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HYBRID SOLUTIONS APPLIED TO COUPLED PROBLEMS OF HEAT AND MASS TRANSFER WITH ADSORPTION

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Abstract. *In this work it is presented the application of the Integral Generalized Transformed Technique (GITT), in its unified version, in the solution of Burgers equations applied in the simulation of a heat and mass transfer coupled problem with a source term that represents the phenomenon of Adsorption. A computational code was developed using the programming language FORTRAN 90/2003 to solve the ODE system resultant of the integral transformation of governing PDE's. In this code the integral coefficients obtained during the process of integral transformation are solved by a semi-analytic procedure and the resultant ODE's systems is solved through subroutine IVPAG of the library IMSL (1991). The obtained results were compared with those derived from the Method of Lines (MOL-Method of Lines) and, as well, with the available in the literature.*

Keywords: *Adsorption, GITT, IVPAG, Method of Lines.*

1. INTRODUCTION

The study of simultaneous transfer of heat and mass with the presence of adsorption has wide application in a variety of fields including not only thermal engineering applications directly, but also mechanical and environmental bioengineering. As an example of these applications, we can mention sensible and latent heat exchangers (also known as the enthalpy exchangers), alternative methods for storage of gases, gas filtration and purification, drying and preserving food. The difficulty in problems involving adsorption phenomenon is that this increases the non-linearity and coupling between the mass and heat transfer, making more complex problems from the viewpoint of modeling and solution.

A constant challenge for the engineering is the problems resolution that involve simultaneous transfer of heat and mass, once the fundamental differential equations that govern the phenomena form a system of coupled partial differential equations, describing the interrelations between heat and mass transfer, what makes more complex the problem in a modeling and solution point of view. Recently, analytic-numeric techniques of resolution come winning highlight in several areas guaranteeing results with greater reliability and lower computational cost.

In this paper, the main objective is to obtain the solution of the system of PDE's that governs the unsteady one-dimensional coupled problem of heat and mass transfer in the presence of adsorption, via the GITT in its unified version. Thus developed an alternative code by applying the technique of processing in a generalized integral version, unified whole by means of semi-analytical (Cotta et al, 2010), differing from a generalized version, the construction simplified algorithm.

A computer code was developed using the programming language Fortran 90/2003, where a convergence analysis for the main potentials was applied in order to observe the influence of the number of terms in the final solution. The results for the dimensionless concentration and temperature fields dimensionless obtained by GITT are produced with different values of the parameters governing the studied system. Moreover, comparisons with the results obtained by the method of lines are conducted in order to validate the numerical code developed in the present work and demonstrate the consistency of the final results.

2. MATHEMATICAL FORMULATION

The problem studied in this work is represented by a system of partial differential equations transient, one-dimensional, non-linear and physically coupled to describe the phenomenon of simultaneous transfer of heat and mass

with the presence of adsorption. To obtain the mathematical formulation of the problem it is assumed, we assume the following hypotheses: initial uniform temperature and concentration, boundary conditions of the first-type, constant thermophysical properties and a system of coupled partial differential equations in dimensionless form written in the following form:

$$\frac{\partial \theta}{\partial \tau}+\frac{\partial \theta}{\partial x}=\frac{\partial^2 \theta}{\partial x^2}+\alpha \Delta H \frac{\partial S}{\partial \tau} \tag{1.a}$$

$$\frac{\partial C}{\partial \tau}+\alpha \frac{\partial S}{\partial \tau}+\frac{\partial C}{\partial x}=\frac{\partial^2 C}{\partial x^2} \tag{1.b}$$

where the initial and boundary conditions are:

$$\tau=0 \rightarrow \begin{cases} \theta(x,0)=\theta_0 \\ C(x,0)=C_0 \end{cases}; \qquad x=0 \rightarrow \begin{cases} \theta(0,\tau)=\theta_e \\ C(0,\tau)=C_e \end{cases}; \qquad x=1 \rightarrow \left\{ \frac{\partial \theta(1,\tau)}{\partial x}=\frac{\partial C(1,\tau)}{\partial x}=0 \right. \tag{1.c-e}$$

where: α is the coefficient, ΔH is the heat of adsorption, $\alpha \Delta H \frac{\partial S}{\partial \tau}$ is the source term of the energy equation and coupling and $\theta_e = C_e = 1$.

Additionally, in equations (1.a-b), S represents the amount of adsorbed on the adsorbent mass, and can be determined by the following equation:

$$S=\frac{KC}{1+KC} \tag{1.f}$$

where, K is the equilibrium constant.

3. SOLUTION METHODOLOGY

The PDE's system described by the coupled Eqs. (1.a-b), will be solved using the Generalized Integral Transform Technique in its unified version and its results will be compared with the solution obtained by the method of lines.

