,l}(\mathbf{x})T_{k,l}(\mathbf{x},t) + P_{k,l}(\mathbf{x},t,\mathbf{T}),$$

$$\mathbf{x} \in V_l, \quad t > 0, \quad k = 1, 2, ..., n, \quad l = 1, 2, ..., n_V \tag{7a}$$

with initial, interface and boundary conditions given, respectively, by

$$T_{k,l}(\mathbf{x},0) = f_{k,l}(\mathbf{x}), \qquad \mathbf{x} \in V_l \tag{7b}$$

$$T_{k,l}(\mathbf{x},t) = T_{k,m}(\mathbf{x},t), \ \mathbf{x} \in S_{l,m}, \ t > 0 \tag{7c}$$

$$K_{k,l}(\mathbf{x})\frac{\partial T_{k,l}(\mathbf{x},t)}{\partial \mathbf{n}} = K_{k,m}(\mathbf{x})\frac{\partial T_{k,m}(\mathbf{x},t)}{\partial \mathbf{n}}, \ \mathbf{x} \in S_{l,m}, \ t > 0 \tag{7d}$$

$$\left[\alpha_{k,l}(\mathbf{x}) + \beta_{k,l}(\mathbf{x})K_{k,l}(\mathbf{x})\frac{\partial}{\partial \mathbf{n}}\right]T_{k,l}(\mathbf{x},t) = \phi_{k,l}(\mathbf{x},t,\mathbf{T}), \ \mathbf{x} \in S_l, \ t > 0 \tag{7e}$$

where $\mathbf{n}$ denotes the outward-drawn normal to the interfaces, $S_{l,m}$, and external surfaces, S_l.

The Generalized Integral Transform Technique (GITT) [5-11] can in principle be applied to solve system (7) above, either by constructing an individual eigenfunction expansion basis for each potential, and then coupling all the transformed systems and potentials for each sub-region, or by constructing a multiregion eigenvalue problem that couples all of the sub-regions into a single set of eigenvalues, which in general involves cumbersome computations in multidimensional applications. Figure 1 provides two possibilities for representation of the single domain, either by keeping the original overall domain after definition of the space variable coefficients, as shown in Figure 1b, or, if desired, by considering a regular overall domain that envelopes the original one, as shown in Figure 1c. Irregular domains can be directly integral transformed and, in principle, there is no need to consider the second representation possibility pointed out above. However, some computational advantages may be achieved by enveloping the original irregular domain by a simple regular region.
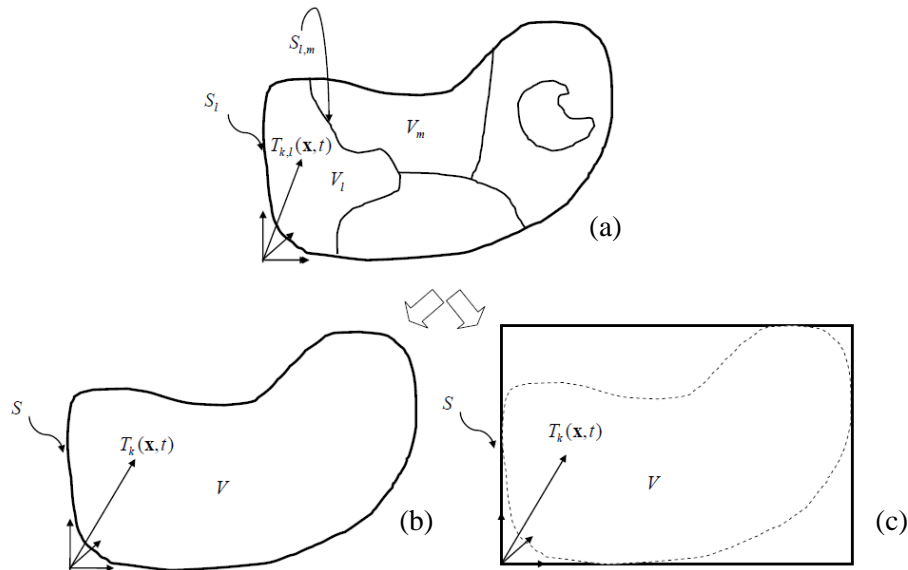

Figure 1: (a) Diffusion or convection-diffusion in a complex multidimensional configuration with n_V sub-regions; (b) Single domain representation keeping the original overall domain; (c) Single domain representation considering a regular overall domain that envelopes the original one [11,15].

Therefore, as already demonstrated in the analysis of specific conjugated problems [11,15-16], it is possible to rewrite problem (7) as a single domain formulation with space variable coefficients and source terms, given by:

$$w_k(\mathbf{x})\frac{\partial T_k(\mathbf{x},t)}{\partial t} = \nabla \cdot \left(K_k(\mathbf{x})\nabla T_k(\mathbf{x},t)\right) - d_k(\mathbf{x})T_k(\mathbf{x},t) + P_k(\mathbf{x},t,\mathbf{T}), \quad \mathbf{x} \in V, \ t > 0 \tag{8a}$$

with initial and boundary conditions given, respectively, by

$$T_k(\mathbf{x},0) = f_k(\mathbf{x}), \qquad \mathbf{x} \in V \tag{8b}$$

$$\left[\alpha_k(\mathbf{x}) + \beta_k(\mathbf{x}) K_k(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \right] T_k(\mathbf{x},t) = \phi_k(\mathbf{x},t,\mathbf{T}), \ \mathbf{x} \in S, \ t > 0 \tag{8c}$$

where

$$V = \sum_{l=1}^{n_V} V_l, \quad S = \sum_{l=1}^{n_V} S_l \tag{8d,e}$$

The space variable coefficients in equations (8), besides the new equation and boundary source terms and initial conditions, now without the subscript l for the sub-regions V_l, incorporate the abrupt transitions among the different sub-regions and permit the representation of system (7) as a single domain formulation, to be directly handled by integral transforms, as described in section 2.

