Proceedings of CHT-17
ICHMT International Symposium on Advances in Computational Heat Transfer

May 28-June 1, 2017, Napoli, Italy

CHT-17-252

NONLINEAR EIGENVALUE PROBLEM APPROACH IN THE INTEGRAL TRANSFORMS ANALYSIS OF METAL SEPARATION BY POLYMERIC DIFFUSIVE MEMBRANES

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ABSTRACT The Generalized Integral Transform Technique (GITT) is a well-established tool in the hybrid numerical-analytical solution of various classes of nonlinear diffusion and convection-diffusion problems. Quite recently, a variant in the GITT approach has been advanced, based on retaining the original nonlinear operator coefficients in the eigenvalue problem proposition, and has been demonstrated in diffusion problems with nonlinear boundary conditions, illustrating the relative gains in convergence enhancement. The present work further demonstrates this nonlinear eigenvalue problem path in the GITT approach, by considering a mass transfer application of metal extraction through a polymeric hollow fiber membrane with diffusive separation. The methodology is here illustrated for this convection-diffusion problem with nonlinear boundary condition coefficient. The novel approach is then critically compared to the methodology employing a linear eigenvalue problem basis, for typical parametric values, but with an alternative convergence enhancement approach based on a nonlinear filter, so as to also demonstrate its convergence enhancement effect with an eventually increased computational effort for a fixed truncation order.

NOMENCLATURE

C	dimensionless concentration
$\bar{C}$	integral transformed concentration
C^*	dimensional concentration, mol m^{-3}
C_i^*	initial solute concentration, mol m^{-3}
D	diffusivity of solute in the fluid phase, m^2 s^{-1}
H	equilibrium distribution coefficient of solute concentration in the membrane to that in the fluid
h^*	dimensionless slope of the distribution coefficient, m^3 mol^{-1}
h_o	distribution coefficient for infinite solute dilution
k_m	membrane permeability coefficient, m s^{-1}
R	inner radius of hollow fiber, m
R_o	outer radius of hollow fiber, m
r	dimensionless radial coordinate

r^*	dimensional radial coordinate, m
s	hollow fiber shape factor
Sh_w	wall Sherwood number
U	dimensionless velocity profile
v	average fluid velocity, m s^{-1}
z	dimensionless axial coordinate
z^*	dimensional axial coordinate, m

Greek symbols

γ	dimensionless slope for a variable distribution coefficient
Ψ, Ω	eigenfunction
$\tilde{\Psi}, \tilde{\Omega}$	normalized eigenfunction
μ, ν	eigenvalues

Subscripts and superscripts

e	entrance position
f	filter solution
i,j,l,m	order of eigenvalues and eigenfunctions
h	homogeneous solution

INTRODUCTION

The Generalized Integral Transform Technique (GITT) is a well-established tool in the hybrid numerical-analytical solution of various classes of linear and nonlinear diffusion and convection-diffusion problems, (Cotta [1990], Cotta [1993], Cotta [1994], Cotta & Mikhailov [1997], Cotta [1998], Cotta & Mikhailov [2006], Cotta et al. [2015]). In most of the previous implementations of this approach, linear eigenvalue problems have been proposed in providing the basis of the eigenfunction expansions, inherent to this class of method. Typically, the original nonlinear problem formulation is first rewritten by retaining characateristic linear coefficients in the transient, diffusive, and dissipation operators of the partial differential equations, while transporting the remaining nonlinear terms to a general nonlinear equation source term. Again, the same formulation interpretation is adopted in case that nonlinear boundary conditions are present. Then, such characteristic equation and boundary condition linear coefficients, naturally lead to the eigenvalue problem choice to be employed in constructing the expansions. Quite recently, a variant in the GITT approach has been advanced, based on retaining the original nonlinear operator coefficients in the eigenvalue problem proposition, Cotta et al. [2016]. This methodology has been only demonstrated in diffusion problems with nonlinear boundary conditions, Cotta et al. [2016], clearly illustrating the relative gains in convergence enhancement, in comparison to other alternative schemes such as filtering and integral balances.