3.1 Solution via the GITT

The Integral Transform method (GITT) has proven to be a powerful tool in different classes of problems, that involve transport phenomena in different physical areas. GITT is a hybrid, numerical-analytical, technique that use eigenfunction expansions for description of an arbitrary function, characterizing as a method that, in general, transforms a system of partial differential equations in a system of ordinary differential equations.

The Generalized Integral Transform Technique (GITT), reviewed in detail by Cotta (1993), Cotta and Mikhailov (1997) and Cotta (1998), has been progressively established as a powerful tool in benchmarking and engineering applications for linear and nonlinear diffusion and convection-diffusion problems. More specifically it is worth mentioning the integral transform solutions of the 2-D and 3-D Navier-Stokes equations under streamfunction-only formulation for incompressible flow within cavities, and the solutions of laminar and turbulent flows inside regular and irregular ducts. Transient and steady natural convection inside rectangular enclosures, under Boussinesq approximation and with variables properties, were investigated by Leal et al. (1999) and Leal et al. (2000), respectively.

The initial procedure of this methodology is through a previous analysis of the original problem before applying the formalism of GITT. It is the non-homogeneity of the problem, which requires the use of filter functions to improve the computational performance and with the aim to obtain expansions of eigenfunctions of better numerical convergence. Therefore, we have chosen a function for the filter that preserves the characteristics of the problem of heat and mass transfer and delete the inhomogeneities of the boundary conditions in spatial direction "x", where the eigenvalue problem will be developed. Thus, the solution of equations (1.a-b) is given by the following equations:

$$\theta(x,\tau)=\theta_H(x,\tau)+\theta_p(x) \tag{2.a}$$

$$C(x,\tau)=C_H(x,\tau)+C_p(x) \tag{2.b}$$

For the purpose of obtaining the solution and resulting from the filtering process, we consider a system of ODE's boundary conditions subject to inhomogeneities in the form:

$$\frac{d^2\theta_p(x)}{dx^2} - \frac{d\theta_p(x)}{dx} = 0 \tag{3.a}$$

$$\frac{d^2C_p(x)}{dx^2} - \frac{dC_p(x)}{dx} = 0 \tag{3.b}$$

where the boundary conditions;

$$x = 0 \rightarrow \begin{cases} \theta_p(0) = \theta_e \\ \phi_p(0) = \theta_e \end{cases} \tag{3.c}$$

$$x = 1 \rightarrow \begin{cases} \dfrac{d\theta_p(1,\tau)}{dx} = \dfrac{dC_p(1,\tau)}{dx} = 0 \end{cases} \tag{3.d}$$

The solution of the differential equations (3.a-b) for the particular problem is presented as follows:

$$\theta_p(x) = \theta_e \tag{3.e}$$

$$C_p(x) = C_e \tag{3.f}$$

The definitions given by equations (2.a) and (2.b) are applied to the original system given by equations (1.a-f) to obtain the following homogeneous problem:

$$\frac{\partial\theta_H(x,\tau)}{\partial\tau} + \frac{\partial\theta_H(x,\tau)}{\partial x} = \frac{\partial^2\theta_H(x,\tau)}{\partial x^2} + \alpha\Delta HE(C)\frac{\partial C_H(x,\tau)}{\partial\tau} \tag{4.a}$$

$$\frac{\partial C_H(x,\tau)}{\partial\tau} + G(C)\frac{\partial C_H(x,\tau)}{\partial x} = G(C)\frac{\partial^2 C_H(x,\tau)}{\partial x^2} \tag{4.b}$$

where the initial and boundary conditions homogeneous:

$$\tau = 0 \rightarrow \begin{cases} \theta_H(x,0) = \theta_0 - \theta_p(x) \\ C_H(x,\tau) = C_0 - C_p(x) \end{cases}; \quad x = 0 \rightarrow \begin{cases} \theta_H(0,\tau) = 0 \\ C_H(0,\tau) = 0 \end{cases}; \quad x = 1 \rightarrow \begin{cases} \dfrac{\partial\theta_H(1,\tau)}{\partial x} = \dfrac{\partial C_H(1,\tau)}{\partial x} = 0 \end{cases} \tag{4. c-e}$$

where;

$$G(C) = \frac{(1+KC)^2}{(1+KC)^2 + \alpha K} \text{ and } E(C) = \frac{K}{(1+KC)^2} \tag{4.f-g}$$

Once inserted the filter in the boundary conditions, it can be observed homogeneous conditions in spatial direction "x", where the eigenvalue problem will be considered. Then, equations (4.a-b) and the boundary conditions given by equations (4.c-e) shall be submitted to the Generalized Integral Transform Technique (GITT) in their unified version to obtain the solution for the potential.