3.3. Eigenvalue Problem: Integral Balance Approach

For an improved convergence of the eigenfunction expansion for the original potential, Eq. (3b), it is of interest to include as much information as possible of the coefficients spatial behavior into the eigenvalue problem, Eqs. (2), via the user chosen coefficients $w_k(\mathbf{x}), k_k(\mathbf{x}),$ and $d_k(\mathbf{x})$. The GITT approach itself is employed in the hybrid numerical-analytical solution of this eigenvalue problem, as discussed in [6,11], after choosing an auxiliary eigenvalue problem with simpler structure, defined by the coefficients $\hat{w}_k(\mathbf{x}), \hat{k}_k(\mathbf{x}),$ and $\hat{d}_k(\mathbf{x})$, which should allow for an analytical solution. The solution of problem (2) is thus itself proposed as an eigenfunction expansion:

$$\psi_{ki}(\mathbf{x}) = \sum_{n=1}^{\infty} \tilde{\Omega}_{kn}(\mathbf{x}) \bar{\psi}_{ki,n}, \qquad inverse \tag{9a}$$

$$\bar{\psi}_{ki,n} = \int_V \hat{w}_k(\mathbf{x}) \psi_{ki}(\mathbf{x}) \tilde{\Omega}_{kn}(\mathbf{x}) dV, \qquad transform \tag{9b}$$

where the normalized auxiliary eigenfunction and its norms are

$$\tilde{\Omega}_{kn}(\mathbf{x}) = \frac{\Omega_{kn}(\mathbf{x})}{\sqrt{N_{\Omega_{kn}}}} \ , \ \text{with} \ N_{\Omega_{kn}} = \int_V \hat{w}_k(\mathbf{x}) \Omega_{kn}^2(\mathbf{x}) dV \tag{10a,b}$$

in terms of the simpler auxiliary eigenvalue problems given as:

$$\nabla \cdot \hat{k}_k(\mathbf{x}) \nabla \Omega_{kn}(\mathbf{x}) + (\lambda_{kn}^2 \hat{w}_k(\mathbf{x}) - \hat{d}_k(\mathbf{x})) \Omega_{kn}(\mathbf{x}) = 0, \ \mathbf{x} \in V \tag{11a}$$

with boundary conditions

$$\alpha_k(\mathbf{x}) \Omega_{kn}(\mathbf{x}) + \beta_k(\mathbf{x}) \hat{k}_k(\mathbf{x}) \frac{\partial \Omega_{kn}(\mathbf{x})}{\partial \mathbf{n}} = 0, \quad \mathbf{x} \in S \tag{11b}$$

Equation (2a) is then operated on with $\int_V \tilde{\Omega}_{ki}(\mathbf{x})(\cdot) dV$, to yield the transformed algebraic systems:

$$(\mathbf{A}_k + \mathbf{C}_k)\{\bar{\psi}_k\} = \mu_k^2 \mathbf{B}_k \{\bar{\psi}_k\} \tag{12a}$$

with the elements of the M x M matrices given by:

$$A_{k,ij} = \int_S \frac{\tilde{\Omega}_{ki}(\mathbf{x}) - \hat{k}_k(\mathbf{x}) \frac{\partial \tilde{\Omega}_{ki}(\mathbf{x})}{\partial \mathbf{n}}}{\alpha_k(\mathbf{x}) + \beta_k(\mathbf{x})} \left[\beta_k(\mathbf{x}) \left(k_k(\mathbf{x}) - \hat{k}_k(\mathbf{x}) \right) \frac{\partial \tilde{\Omega}_{kj}(\mathbf{x})}{\partial \mathbf{n}} \right] dS - \int_S \left(k_k(\mathbf{x}) - \hat{k}_k(\mathbf{x}) \right) \tilde{\Omega}_{ki}(\mathbf{x}) \frac{\partial \tilde{\Omega}_{kj}(\mathbf{x})}{\partial \mathbf{n}} dS +$$

$$+ \int_V \left(k_k(\mathbf{x}) - \hat{k}_k(\mathbf{x}) \right) \nabla \tilde{\Omega}_{ki}(\mathbf{x}) \cdot \nabla \tilde{\Omega}_{kj}(\mathbf{x}) dV + \int_V \left(d_k(\mathbf{x}) - \hat{d}_k(\mathbf{x}) \right) \tilde{\Omega}_{ki}(\mathbf{x}) \tilde{\Omega}_{kj}(\mathbf{x}) dV$$

$$\tag{12b}$$

$$C_{k,ij} = \lambda_{ki}^2 \delta_{ij} \qquad\qquad B_{k,ij} = \int_V w_k(\mathbf{x}) \tilde{\Omega}_{ki}(\mathbf{x}) \tilde{\Omega}_{kj}(\mathbf{x}) dV \tag{12c,d}$$

where δ_{ij} is the Kronecker delta.

Therefore, the eigenvalue problem given by Eqs. (2) is reduced to the standard algebraic eigenvalue problems given by Eqs. (12), which can be solved with existing software for matrix eigensystem analysis, yielding the eigenvalues μ_k, whereas the corresponding calculated eigenvectors from this numerical solution, $\bar{\psi}_{ki}$, are to be used in the inversion formula, given by Eq. (9a), to find the desired eigenfunction.

However, when dealing with the GITT solution of this eigenvalue problem with markedly variable spatial coefficients, it is not always possible to employ an auxiliary eigenvalue problem that incorporates even part of this information, since it may result unsolvable in analytic explicit form. Therefore, in many cases it is required to choose simpler expressions for the auxiliary coefficients, $\hat{w}_k(\mathbf{x}), \hat{k}_k(\mathbf{x}),$ and $\hat{d}_k(\mathbf{x})$, which may lead to slowly converging expansions for the original eigenfunctions. This is particularly important when multiple spatial scales and/or very abrupt variations of the coefficients need to be handled. In such cases, an integral balance procedure [21-22] can be particularly beneficial in accelerating the convergence of such eigenfunction expansions by analytically rewriting the expansion for the eigenfunction itself, while explicitly accounting for the space variable coefficients local variation. The integral balance procedure employed is a convergence acceleration technique [8,21-22] here aimed at obtaining eigenfunction expansions of improved convergence behavior for both the eigenfunction and its derivatives, through integration over the spatial domain, thus benefiting from the better convergence characteristics of the integrals of eigenfunction expansions. It consists of the double integration of the original equation that governs the potential for which the convergence improvement is being sought, in this case, the eigenvalue problem itself. Through a single integration of the original equation, in a chosen coordinate, an improved expression for the eigenfunction derivative is obtained, and a second integration then offers an improved relation for computation of the eigenfunction itself. Then, the problem boundary conditions in that coordinate are accounted for, so that the eigenfunctions and respective derivatives at the boundaries can be eliminated. The expressions provided by the integral balance approach can then be employed back into the solution of the eigenvalue problem (2), following the integral transformation procedure above described, yielding the algebraic eigenvalue which provides the eigenvalues and the eigenvectors, that can be readily substituted back in the inversion formula, Eqs. (9a). This approach is illustrated in details in [21-22].