The present contribution further advances this nonlinear eigenvalue problem path in the GITT approach, by proposing the analysis of a convection-diffusion mass transfer problem, related to the metal extraction process through polymeric hollow fiber membranes and diffusive separation. The novel approach is then critically compared to the methodology employing a linear eigenvalue problem basis, for typical parametric values, but employing a nonlinear filter scheme for convergence enhancement. The aim is to demonstrate the convergence enhancement achieved by both approaches, with some applicability advantages allowed for by the nonlinear eigenvalue problem approach.

In this study of hollow-fiber membranes, the GITT methodology is also employed in analyzing the influence of the governing parameters on the mass separation process in tubular membranes. In this class of extraction processes, liquid extractants are used in the pores of the fiber membrane to facilitate the mass separation. Comparisons were also made with results from the literature in order to verify the implementation and demonstrate the potential of this technique in dealing with such nonlinear problems.

PHYSICAL PROBLEM

Membranes are synthetic structures that can promote the separation of two or more phases, restricting the transport of many chemical species and selectively transporting other species [Porter 1990]. They have application in several areas, such as, dialysis, metal extraction, non dispersive solvent extraction, gas separation, artificial oxygenation, and removal of pollutants from industrial waste streams [Urtiaga et al. 1992].

There is great interest in the study of supported liquid membranes because they can promote the selective separation of a solute between two aqueous solutions. The procedure consists in immobilizing an organic liquid (solvent) in the micropores contained in the pores of the membrane to promote the transfer of the solute by the membrane through diffusion, accompanied or not of chemical reaction [Urtiaga et al. 1992; Kim and Stroeve 1988, 1990; Cardoso et al. 2009].

The problem that will be analyzed in this work was proposed by Urtiaga [1992] and consists of a separation process in a module of supported liquid membranes. The analysis of the performance of the separator will be performed based on the study of only one membrane, assuming that the others present similar behavior. A schematic diagram of the hollow fiber membrane is shown in Figure 1.

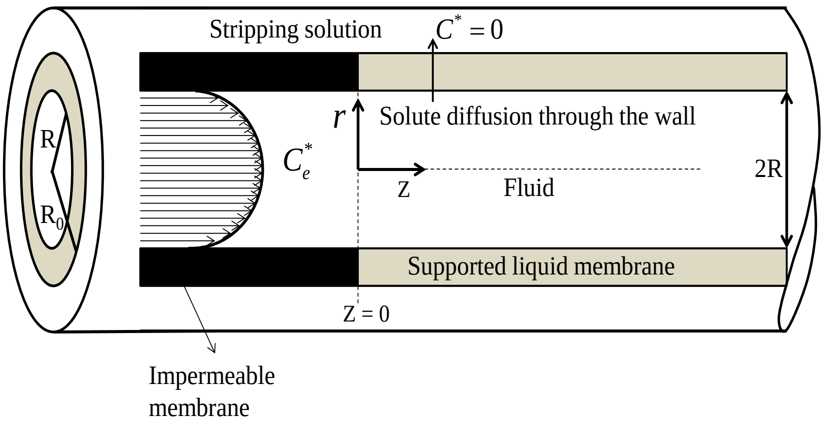

Figure 1. Diagram of the hollow fiber membrane with the solute fluid stream

The mathematical model was obtained from the mass conservation equations assuming fully developed one-dimensional laminar flow of a Newtonian fluid containing the solute to be separated. The fluid enters the separator with known concentration C_e^* and the separation process starts at z = 0, where the fluid comes into contact with the supported liquid membrane. The solute permeates through the liquid membrane by diffusion and on the outside of the fiber reacts instantaneously with the stripping solution, so that its concentration is equal to zero. The distribution coefficient H is a very important parameter of this mass transfer process, and it is defined as equilibrium distribution ratio of the solute concentration in the liquid membrane to the concentration in the fluid side. In this work, the distribution coefficient will be considered as a linear function of the concentration potential of solute in the aqueous phase, $H\left(C\left(1,z\right)\right)=1+\gamma C(1,z)$. The axial diffusion effect is neglected compared to axial convection and radial diffusion. The dimensionless mathematical model proposed by [Urtiaga et al. 1992] is given by:

$$U(r)\frac{\partial C(r,z)}{\partial z}=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C(r,z)}{\partial r}\right),\ 0<r<1,\ z>0 \tag{1.a}$$

$$C(r,0)=1,\ 0<r<1 \tag{1.b}$$

$$\left.\frac{\partial C(r,z)}{\partial r}\right|_{r=0}=0,\ z>0 \tag{1.c}$$

$$-\left.\frac{\partial C(r,z)}{\partial r}\right|_{r=1}=Sh_w H\left(C(1,z)\right)C(1,z)=Sh_w\left(1+\gamma C(1,z)\right)C(1,z),\ z>0 \tag{1.d}$$

where

$$r=\frac{r^*}{R};\ C(r,z)=\frac{C^*}{C_e^*};\ z=\frac{z^*D}{vR^2};\ \gamma=\frac{C_e^*h^*}{h_o};\ Sh_w=\frac{k_w sRh_o}{D};$$
$$U(r)=2\left(1-r^2\right);\ s=\frac{L/R_0}{\ln\left[1/\left(1-L/R_0\right)\right]}; \tag{2.a-g}$$

Eq. (1.c) represents the symmetry condition at the channel centerline, while Eq. (1.d) imposes the continuity of solute flux across the membrane-fluid interface. Eq. (1.d) is a nonlinear boundary condition and, therefore, makes it unlikely to obtain a fully analytical solution for this problem. In this case, a reliable numerical or hybrid method should be employed to obtain an accurate solution of the problem.

SOLUTION METHODOLOGY

Nonlinear Eigenvalue Problem

As an alternative to classical numerical methods, the hybrid method known as GITT (Generalized Integral Transform Technique) will be used to construct the solution of the given problem. The GITT is a technique that consists of representing the desired potential as an expansion of orthogonal eigenfunctions defined from an eigenvalue problem that in general incorporates the spatial operators of the original problem. This same problem has been previously solved by the GITT [Cardoso et al. 2009], in its traditional form, by choosing a linear eigenvalue problem as a basis for the eigenfunction expansion, thus avoiding the inclusion of the nonlinear boundary condition in its formulation. Then, from application of Green´s second identity, the contribution of the nonlinear boundary source term reappears in the transformed ordinary differential system. Besides, in [Cardoso et al. 2009], the most direct approach was employed, without the adoption of an analytical filtering solution, aimed at improving convergence of the proposed expansion. Nevertheless, the final numerical results were demonstrated to be fully converged to four significant digits at least, but at the cost of large truncation orders in the infinite eigenfunction expansions.

Here, a recently introduced alternative approach [Cotta et al. 2016], based on the adoption of a nonlinear eigenvalue problem, will be further investigated. A natural eigenvalue problem choice can be derived from separation of variables applied to the partial differential equation (1.a), including the nonlinear boundary condition, in the form:

$$\frac{\partial}{\partial r}\left[r\frac{\partial \psi_i}{\partial r}\right]+\mu_i^2(z)rU(r)\psi_i(r;z)=0 \tag{3.a}$$

$$\left.\frac{\partial \psi_i}{\partial r}\right|_{r=0} = 0;\ \left.\frac{\partial \psi_i}{\partial r}\right|_{r=1} + Sh_w\left(1+\gamma C\left(1,z\right)\right)\psi_i(1,z) = 0 \qquad (3.b\text{-}c)$$