Following the formalism of the technique (GITT), eigenvalues problems with their respective eigenvalues and eigenfunctions are defined as follows:

$$\frac{d^2\psi_i(x)}{dx^2} + \mu_i^2\frac{d\psi_i(x)}{dx} = 0 \tag{5.a}$$

$$x = 0 \rightarrow \{\psi_i(x) = 0\,; \qquad x = 1 \rightarrow \begin{cases} \dfrac{d\psi_i(x)}{dx} = 0\,; \end{cases} \tag{5. b-c}$$

where: μ_i and $\psi_i(x)$ are respectively the eigenvalues and eigenfunctions for the eigenvalue problem in the spatial direction "x", which are given by:

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$$\psi_i(x) = \sin(\mu_i x); \qquad \mu_i = \left((2i-1)/2\right)\pi \quad , \qquad \text{for } i = 1,2,3... \tag{5.d-e}$$

Equations (4.a) and (4.b) have the same solution by separation of variables homogeneous version of the problem, which refers the same eigenvalue problem common to both equations, so the eigenfunctions $\psi_i(x)$ and the eigenvalues μ_i satisfy the system ODE's for the two potentials.

The eigenfunctions of this eigenvalue problem have the following orthogonality property:

$$\int_0^1 \psi_i(x)\psi_j(x)dx = \begin{cases} 0, i \neq j \\ N_i, i = j \end{cases} \tag{5.f}$$

and the normalization integrals is calculated from:

$$N_i = \int_0^1 \psi_i^2(x)dx = \frac{1}{2} \tag{5.g}$$

The problem given by equations (4.a-e) allows the definition of the followingintegral transform pairs:

$$\overline{\theta}_{Hi}(\tau) = \int_0^1 \overline{\psi}_i(x)\theta_H(x,\tau)dx\,, \quad \text{transform;} \qquad \theta_H(x,\tau) = \sum_{i=1}^{\infty} \overline{\psi}_i(x)\overline{\theta}_{Hi}(\tau)\,, \quad \text{inverse} \tag{6.a-b}$$

$$\overline{C}_{Hi}(\tau) = \int_0^1 \overline{\psi}_i(x)C_H(x,\tau)dx\,, \quad \text{transform;} \qquad C_H(x,\tau) = \sum_{i=1}^{\infty} \overline{\psi}_i(x)\overline{C}_{Hi}(\tau)\,, \quad \text{inverse} \tag{7.a-b}$$

where:

$$\overline{\psi}_i(x) = \frac{\psi_i(x)}{\sqrt{N_i}} \tag{8}$$

Using the integral transformation operators defined in equations (6.a) and (7.a), the problem of partial differential equations are transformed homogeneous, obtaining the following system of coupled differential equations:

$$\frac{d\overline{\theta}_{Hi}}{dx} = -\mu_i^2\overline{\theta}_{Hi} + \overline{Q}_i \qquad \text{for } \tau \geq 0 \text{ and } i = 1,2,3... \tag{10.a}$$

$$\frac{d\overline{C}_{Hi}}{dx} = \overline{P}_i \qquad \text{for } \tau \geq 0 \text{ and } i = 1,2,3... \tag{10.b}$$

$$\overline{\theta}_{Hi}(0) = [\theta_0 - \theta_p(x)]f_i\,; \qquad \overline{C}_{Hi}(0) = [C_0 - C_p(x)]f_i \tag{10.c-d}$$

$$f_i = \int_0^1 \overline{\psi}_i(x)dx \tag{10.e}$$

where the portions of equations (10.a-b) are embedded in the non-transformed source terms, without loss of generality:

$$\overline{Q}_i = \int_0^1 \overline{\psi}_i(x)\left[\alpha\Delta HE(C)\frac{\partial C}{\partial \tau} - \frac{\partial \theta_H(x,\tau)}{\partial \tau}\right]dx \tag{10.f}$$

$$\overline{P}_i = \int_0^1 \overline{\psi}_i(x)G(C)\left[\frac{\partial^2 C_H}{\partial x^2} - \frac{\partial C_H}{\partial \tau}\right]dx \tag{10.g}$$

The coupled system of ordinary differential equations, equations (10.a-b), is solved by an efficient numerical algorithm for initial value problems by IVPAG subroutine from IMSL library (1991). To solve the system of ODE's via GITT, the system must be truncated to finite order one large enough to achieve converged solutions for a given desired accuracy.

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The source terms $\overline{P}_i$ and $\overline{Q}_i$ the system of ODE's, equations (10.a-b), are calculated by a semi-analytical procedure within the subroutine IVPAG, since they are non-linear coefficients.. Therefore, in order to offer an alternative semi-analytic integration of the code UNIT terms sources are approximated by simple polynomials in segments, allowing the analytical integration in each subinterval.