3.4. Convective Eigenvalue Problem

An interesting approach towards enhancing convergence of eigenfunction expansions for convection-diffusion problems with strong convective effects, involves incorporating the convective effects into the chosen eigenvalue problem that forms the basis of the proposed eigenfunction expansion. The aim is to improve convergence, especially in such cases of highly convective formulations, by directly accounting for the relative importance of convective and diffusive effects within the eigenfunctions themselves [23], in contrast to the traditional approach via a purely diffusive eigenvalue problem, above revised. Through a straightforward transformation of the original convection-diffusion problem, basically by redefining the coefficients associated with the transient and diffusive terms, the convective terms are merged into a generalized diffusion term with a space variable diffusion coefficient. The generalized diffusion problem then naturally leads to the eigenvalue problem to be adopted for deriving the eigenfunction expansion in the linear situation, as well as for the appropriate linearized version in the case of a nonlinear application. The resulting eigenvalue problem with space variable coefficients is then solved through the GITT, yielding the corresponding algebraic eigenvalue problem upon selection of a simple auxiliary eigenvalue problem of known analytical solution [6,11]. The GITT is also applied in the solution of the generalized diffusion problem, and the resulting transformed ordinary differential equations system is solved either analytically, for the linear case, or numerically for the nonlinear formulation. This approach is here briefly illustrated by considering a fairly general nonlinear one-dimensional parabolic formulation:

$$w_k(x)\frac{\partial T_k(x,t)}{\partial t} + u_k(x)\frac{\partial T_k(x,t)}{\partial x} = \frac{\partial}{\partial x}[k_k(x)\frac{\partial T_k(x,t)}{\partial x}] - d_k(x)T_k(x,t) + P_k(x,t,\mathbf{T}), \quad x_0 < x < x_1, t > 0 \quad (13)$$

where $u_k(x)$ is a characteristic linear representation of the convective term coefficient, while the remaining of the nonlinear convective operator (or of any other operator) is incorporated into the nonlinear source term, $P_k(x,t,\mathbf{T})$. Problem (13) can be readily rewritten as a generalized diffusion problem, through a simple transformation of the diffusive and transient terms as:

$$\hat{w}_k(x)\frac{\partial T_k(x,t)}{\partial t} = \frac{\partial}{\partial x}[\hat{k}_k(x)\frac{\partial T_k(x,t)}{\partial x}] - \hat{d}_k(x)T_k(x,t) + \hat{P}_k(x,t,T), \quad x_0 < x < x_1, t > 0 \quad (14)$$

where,

$$\hat{w}_k(x) = w_k(x)\hat{k}_k(x)/k_k(x); \hat{d}_k(x) = d_k(x)\hat{k}_k(x)/k_k(x); \hat{P}_k(x,t,T) = P_k(x,t,\mathbf{T})\hat{k}_k(x)/k_k(x);$$

$$u_k^*(x) = \frac{1}{k_k(x)}\left[u_k(x) - \frac{dk_k(x)}{dx}\right]; \text{ and } \hat{k}_k(x) = e^{-\int u_k^*(x)dx} \quad (15a\text{-}e)$$

Equation (14) is a special case of the nonlinear diffusion problems that have been extensively handled through the GITT, as described in section 2, but are now treated through an eigenfunction expansion basis that includes convective effects through the characteristic convective term coefficient, $u_k(x)$. The self-adjoint eigenvalue problem with space variable coefficients to be considered would then be given by the following equation:

$$\frac{d}{dx}[\hat{k}_k(x)\frac{d\psi_k(x)}{dx}] + [\mu_k^2\hat{w}_k(x) - \hat{d}_k(x)]\psi_k(x) = 0, \quad x_0 < x < x_1 \quad (16)$$

which can be readily solved by the GITT itself, as discussed above, yielding the corresponding algebraic eigenvalue problems. The extension of this analysis to multidimensional problems is straightforward [23].

3.5. Nonlinear Eigenvalue Problem

A whole new frontier for the GITT methodology has been recently envisioned [24], when eigenfunction expansions based on nonlinear eigenvalue problems, that incorporate the original nonlinear equation and boundary condition coefficients, have been proposed. The aim is to achieve improved convergence behavior, in comparison to the classical approach with a linear eigenvalue problem, here in particular for problems with nonlinear boundary conditions. For the sake of illustration, the nonlinear single-potential parabolic problem below is considered, with no need of collapsing the nonlinear boundary condition coefficients information into the nonlinear source terms, as previously prefered:

$$w(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial t} = \nabla.k(\mathbf{x})\nabla T - d(\mathbf{x})T + P(\mathbf{x},t,T) , \quad \text{in } \mathbf{x} \in V, \ t > 0 \quad (17a)$$

with initial and boundary conditions

$$T(\mathbf{x},0) = f(\mathbf{x}) , \quad \mathbf{x} \in V \quad (17b)$$

$$\alpha(\mathbf{x},t,T) \ T + \beta(\mathbf{x},t,T) \ k(\mathbf{x}) \ \frac{\partial T}{\partial \mathbf{n}} = \phi(\mathbf{x},t,T) , \quad \mathbf{x} \in S , \ t > 0 \quad (17c)$$

where α and β are the nonlinear boundary condition coefficients and $\mathbf{n}$ is the outward drawn normal vector to surface S. All the boundary condition coefficients and source terms are allowed to be nonlinear, besides being explicitly dependent also on the space and time variables for the sake of generality.

Here, it suffices to proceed with the formal integral transform solution for the non-filtered potential. Taking a different path from the usual formalism in the GITT, as presented in section 2, a nonlinear eigenvalue problem that preserves the original boundary condition coefficients is preferred instead of the one with linear characteristic coefficients, as in eqs.(2), in the form:

$$\nabla.k(\mathbf{x})\nabla\psi_i(\mathbf{x};t)+\left(\mu_i^2(t)w(\mathbf{x})-d(\mathbf{x})\right)\psi_i(\mathbf{x};t)=0\ ,\ \mathbf{x}\in V \tag{18a}$$

with boundary conditions

$$\alpha(\mathbf{x},t,T)\psi_i(\mathbf{x};t)+\beta(\mathbf{x},t,T)k(\mathbf{x})\frac{\partial\psi_i(\mathbf{x};t)}{\partial\mathbf{n}}=0,\quad \mathbf{x}\in S \tag{18b}$$

and the solution for the associated t-dependent eigenfunctions, $\psi_i(\mathbf{x};t)$, and eigenvalues, $\mu_i(t)$, is at this point assumed to be known.

Problem (18) allows for the definition of the following integral transform pair:

$$\bar{T}_i(t)=\int_V w(\mathbf{x})\ \psi_i(\mathbf{x};t)\,T(\mathbf{x},t)\ dv\ ,\qquad \text{transform} \tag{19a}$$

$$T(\mathbf{x},t)=\sum_{i=1}^{\infty}\frac{1}{N_i(t)}\psi_i(\mathbf{x};t)\bar{T}_i(t)\ ,\qquad\qquad \text{inverse} \tag{19b}$$

and the normalization integrals

$$N_i(t)=\int_V w(\mathbf{x})\psi_i^2(\mathbf{x};t)\ dv \tag{19c}$$

After application of the integral transformation procedure, the resulting ODE system for the transformed potentials, $\bar{T}_i(t)$, is written as:

$$\frac{d\bar{T}_i(t)}{dt}+\sum_{j=1}^{\infty}A_{i,j}(t,\bar{\mathbf{T}})\bar{T}_j(t)=\bar{g}_i(t,\bar{\mathbf{T}}),\quad t>0,\ \ i,j=1,2\ldots \tag{20a}$$

with initial conditions

$$\bar{T}_i(0)=\bar{f}_i \tag{20b}$$

where,

$$A_{i,j}(t,\bar{\mathbf{T}})=\delta_{ij}\mu_i^2(t)+A_{i,j}^*(t,\bar{\mathbf{T}}) \tag{20c}$$

and

$$A_{i,j}^*(t,\bar{\mathbf{T}})=-\frac{1}{N_j(t)}\int_V w(\mathbf{x})\ \frac{\partial}{\partial t}[\psi_i(\mathbf{x};t)]\psi_j(\mathbf{x};t)\ dv \tag{20d}$$

$$\bar{g}_i(t,\bar{\mathbf{T}})=\int_V \psi_i(\mathbf{x};t)P^*(\mathbf{x},t,T)\ dv+\int_S\phi(\mathbf{x},t,T)\left(\frac{\psi_i(\mathbf{x};t)\ -k(\mathbf{x})\dfrac{\partial\psi_i}{\partial\mathbf{n}}}{\alpha(\mathbf{x},t,T)+\beta(\mathbf{x},t,T)}\right)ds \tag{20e}$$

$$\bar{f}_i=\int_V w(\mathbf{x})\ \psi_i(\mathbf{x};0)\,f(\mathbf{x})\ dv \tag{20f}$$

System (20) is again numerically solved through well-established initial value problem solvers [25]. It should be recalled that the eigenvalue problem in eqs.(18) has now to be solved simultaneously with the transformed system given by eqs. (19), yielding the time variable eigenfunctions, eigenvalues and norms, as is further discussed in [24]. The desired final solution is then reconstructed from the inverse formula (19b). The GITT itself is employed in the solution of the nonlinear eigenvalue problem, eqs.(18). The basic idea is to reduce the eigenvalue problem described by the partial differential equation into a nonlinear algebraic eigenvalue problem, which can be solved by known approaches for matrix nonlinear eigensystem analysis. Therefore, the eigenfuctions of the original auxiliary problem can be expressed by eigenfunction expansions based on a simpler auxiliary eigenvalue problem, with linear coefficients, for which exact analytic solutions exist, as previously discussed and detailed in [24].

4. Applications and Results

The developments above discussed are now in part illustrated through a couple of applications recently dealt with via the GITT. The first one is associated with conjugated heat transfer in a non-straight microchannel configuration, which demonstrates both the single domain reformulation strategy as well as the comparison of different reordering schemes on the expansions convergence behavior. The second application brings a coupled three-dimensional nonlinear reactive-convective-diffusive problem, associated with the continuous synthesis of biodiesel in micro-reactors. Here, two different choices of eigenvalue problems were critically compared, either by accounting only for the diffusion effects or by incorporating information on the convective effects through a space variable coefficient.

4.1. Conjugated Heat Transfer in Microsystems

This example is aimed at illustrating the combination of the single domain formulation with the Generalized Integral Transform Technique to tackle conjugated heat transfer problems in arbitrarily shaped channels [15-17, 19].

As an illustration, a two-dimensional horseshoe-shaped microchannel on a rectangular substrate is considered, as depicted in Figure 2, undergoing a transient heat transfer process. The channel substrate participates on the heat transfer process through both transversal and longitudinal heat conduction. The single domain dimensionless formulation for this problem can be written as [19]:

$$\frac{\partial \theta(X,Y,t)}{\partial t} + U(X,Y)W(X,Y)\frac{\partial \theta(X,Y,t)}{\partial X} + \mathrm{Pe}V(X,Y)W(X,Y)\frac{\partial \theta(X,Y,t)}{\partial Y} =$$

$$= \frac{1}{\mathrm{Pe}^2}\frac{\partial}{\partial X}\left(K(X,Y)\frac{\partial \theta(X,Y,t)}{\partial X}\right) + \frac{\partial}{\partial Y}\left(K(X,Y)\frac{\partial \theta(X,Y,t)}{\partial Y}\right) \tag{21a}$$

with initial and boundary conditions:

$$\theta(X,Y,0) = 0; \quad \theta(0,Y,t) = 1; \quad \theta(X,0,t) = 0; \quad \theta'(L_x,Y,t) = 0; \quad \theta'(X,L_y,t) = 0 \tag{21b-f}$$

In this formulation, the spatially varying coefficients $U(X,Y)$, $V(X,Y)$, $W(X,Y)$ and $K(X,Y)$ are responsible for incorporating the two physical domains (solid and fluid stream) into the single domain model given by Eq. (21a), by presenting characteristic values at the different regions with abrupt transitions at the interfaces. Besides the assumption of constant physical properties, the inertia terms are disregarded in the flow problem. The obtained dimensionless velocity component $U(X,Y)$ is represented in Figure 2. One should note that by letting $U(X,Y) = 0$ and $V(X,Y) = 0$ at the solid region, Eq. (21a) reduces to the heat conduction equation in the substrate.
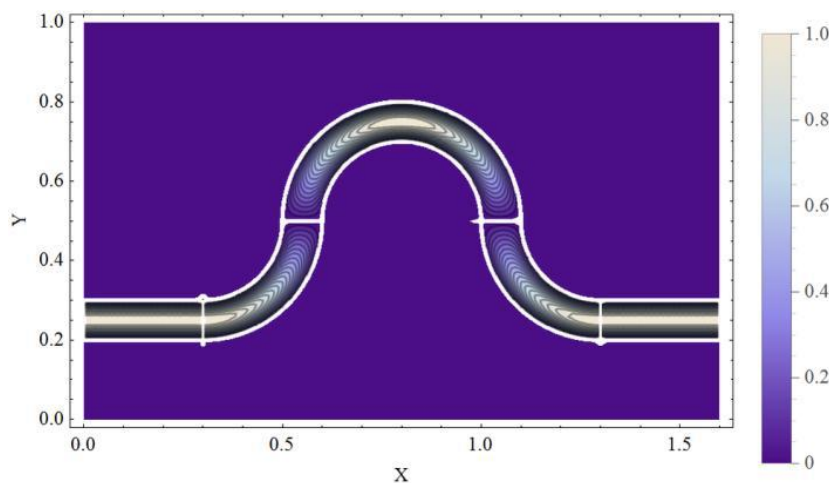

Figure 2 – Horseshoe-shaped microchannel in rectangular substrate with contours of the *X*-direction velocity component.