Assuming, $Q = a_k x + b_k$ and $P = c_k x + d_k$, we can approximate the terms by series:

$$\overline{Q}_i = \sum_{j=1}^{J} \int_{x_{j-1}}^{x_j} \overline{\psi}_i(x)\left[a_k x + b_k\right]dx = \sum_{j=1}^{J} a_k \int_{x_{j-1}}^{x_j} x\overline{\psi}_i(x)dx + b_k \int_{x_{j-1}}^{x_j} \overline{\psi}_i(x)dx \tag{11.a}$$

$$\overline{P}_i = \sum_{j=1}^{J} \int_{x_{j-1}}^{x_j} \overline{\psi}_i(x)\left[c_k x + d_k\right]dx = \sum_{j=1}^{J} c_k \int_{x_{j-1}}^{x_j} x\overline{\psi}_i(x)dx + d_k \int_{x_{j-1}}^{x_j} \overline{\psi}_i(x)dx \tag{11.b}$$

where:

$$a_k = \frac{Q_k - Q_{k-1}}{x_k - x_{k-1}}\ , \qquad b_k = Q - a_k x \tag{11.c-d}$$

$$c_k = \frac{P_k - P_{k-1}}{x_k - x_{k-1}}\ , \qquad d_k = P - c_k x \tag{11.e-f}$$

For the characteristic of the hybrid technique, as $\psi_i(x)$ is known, the integrals of equations (11.a,b) will be solved analytically and the coefficients, calculated in each step of the integration process.

3.2 Solution via the Method of Lines

The method of lines (Schiesser, 1991), is a method of numerical solution of nonlinear PDE's, approaching this type of equations by systems of ordinary differential equations (ODE's). The idea of the method is, for PDEs, discretize all variables except one, thus obtaining a system of ODE's. Is this approach called semi-discretization, time is left continuous and the spatial variables discretized. Recently, Brito (2010), recently described in a general way that the numerical solution of an EDP using the method of lines, is to approximate the original problem defined in the continuous domain to a system of algebraic equations in a discrete domain. For the problem at hand we discretize the spatial variable by finite differences.

$$\frac{d\theta_i}{d\tau} = \delta_{\theta_i} - \gamma_{\theta_i} + \alpha\Delta HE(C_i)\frac{dC_i}{d\tau} \quad \text{, for} \qquad 0 < x < 1 \text{ and } 1 \le i \le M \tag{12.a}$$

$$\frac{dC_i}{d\tau} = G(C_i)[\delta_{C_i} - \gamma_{C_i}] \quad \text{, for} \qquad 0 < x < 1 \text{and } 1 \le i \le M \tag{12.b}$$

$$\tau = 0 \rightarrow \theta_i(x,0) = \theta_0 \qquad \text{and} \qquad C_i(x,0) = C_0 \tag{12.c-d}$$

where:

$$G(C_i) = \frac{(1+KC_i)^2}{(1+KC_i)^2 + \alpha K} \qquad \text{and} \qquad E(C_i) = \frac{K}{(1+KC_i)^2} \tag{12.e-f}$$

by central differences:

$$\delta_{\theta_i} = \frac{\partial^2\theta_i}{\partial x^2} = \frac{\theta_{i+1} - 2\theta_i + \theta_{i-1}}{\Delta x^2}; \qquad \delta_{C_i} = \frac{\partial^2 C_i}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2}, \tag{12.h-i}$$

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For and by first-order backward finite difference scheme for;

$$\gamma_{\theta_i} = \left.\frac{\partial \theta_i}{\partial x}\right|_{x=i} = \frac{\theta_i - \theta_{i-1}}{\Delta x}; \qquad \gamma_{C_i} = \left.\frac{\partial C_i}{\partial x}\right|_{x=i} = \frac{C_i - C_{i-1}}{\Delta x} \tag{12.j-k}$$

To meet the boundary conditions at x = 1, we will use the first order Upwind scheme to set the value of the derivatives and the value of the potential.

$$\left.\frac{\partial \theta}{\partial x}\right|_{x=i} = \frac{\theta_{i-2} - 4\theta_{i-1} + 3\theta_i}{\Delta x} = 0 \quad \rightarrow \quad \theta_i = \frac{4\theta_{i-1} - \theta_{i-2}}{3} \quad \text{at} \quad x = 1 \text{ e } \tau \geq 0 \tag{12.l}$$

$$\left.\frac{\partial C}{\partial x}\right|_{x=i} = \frac{C_{i-2} - 4C_{i-1} + 3C_i}{\Delta x} = 0 \quad \rightarrow \quad C_i = \frac{4C_{i-1} - C_{i-2}}{3} \quad \text{at} \quad x=1 \text{ e } \tau \geq 0 \tag{12.m}$$

4. RESULTS AND DISCUSSION

Numerical results for the fields of temperature and concentration are generated as a function of spatial and temporal variables for cases where the dimensionless parameters are listed in Table (1). Two computer codes were developed in the programming language FORTRAN 95/2003 and implemented on a computer INTEL DUAL CORE i7 2.00 GHz Process Simulation Laboratory, School of Chemical Engineering, Federal University of Pará (LSP / FEQ / UFPA). The subroutine IVPAG from IMSL Library (1991) was used to solve the coupled system of ODE's transformed to potential given by Equations (10.a-b) and Eqs. (12.a-b) via the MOL, with a relative error prescribed by user 10^{-8} and equal truncation orders for all fields.