Following the formal solution procedure described in Section 2, first a filter is proposed, based on the steady state two-dimensional heat conduction equation with constant thermal properties, yielding homogeneous boundary conditions in both space coordinates in the filtered version of Problem (21). In this example, the simplest possible eigenvalue problem is chosen, given by:

$$\frac{\partial^2 \Omega(X,Y)}{\partial X^2} + \frac{\partial^2 \Omega(X,Y)}{\partial Y^2} + \beta_i^2 \Omega(X,Y) = 0 \tag{22a}$$

$$\Omega(0,Y) = 0; \quad \Omega(X,0) = 0; \quad \Omega'(L_x,Y) = 0; \quad \Omega'(X,L_y) = 0 \tag{22b-e}$$

which allows for the definition of the following integral transform pair:

$$\text{Transform: } \overline{\theta}_i(t) = \int_0^{L_y} \int_0^{L_x} \tilde{\Omega}_i(X,Y)\theta^*(X,Y,t)dXdY \tag{23a}$$

$$\text{Inverse: } \theta^*(X,Y,t) = \sum_{i=1}^{\infty} \tilde{\Omega}_i(X,Y)\overline{\theta}_i(t) \tag{23b}$$

where $\theta^*(X,Y,t)$ is the filtered dimensionless temperature field and the normalized eigenfunctions are given by:

$$\tilde{\Omega}_i(X,Y) = \frac{\Omega_i(X,Y)}{\sqrt{N_i}} \text{ with } \qquad N_i = \int_0^{L_y} \int_0^{L_x} \left[\tilde{\Omega}_i(X,Y) \right]^2 dXdY \tag{24a,b}$$

Operating on the filtered problem with $\int_0^{L_y} \int_0^{L_x} \tilde{\Omega}_i(X,Y)(\cdot)dXdY$ and making use of the eigenfunctions orthogonality property, the obtained transformed problem allows for analytical solution for the transformed potentials, $\overline{\theta}_i(t)$. Afterwards, the inverse formula, eq.(23b) can be readily employed to yield an analytical expression for the desired dimensionless temperature field, $\theta(X,Y,t)$.

In order to illustrate some numerical results for the example involving conjugated heat transfer in arbitrarily shaped microchannels, the working fluid was taken as water ($c_{p,f} = 4.11 \times 10^6$ J/m³K and $k_f = 0.62$ W/mK) and the substrate as acrylic ($c_{p,s} = 1.75 \times 10^6$ J/m³K and $k_s = 0.19$ W/mK), with $\text{Pe} = 1$, in the numerical results that follow.

Table 1 presents the eigenfunction expansion convergence behavior of the calculated steady state temperature field at some selected points in both the solid and fluid regions, with truncation orders from *N*=40 up to 400. A convergence to at least three significant digits for a truncation order of $N < 400$ is here demonstrated, in the whole region under analysis. For comparison purposes, the same problem has also been numerically solved via the Finite Element Method, employing the commercial CFD solver Comsol Multiphysics, and the results are shown in the last row of Table 1, showing an agreement of two significant digits in comparison with the converged GITT solution with *N*=400.

In order to illustrate the solution behavior throughout the domain, Figure 3 depicts the calculated steady state temperature field in the horseshoe-shaped microchannel and substrate. One can clearly notice the effects of the internal convection occurring due to the fluid stream inside the microchannel, distorting the isotherms in the substrate region. The results clearly illustrate that the effects of the conjugated heat transfer are fully captured by the single domain formulation approach.

It is also performed a convergence analysis considering two different reordering schemes to achieve a single sum representation for the inverse formula, namely the traditional scheme through the sum of the squared eigenvalues, already illustrated in the results shown above, and a more elaborate one, considering the most important elements appearing in the diagonal of the coefficients matrix of the transformed problem. In this analysis, a sufficiently large number of diagonal elements of this

matrix were calculated and sorted in ascending order, and the first four hundred terms were used for the comparative calculation. It is possible to observe in Figures 4a,b that a slightly better convergence rate is obtained with the second reordering scheme, which accounts for more information from the non-transformed convective terms in the original formulation.

Table 1 – Convergence of the GITT solution for steady state temperature in conjugated problem

| N	$\theta(Y,Z), X = 0.1$			$\theta(Y,Z), X = 0.25$			$\theta(Y,Z), Y = 0.25$		
	$Y = 0.1$	$Y = 0.4$	$Y = 0.7$	$Y = 0.1$	$Y = 0.4$	$Y = 0.7$	$X = 0.25$	$X = 0.75$	$X = 1.5$
40	0.54098	0.84764	0.89491	0.31052	0.63804	0.73238	0.57969	0.21257	0.10320
160	0.53301	0.84937	0.89171	0.29591	0.64935	0.73364	0.57562	0.20870	0.10251
300	0.53338	0.84919	0.89129	0.29734	0.64648	0.73463	0.57424	0.20828	0.10177
360	0.53351	0.84944	0.89151	0.29733	0.64730	0.73489	0.57434	0.20802	0.10199
400	0.53356	0.84981	0.89121	0.29741	0.64764	0.73448	0.57408	0.20795	0.10190
COMSOL	0.53160	0.85149	0.89320	0.29569	0.65310	0.73912	0.57770	0.21008	0.10662
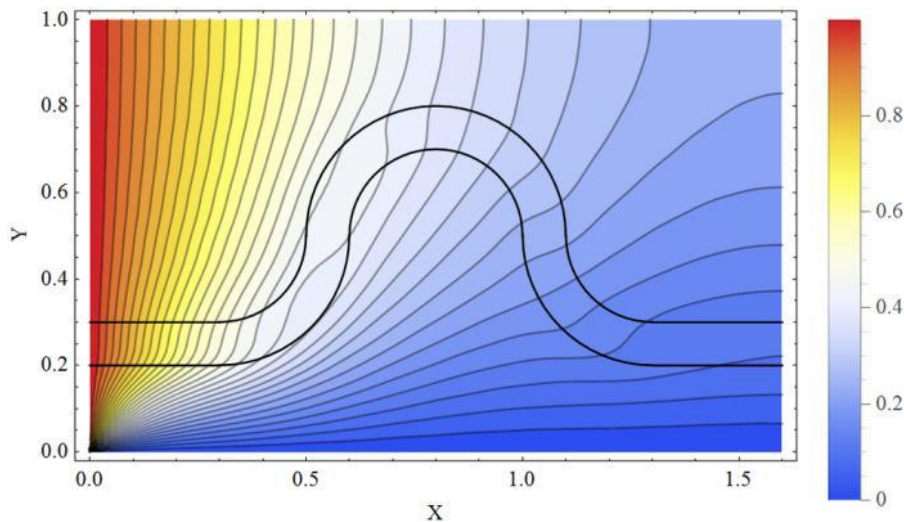
Figure 3 – GITT solution for the steady state temperature in both liquid and solid regions of the microsystem
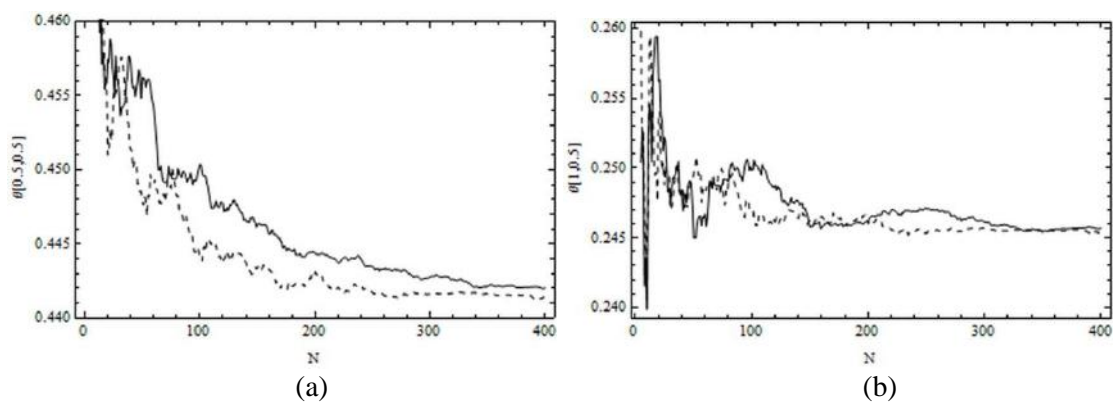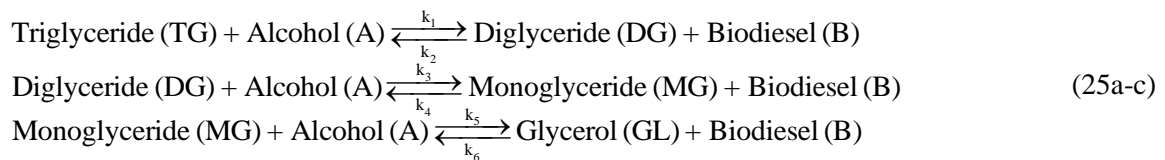

(a)   (b)

Figure 4 – Temperature convergence behaviour at (a) (X,Y) = (0.5, 0.5) and (b) (X,Y) = (0.1, 0.5). Solid line: squared eigenvalues reordering; Dashed line: coefficients matrix diagonal reordering

4.2. Biodiesel Synthesis in Microreactors

The use of microreactors for the transesterification reaction in continuous biodiesel synthesis, ensures high ration of interface area to volume and shorter diffusion paths for the reactive system, resulting in enhanced mass transfer and faster reactions, with lower energy and material consumption [26-27]. To illustrate this application, a 3D nonlinear mathematical model is proposed to describe the transesterification reaction between soybean oil and methanol, catalyzed by sodium hydroxide in microreators, considering the associated dispersion, reaction and convection phenomenon. The set of coupled nonlinear partial differential equations is then solved by the Generalized Integral Transform Technique (GITT).

Biodiesel can be obtained from the transesterification reaction between triglycerides and alcohol (alcoholysis reaction) in the presence of a catalyst, typically sodium or potassium hydroxide, which yields esters of fatty acids and glycerol. A general mechanism widely accepted in the literature considers the transesterification as a second order reversible and homogeneous reaction exhibiting elementary kinetics, as follows [26-28]:

$$\text{Triglyceride (TG)} + \text{Alcohol (A)} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \text{Diglyceride (DG)} + \text{Biodiesel (B)}$$

$$\text{Diglyceride (DG)} + \text{Alcohol (A)} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} \text{Monoglyceride (MG)} + \text{Biodiesel (B)} \qquad (25a\text{-}c)$$

$$\text{Monoglyceride (MG)} + \text{Alcohol (A)} \underset{k_6}{\overset{k_5}{\rightleftharpoons}} \text{Glycerol (GL)} + \text{Biodiesel (B)}$$

Diglycerides and monoglycerides are considered intermediates and as contaminants in the final product [29].

The reactants for the transesterification reaction, triglycerides and alcohol, present an immiscible nature and, therefore, in a continuous process inside a microreactor they form a multiphase flow. In this work, will be considered a stratified flow between two reacting fluids. A schematic description of the stratified velocity profiles is shown in Fig. 5.
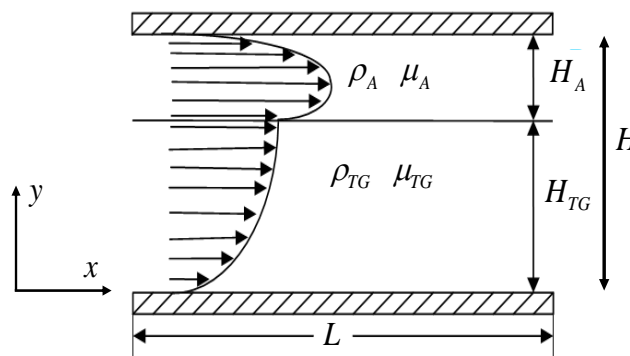

Figure 5 – Stratified two-phase flow of immiscible liquids in rectangular microchannel

The mathematical model that describes the velocity profile scheme presented in Fig. 5, can be obtained from de Navier-Stokes equations assuming fully developed stratified laminar flow of two immiscible Newtonian fluids, with constant physical properties in a rectangular cross section micro-reactor, subject to a constant pressure drop and under isothermal steady conditions. The body forces are neglected and it is considered the existence of a flat plane interface between the two fluids, located at H_{TG}. At the interface it is assumed continuity of velocity and shear stress between the two fluid layers, while at the walls it is adopted the usual no-slip conditions. From these assumptions, the Navier-Stokes equations are simplified and can be written as:

$$\frac{\partial P}{\partial x} = \mu_{TG}\left(\frac{\partial^2 u_{TG}}{\partial y^2} + \frac{\partial^2 u_{TG}}{\partial z^2}\right); \quad \frac{\partial P}{\partial x} = \mu_A\left(\frac{\partial^2 u_A}{\partial y^2} + \frac{\partial^2 u_A}{\partial z^2}\right), \; 0 < z < W, \; H_{TG} < y < H \quad (26\text{a,b})$$

$$u_{TG}(y,0) = u_{TG}(y,W) = u_A(y,0) = u_A(y,W) = 0 \quad (26\text{c-f})$$

$$u_{TG}(0,z) = u_A(H,z) = 0 \quad (26\text{g,h})$$

$$u_{TG}(H_{TG},z) = u_A(H_{TG},z); \quad -\mu_{TG}\left.\frac{\partial u_{TG}}{\partial y}\right|_{y=H_{TG}} = -\mu_A\left.\frac{\partial u_A}{\partial y}\right|_{y=H_{TG}} \quad (26\text{i,j})$$