Table 1 – Parameters used in the calculation of the concentration fields (C) and temperature (θ).

GITT / MOL		
Dimensionless Parameters	Case 1	Case 2
ΔH	1	100
α	0.5	0.8
K	0.1	10

Initially a convergence analysis is effectuated and then the results for the dimensionless temperature and concentration via GITT (UNIT) is compared with the method of lines, at different times and locations during the transient process.

The results for the fields of temperature and concentration for the simulated cases are presented, in Table (2). The convergence of the solution is checked by comparing potential values obtained with the series truncated to different numbers of terms.

Table (2) shows the behavior of the convergence of the solution code UNIT for the system of differential equations and cases analyzed, with five significant digits for the potential for different values of times, τ = 0.3, τ = 0.7; τ = 0.9 and positions x = 0.1, x = 0.5 and x = 0.9.

For Case 1, analyzing the results for the temperature and concentration, there was excellent convergence rates such that the results were achieved with five significant digits, for NT = 40 terms in the series, for the instants of time and analyzed positions. For this case the results obtained by the method of lines showed good agreement with those obtained via UNIT with NT = 40, at different times and locations.

For case 2, was analyzed for convergence of the solution temperature and concentration in dimensionless terms of the number NT at the instants τ = 0.3, τ = 0.7, τ = 0.9 and positions x = 0, 1, x = 0.5 and x = 0.9. It is shown in Table (2) convergence to field fluctuations in the temperature display time instants analyzed, so that the values are converged to five significant figures NT between 240 and 275 words for all positions shown.

The potential field concentration, *C (x, τ),* has good convergence rates for NT between 240 and 275 words with five significant digits for the instant of time and position analyzed. For τ = 0.3, τ = 0.7, τ = 0.9, there is good convergence rates for field concentration *C (x, τ)*, although there is still small oscillations for the positions studied.

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Table 2 – Convergence of the fields of temperature, $\theta(x,\tau)$, and concentration, $\phi(x,\tau)$, for GITT and comparison with Method of Lines (MOL).

	$\tau = 0.3$					
	$\theta(x,\tau)$			$C(x,\tau)$		
NT	x = 0.1	x = 0.5	x = 0.9	x = 0.1	x = 0.5	x = 0.9
40	1.00289[a] 5.57982[b]	1.01524[a] 27.68983[b]	1.02315[a] 49.25121[b]	0.93932[a] 0.89633[b]	0.67793[a] 0.42625[b]	0.50775[a] 0.04838[b]
80	1.00289[a] 5.47681[b]	1.01524[a] 27.17479[b]	1.02315[a] 48.74789[b]	0.93932[a] 0.89738[b]	0.67793[a] 0.43141[b]	0.50775[a] 0.05341[b]
120	1.00289[a] 5.46817[b]	1.01524[a] 27.13177[b]	1.02315[a] 48.70607[b]	0.93932[a] 0.89746[b]	0.67793[a] 0.43184[b]	0.50775[a] 0.05383[b]
160	1.00289[a] 5.50516[b]	1.01524[a] 27.31429[b]	1.02315[a] 48.87385[b]	0.93932[a] 0.89709[b]	0.67793[a] 0.43001[b]	0.50775[a] 0.05215[b]
200	1.00289[a] 5.51874[b]	1.01524[a] 27.37958[b]	1.02315[a] 48.92663[b]	0.939320[a] 0.89696[b]	0.67793[a] 0.42936[b]	0.50775[a] 0.05162[b]
240	1.00289[a] 5.48192[b]	1.01524[a] 27.19851[b]	1.02315[a] 48.76359[b]	0.939320[a] 0.89742[b]	0.67793[a] 0.43119[b]	0.50775[a] 0.05326[b]
275	1.00289[a] 5.47876[b]	1.01524[a] 27.1874[b]	1.02315[a] 48.76969[b]	0.93932[a] 0.89757[b]	0.67793[a] 0.43185[b]	0.50775[a] 0.05382[b]
MOL*	1.00289[a] 5.46098[b]	1.01524[a] 27.09476[b]	1.02314[a] 48.68349[b]	0.93931[a] 0.89756[b]	0.67831[a] 0.43241[b]	0.50843[a] 0.05440[b]
	$\tau = 0.7$					
	$\theta(x,\tau)$			$C(x,\tau)$		
NT	x = 0.1	x = 0.5	x = 0.9	x = 0.1	x = 05	x = 0.9
40	1.00154[a] 3.35064[b]	1.00821[a] 13.6294[b]	1.01259[a] 20.5819[b]	0.98493[a] 0.96295[b]	0.91983[a] 0.80175[b]	0.87717[a] 0.69393[b]
80	1.00154[a] 3.29553[b]	1.00821[a] 13.3324[b]	1.01259[a] 20.1158[b]	0.98493[a] 0.9635[b]	0.91983[a] 0.80472[b]	0.87717[a] 0.6986[b]
120	1.00154[a] 3.29106[b]	1.00821[a] 13.3082[b]	1.01259[a] 20.0779[b]	0.98493[a] 0.96355[b]	0.91983[a] 0.80496[b]	0.87717[a] 0.69898[b]
160	1.00154[a] 3.30942[b]	1.00821[a] 13.4079[b]	1.01259[a] 20.2343	0.98493[a] 0.96337	0.91983[a] 0.80396[b]	0.87717[a] 0.69741[b]
200	1.00154[a] 3.31557[b]	1.00821[a] 13.4413[b]	1.01259[a] 20.2867[b]	0.98493[a] 0.96330[b]	0.91983[a] 0.80363[b]	0.87717[a] 0.69689[b]
240	1.00154[a] 3.29751[b]	1.00821[a] 13.3433[b]	1.01259[a] 20.1329	0.98493[a] 0.96352[b]	0.91983[a] 0.80461[b]	0.87717[a] 0.69843[b]
275	1.00154[a] 3.29123[b]	1.00821[a] 13.3092[b]	1.01259[a] 20.0794[b]	0.98493[a] 0.96358[b]	0.91983[a] 0.80496[b]	0.87717[a] 0.69896[b]
MOL*	1.00154[a] 3.28493[b]	1.00821[a] 13.2728[b]	1.01259[a] 20.0201[b]	0.98495[a] 0.96363[b]	0.92005[a] 0.80542[b]	0.87754[a] 0.69973[b]
	$\tau = 0.9$					
	$\theta(x,\tau)$			$C(x,\tau)$		
NT	x = 0.1	x = 0.5	x = 0.9	x = 0.1	x = 0.5	x = 0.9
40	1.00096[a] 2.27070[b]	1.00513[a] 7.77466[b]	1.00786[a] 11.41488[b]	0.99248[a] 0.98073[b]	0.96001[a] 0.89739[b]	0.93873[a] 0.84244[b]
80	1.00096[a] 2.24080[b]	1.00513[a] 7.61619[b]	1.00786[a] 11.17077[b]	0.99248[a] 0.98103[b]	0.96001[a] 0.89897[b]	0.93873[a] 0.84488[b]
120	1.00096[a] 2.23838[b]	1.00513[a] 7.60329[b]	1.00786[a] 11.15091[b]	0.99248[a] 0.98106[b]	0.96001[a] 0.89910[b]	0.93873[a] 0.84508[b]
160	1.00096[a] 2.24833[b]	1.00513[a] 7.65647[b]	1.00786[a] 11.23284[b]	0.99248[a] 0.98096[b]	0.96001[a] 0.89857[b]	0.93873[a] 0.84426[b]
200	1.00096[a] 2.25167[b]	1.00513[a] 7.67429[b]	1.00786[a] 11.26029[b]	0.99248[a] 0.98092[b]	0.96001[a] 0.89839[b]	0.93873[a] 0.84398[b]
240	1.00096[a] 2.24188[b]	1.00513[a] 7.62200[b]	1.00786[a] 11.17973[b]	0.99248[a] 0.98104[b]	0.96001[a] 0.89892[b]	0.93873[a] 0.84479[b]
275	1.00096[a] 2.24184[b]	1.00513[a] 7.62180[b]	1.00786[a] 11.17941[b]	0.99248[a] 0.98103[b]	0.96001[a] 0.89893[b]	0.93873[a] 0.8448[b]
MOL*	1.00096[a] 2.23448[b]	1.00513[a] 7.58147[b]	1.00786[a] 11.11632[b]	0.99248[a] 0.98111[b]	0.96001[a] 0.89939[b]	0.93873[a] 0.84553[b]

*Results obtained by MOL [a]280 and [b]560 points in the mesh. [a]Case 1 and [b]Caso 2.

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The validation of the proposed model was made by comparing results obtained with the GITT (NT = 275 terms) for the fields of temperature and concentration dimensionless with the results obtained by the method of lines with 280 points in the mesh for Case 1 and Case 2 to 560.