A three-dimensional mathematical model that governs the concentration of the species involved in the transesterification reaction in a micro-reactor of rectangular cross section can be obtained from the general species balance equations, assuming an isothermal and steady system with constant physical properties. It is considered that the reactive effects occur predominantly in the triglyceride phase and that only the alcohol species migrates through the interface and the other species remain confined in the triglyceride phase [20,27]. As the reaction occurs predominantly in the triglyceride phase, it is reasonable to assume that reactants, intermediates and products are subject to the same convective effects within the triglyceride phase. At the walls of the micro-reactor, it is assumed no penetrability conditions. At the inlet of the micro-reactor all species have known concentrations, while at the micro-reactor outlet it is assumed a zero flux condition for all species. Therefore, the dimensionless reaction-convection-diffusion equations that govern the concentration of the species in the triglyceride phase, with the specific nonlinear chemical kinetics terms, can be written as:

$$U_{TG}(Y,Z)\frac{\partial F_s}{\partial X} = \frac{1}{Pe_s}\frac{\partial^2 F_s}{\partial X^2} + \xi_s\left(\frac{\partial^2 F_s}{\partial Y^2} + \omega\frac{\partial^2 F_s}{\partial Z^2}\right) + \varsigma G_s, \; \text{where } s = TG, DG, MG, B, A, GL \quad (27\text{a})$$

$$F_{TG}(0,Y,Z) = 1; \; F_s(0,Y,Z) = 0, \; \text{where } s = DG, MG, B, A, GL \quad (27\text{b,c})$$

$$\left.\frac{\partial F_s}{\partial X}\right|_{X=1} = \left.\frac{\partial F_s}{\partial Y}\right|_{Y=0} = \left.\frac{\partial F_s}{\partial Z}\right|_{Z=0} = \left.\frac{\partial F_s}{\partial Z}\right|_{Z=1} = 0, \; \text{where } s = TG, DG, MG, B, A, GL \quad (27\text{d-g})$$

$$F_A(X,1,Z) = F_{Ao}; \; \left.\frac{\partial F_s}{\partial Y}\right|_{Y=1} = 0, \; \text{where } s = TG, DG, MG, B, GL \quad (27\text{h,i})$$

where G_s represents the reaction kinetics term for each species involved in the transesterification. Considering a second-order consecutive elementary reversible reaction [26-28], the reaction kinetics terms for the species involved in the transesterification can be written according to Table 2 below.

Table 2 - Dimensionless chemical kinetics expressions for the species s.

Specie s	G_s
TG	$-k_1 F_{TG} F_A + k_2 F_{DG} F_B$
A	$\left(-k_1 F_{TG} - k_3 F_{DG} - k_5 F_{MG}\right) F_A + \left(k_2 F_{DG} + k_4 F_{MG} + k_6 F_{GL}\right) F_B$
DG	$\left(k_1 F_{TG} - k_3 F_{DG}\right) F_A + \left(-k_2 F_{DG} + k_4 F_{MG}\right) F_B$
MG	$\left(k_3 F_{DG} - k_5 F_{MG}\right) F_A + \left(-k_4 F_{MG} + k_6 F_{GL}\right) F_B$
GL	$k_5 F_{MG} F_A - k_6 F_{GL} F_B$
B	$\left(k_1 F_{TG} + k_3 F_{DG} + k_5 F_{MG}\right) F_A + \left(-k_2 F_{DG} - k_4 F_{MG} - k_6 F_{GL}\right) F_B$

The dimensionless groups used in Eqs. (27) were defined as:

15

$$F_{TG} = \frac{C_{TG}}{C_{TGo}};\ F_A = \frac{C_A}{C_{TGo}};\ F_{DG} = \frac{C_{DG}}{C_{TGo}};\ F_{MG} = \frac{C_{MG}}{C_{TGo}};\ F_M = \frac{C_M}{C_{TGo}};\ F_{GL} = \frac{C_{GL}}{C_{TGo}};\ F_{Ao} = \frac{C_A^*}{C_{TGo}};\ X = \frac{x}{L};$$

$$Y = \frac{y}{H_{TG}};\ Z = \frac{z}{W};\ Pe_s = \frac{u_{TG,Av}L}{D_s};\ U_{TG} = \frac{u_{TG}}{u_{TG,Av}};\ \varsigma = \frac{LC_{TGo}}{u_{TG,Av}};\ \xi_s = \frac{LD_s}{u_{TG,Av}H_{TG}^2};\ \omega = \frac{H_{TG}^2}{W^2}$$

(28a-o)

where C_A^* is the equilibrium concentration of the alcohol species at the interface.

Equations (27) form a system of nonlinear partial differential equations, coupled by the reaction kinetic terms, that can be solved by GITT, following the formalism presented in section 2. Here, two different solution paths were considered for comparison purposes, through different choices of the eigenvalue problem that offers the basis for the eigenfunction expansions. Both the path with a purely diffusive constant coefficients eigenvalue problem and with a spatially variable coefficients eigenvalue problem were analyzed. In the second case, the space variable velocity profile is accounted for in the eigenvalue problem, adding information on the convective effects to the eigenfunction expansions.

Although the reaction system is here considered to be isothermal, the transesterification reaction can be evaluated at different temperature levels, since this parameter is related to the energy state of the molecules. It is expected that higher temperatures provide better triglyceride conversion rates. The Arrhenius equation can be used to represent the relation between the kinetics constants and temperature:

$$k_{i,1} = \alpha_i Exp\left[-\frac{E_i}{RT_1}\right],\quad i = 1, 2, ..., 6$$

(29)

where $k_{i,1}$ is the kinetic constant of index i at the temperature T_1. The correction of the value of the kinetic constant $k_{i,1}$ for a different temperature T_2 can be accomplished by Eq. (30), directly obtained from Eq. (29), by assuming that the activation energy, E_i, and the pre-exponential factor, α_i, do not present significant changes within the temperature range considered. Thus:

$$\ln\left(\frac{k_{i,2}}{k_{i,1}}\right) = \frac{E_i}{R}\left[\frac{1}{T_1} - \frac{1}{T_2}\right],\quad i = 1, 2, ..., 6$$

(30)

where $k_{i,2}$ is the kinetic constant of index i at temperature T_2.

Due to the absence of specific data on the reaction kinetics for microfluidic devices with the reaction system involving methanol and soybean oil, activation energy and pre-exponential data from a batch system were used to investigate the temperature effects on the process [28].

The reaction efficiency is analyzed through the fractional conversion of triglycerides, for different residence times, by the following equation:

$$Conversion\, TG(\%) = \left[\frac{F_{TG,AV}(0) - F_{TG,Av}(1)}{F_{TG,Av}(0)}\right] \times 100$$

(31)

The residence time provides an average time that the reacting fluids are subjected to the reactive, diffusive and convective conditions inside the micro-reactor. It is expected that higher conversion of triglyceride will occur at higher residence times. Therefore, the residence time is calculated taking into account only the volume of the triglyceride phase, which is where the reaction takes place predominantly, according to the following equation:

$$\tau = \frac{LWH_{TG}}{Q_{TG}} \tag{32}$$

The input data employed in the present study is shown in Table 3 [26,27].