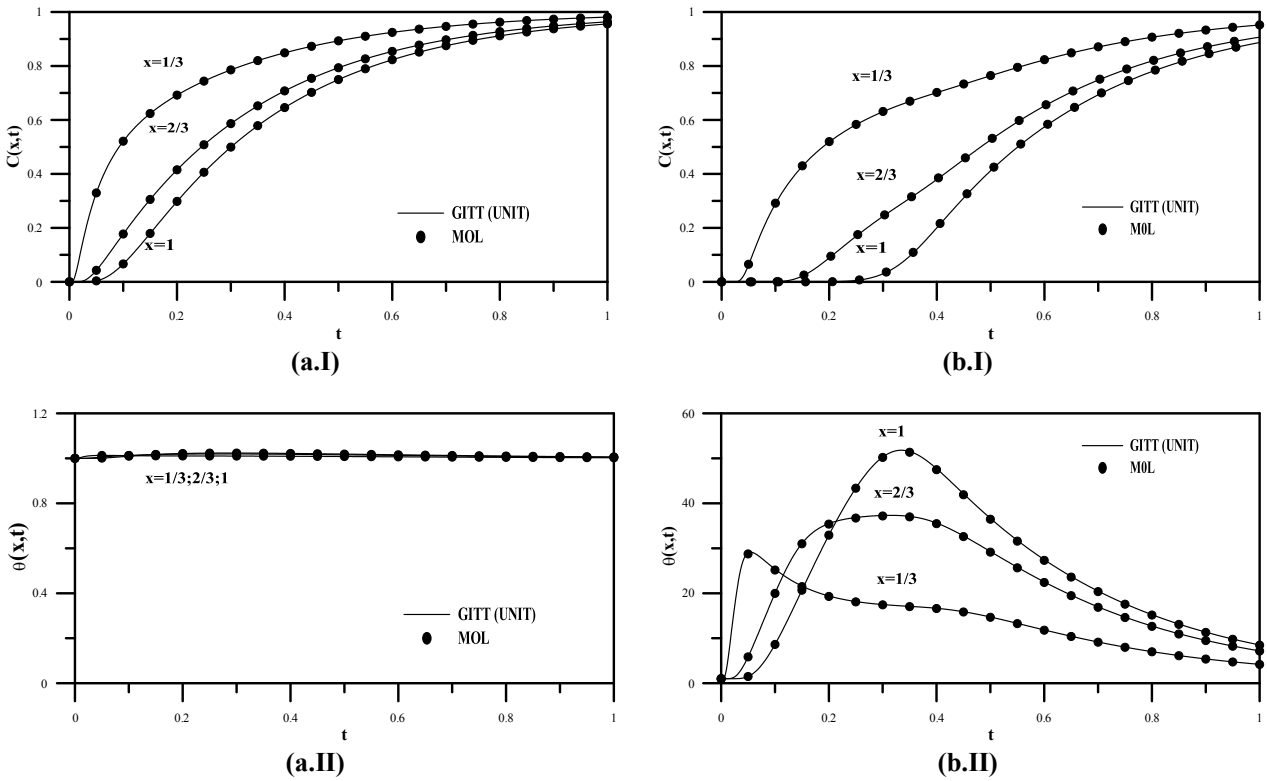
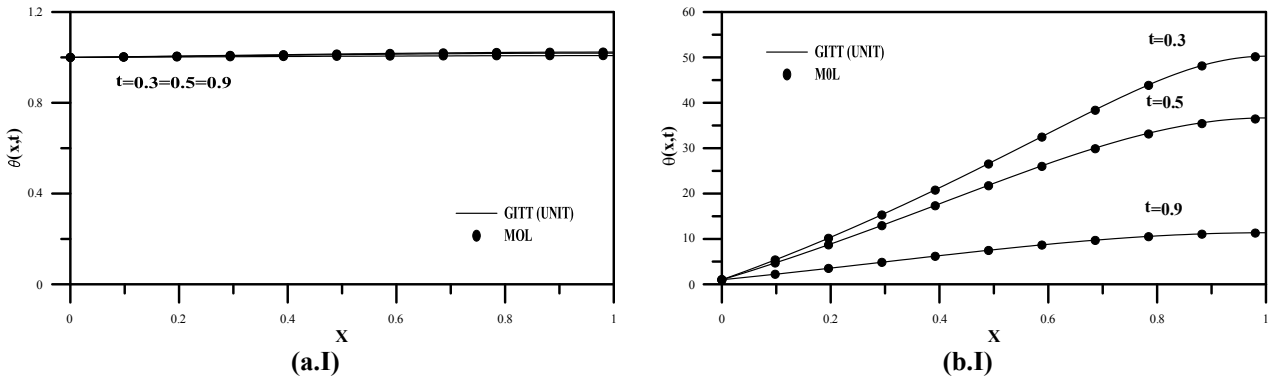


Figure 2. Comparison of the concentration fields and temperature for diferente times and parameters. (a) Case 1; (b) Case 2.

The figures (2.aI) and (2.a.II) show the behavior of the fields of temperature and concentration respectively, as a function of dimensionless time for the x = 1, x = 1/3 and x = 2/3 also is shown comparisons of the results obtained by the two methods for Case 1. Observed a good correlation between the concentration and temperature fields for positions analyzed along the dimensionless time, as in Figures (2.bI) and (2.b.II) for Case 2. The results obtained by GITT agree with those obtained by the method of lines, which demonstrates the efficiency of the hybrid technique in a unified version applied in the cases studied.

For Case 2, Figure (2.b.II), it is observed that the concentration field behaves similarly to that described for Case 1, Figure (2.a.II), where concentration gradients present a behavior decreasing as the variable space increases. It is observed that increasing the values of the parameters for $\Delta H = 100$, $\alpha = 0.8$ and $K = 10$, the curves of the potential concentration in the analyzed moments of time decrease more significantly when compared with curves of Case 1, the increase these parameters in this case causes the mass to be consumed more rapidly as the phenomenon progresses in time to achieve equilibrium with the environment and thus causes an increase in the amount of heat generated by the source term, causing the occurrence of high gradient Case 2 temperature to Figure (2.a.II).



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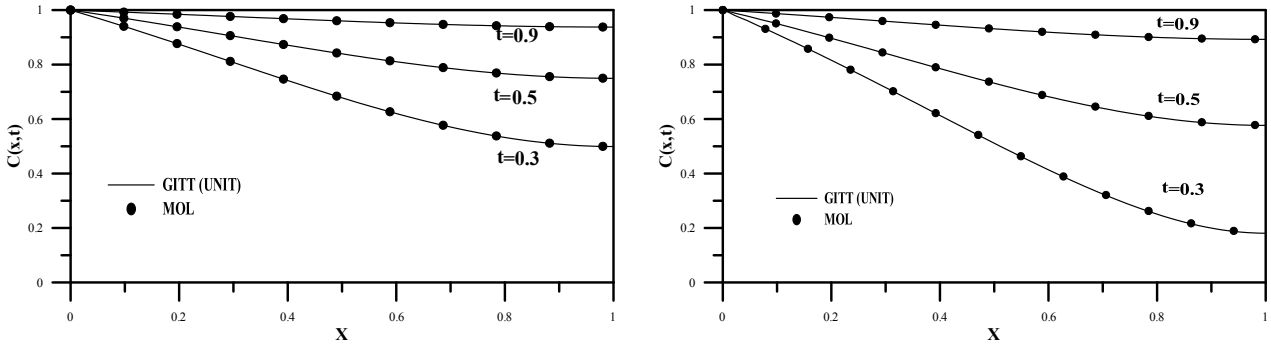

Figure 3. Comparison of the concentration fields and temperature for different positions and parameters. (a) Case 1; (b) Case 2.

In Figure (3.aI) and (3.bI) are analyzed development of the temperature distribution along the coordinate space for the Case 1 and Case 2 respectively evaluated at time instants $\tau = 0.3$, $\tau = 0\ 7$, $\tau = 0.9$. For both cases, good agreement can be observed between the results obtained by GITT and MOL for the potential temperature for different times and varying along the position.

For Case 1, Figure (3.a.I), analyzing the results of the temperature as a function of spatial variable, it is observed that the temperature field has a the same behavior as the phenomenon of heat transfer progresses with time variable. For this case with dimensionless parameter $\Delta H = 1$, the temperature gradient increases slowly with the advance of the coordinate space such that the closer the position $x = 1$, the values tend to increase. Analyzing the curves for Case 2, Figure (3.b.I), where the parameter $\Delta H = 100$, as the spatial coordinate increases, temperature gradients increase rapidly, and the heat transfer by diffusion across the field. It is observed in this case that in the initial times $\tau = 0.3$, $\tau = 0.5$ temperature gradients are larger extent and heat transfer phenomenon advances with time these gradients decrease until it reaches equilibrium with the environment.

In Figures (3.a.II) and (3.b.II) behavior of the concentration distribution along the coordinate space is analyzed for Case 1 and Case 2, respectively, in the time instants $\tau = 0.3$, $\tau = 0.5$ and $\tau = 0.9$. For both cases, there is good agreement between the results obtained by the two methods. Analyzing the potential concentration curves for Case 1, Figure (3.a.II), it was found that the concentration profiles show similar behavior for the different times analyzed, the concentration gradients decrease over a spatial variable. This behavior concentration due to the coupling between the phenomena of heat transfer and mass adsorption, causing an increase in the temperature gradient by the introduction of heat, which shows decreased concentration gradients. For Case 1, the parameters are dimensionless $\Delta H = 1$, $\alpha = 0.1$ and $K = 0.1$, in this case the concentration curves decreases more slowly along the position at different times.

5. CONCLUSIONS

This paper proposed a solution to mathematical models that describe the physical phenomenon of simultaneous transfer of heat and mass coupled with the presence of chemical adsorption, with boundary conditions of the second type. The proposal was to solve the system of equations by applying the GITT the unified version, in which the numerical results were evaluated in relation to the Method of Lines-MOL, for different parameters that govern the phenomenon of mass transfer and heat.

The results from the fields of temperature and concentration for Case 1, obtained by GITT, showed excellent rate of convergence with low numbers of terms, however for Case 2, was more difficult to achieve the same rates of convergence, this is due to increasing parameters, which causes gradients of greater magnitude. For due cases the results were in good agreement with numerical results (MOL), so the GITT in its unified version proves a powerful tool in achieving results in nonlinear problems and coupled.

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