Table 3 - Input data for simulation of a micro-reactor for biodiesel synthesis [26,27]

Parameter	Value	Parameter	Value
μ_{TG}	5.825×10^{-2} [Pa.s]	k_1	4.368×10^{-6} [mol/(m³.s)]
μ_A	5.47×10^{-4} [Pa.s]	k_2	9.623×10^{-6} [mol/(m³.s)]
D_{TG}	1.58×10^{-9} [m²/s]	k_3	1.88×10^{-5} [mol/(m³.s)]
D_A	1.182×10^{-10} [m²/s]	k_4	1.074×10^{-4} [mol/(m³.s)]
D_{DG}, D_{MG}, D_{GL} and D_B	1.38×10^{-9} [m²/s]	k_5	2.117×10^{-5} [mol/(m³.s)]
ρ_{TG}	885 [kg/m³]	k_6	9.0×10^{-7} [mol/(m³.s)]
Q_{TG}	0.4154 [μl/min]	**Reaction**	**Activation Energy [cal/mol]**
Q_{TG}/Q_A	3.402	$TG \rightarrow DG$	13145
C_{TGo}	1014 [mol/m³]	$DG \rightarrow TG$	9932
F_{Ao}	4.4	$DG \rightarrow MG$	19860
L	0.0233 [m]	$MG \rightarrow DG$	14639
$W = H$	100 [μm]	$MG \rightarrow GL$	6421
R	1.987 [cal/(mol.K)]	$GL \rightarrow MG$	9588

Table 4 presents the convergence analysis of the eigenfunction expansions for the average concentrations of both the triglyceride (TG) and biodiesel (B) species in the micro-reactor, at $T = 25°C$ and residence time of $\tau = 0.5$min. The two alternative solution paths here adopted are critically compared, for the constant and variable coefficients eigenvalue problems. It can be seen that the solution obtained by the GITT with an eigenvalue problem including convective effects converges to practically five significant digits, for a lower truncation order (N<50) than for the eigenvalue problem with constant coefficients, which itself converges to at least three significant digits with N<100.

Table 4 - Convergence analysis of the average concentrations of triglyceride and biodiesel

Square Cross Section Microreactor					
Eigenvalue problem with constant coefficients					
Point	$X = 0.3$		$X = 0.5$		$X = 0.7$
NT	TG	B	TG	B	TG	B
20	0.955411	0.049206	0.904022	0.117023	0.844553	0.210476
40	0.955648	0.048923	0.904303	0.116622	0.844850	0.209973
60	0.955815	0.048725	0.904513	0.116322	0.845079	0.209585
80	0.955802	0.048740	0.904492	0.116351	0.845054	0.209627
100	0.955752	0.048799	0.904426	0.116445	0.844981	0.209751
Eigenvalue problem with variable coefficients					
Point	$X = 0.3$		$X = 0.5$		$X = 0.7$
NT	TG	B	TG	B	TG	B
10	0.955449	0.049150	0.904122	0.116853	0.844666	0.210240
20	0.955705	0.048851	0.904378	0.116504	0.844923	0.209831
30	0.955751	0.048798	0.904427	0.116438	0.844977	0.209748
40	0.955761	0.048785	0.904438	0.116423	0.844988	0.209729
50	0.955766	0.048781	0.904444	0.116415	0.844997	0.209717

Figures 6a,b illustrate the temperature effects in a microreactor with fixed dimensions $L = 2.33$ cm, and respectively, (a) $H=W=100$ µm and (b) $H=W=400$ µm, on the triglyceride conversion. The temperature increase influences the kinetics constants of the transesterification process, which as a consequence, influence the reaction process, achieving higher conversion rates in shorter residence times. Also, comparing the two figures, Figs. 6.a and 6.b, for a fixed residence time and reaction temperature, it can be observed a higher conversion for the micro-reactor with the lower hydraulic diameter, due to a higher surface area to volume ratio and shorter diffusion pathways, ensuring improved mass transfer and triglyceride conversion.
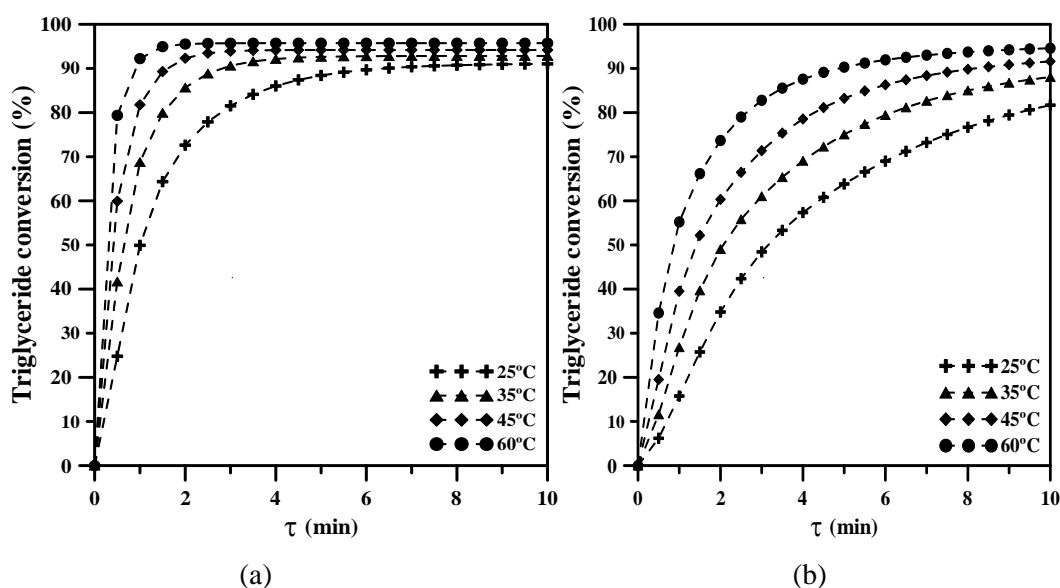

Figure 6 – Conversion rates of triglyceride in a square cross section micro-reactor for different temperatures and different cross sections: (a) H=W=100 µm and (b) H=W=400 µm.

5. Conclusions

The Generalized Integral Transform Technique (GITT) has been reviewed and presented in an unified framework, as an automatic hybrid numerical-analytical treatment of nonlinear coupled convection-diffusion problems. Besides the formal solution, this work systematically presents a few recent advancements to the hybrid approach, involving reordering schemes for multidimensional expansions, single domain reformulation for complex geometries, an integral balance approach for multiscale problems, the adoption of convective eigenvalue problems, and the proposition of nonlinear eigenvalue problems. The compilation of such recent developments is then concluded through the selection of a couple of applications that make use of some of these methodology extensions. Two applications are more closely analyzed in relation with conjugated heat transfer in arbitrarily shaped micro-systems and with nonlinear reactive systems for continuous biodiesel synthesis in micro-reactors. Such examples certainly add to the portfolio of challenging projects tackled by the integral transforms approach in its generalized hybrid numerical-analytical context. Future work should involve the incorporation of such recent developments into the multipurpose unifying structure of the UNIT algorithm [11-14], providing alternative solution paths for convergence improvement and extension of its applicability limits.

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