This eigenvalue problem, equation (3.a), has a known analytical solution given in terms of special functions, and in principle, the solution procedure could follow this path. However, there is some computational advantage in adopting a simpler eigenvalue problem formulation, but still incorporating the nonlinear boundary condition information. Following this alternative, the following nonlinear eigenvalue problem shall be considered:

$$\frac{\partial^2 \Psi_i}{\partial r^2} + \mu_i^2\left(z\right)\Psi_i(r;z) = 0 \qquad (4.a)$$

$$\left.\frac{\partial \Psi_i}{\partial r}\right|_{r=0} = 0;\ \left.\frac{\partial \Psi_i}{\partial r}\right|_{r=1} + Sh_w\left(1+\gamma C\left(1,z\right)\right)\Psi_i(1,z) = 0 \qquad (4.b\text{-}c)$$

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

$$\bar{C}_i\left(z\right) = \int_0^1 \Psi_i(r;z)C\left(r,z\right)dr \qquad \text{transforms} \qquad (5.a)$$

$$C\left(r,z\right) = \sum_{i=1}^{\infty}\frac{1}{N_i(z)}\Psi_i(r;z)\bar{C}_i\left(z\right) \qquad \text{inverses} \qquad (5.b)$$

where the kernels $\Psi_i(r;z)$ are given by the solution of the eigenvalue problem above, eqs.(4). This eigenvalue problem has a known analytical solution given by:

$$\Psi_i(r;z) = \cos\left(\mu_i\left(z\right)r\right) \qquad (6.a)$$

with $N_i(z)$, the normalization integral, given by:

$$N_i(z) = \int_0^1 \Psi_i^2(r;z)dr = \frac{1}{4}\left(2 + \frac{sen\left(2\mu_i\left(z\right)\right)}{\mu_i\left(z\right)}\right) \qquad (6.b)$$

The eigenvalue problem proposed is typical of diffusion problems in Cartesian coordinates, but it was chosen to allow an analytical solution for integrals obtained during the integral transformation procedure, thus avoiding costly numerical integrations. The eigenvalue problem of eqs.(3) would result on hypergeometric functions that would require numerical integration.

The integral transformation of eq.(1a) is accomplished by applying the operator $\int_0^1 \Psi_i(r;z)(.)dr$ and making use of the boundary conditions given by eqs. (1c-d) and (4b-c), yielding the transformed system of ordinary differential equations below:

$$\sum_{j=1}^{\infty} A_{i,j}(z)\frac{d\bar{C}_j\left(z\right)}{dz} = \sum_{j=1}^{\infty} B_{i,j}(z)\bar{C}_j\left(z\right) - \mu_i^2\left(z\right)\bar{C}_i\left(z\right),\quad i = 1,2,3,... \qquad (7.a)$$

where:

$$A_{i,j}(z)=\frac{1}{N_j(z)}\int_0^1 U(r)\Psi_i(r;z)\Psi_j(r;z)dr \tag{7.b}$$

$$B_{i,j}(z)=\int_0^1\left\{\frac{U(r)\Psi_i(r;z)}{N_j^2(z)}\left[-\frac{\partial\Psi_j}{\partial z}N_j(z)+\Psi_j(r;z)\frac{dN_j}{dz}\right]+\frac{\Psi_i(r;z)}{r\,N_j(z)}\frac{\partial\Psi_j}{\partial r}\right\}dr \tag{7.c}$$

The inlet boundary conditions in the z variable given by eq. (1b) are transformed through the operator $\int_0^1 \Psi_i(r;z)(.)dr$, to provide:

$$\bar{C}_i(0)=F_i \tag{7.d}$$

where:

$$F_i=\int_0^1 \Psi_i(r;0)dr \tag{7.e}$$

For the solution of the infinite coupled system of nonlinear ordinary differential equations given by eqs. (6), 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 NDSolve of the *Mathematica* system, Wolfram [2015], may be employed, which is able to provide reliable solutions under automatic absolute and relative errors control. Then, the inversion formula can be recalled to yield the concentration field representation at any desired position r and z.

Replacing the solution, eq. (6.a), obtained for the eigenfunction $\Psi_i(r;z)$, into the nonlinear boundary condition, eq.(4.c), one may reach the transcendental equation for $\mu_i(z)$:

$$-\mu_i(z)sin(\mu_i(z))+Sh_w(1+\gamma C(1,z))\cos(\mu_i(z))=0 \tag{8.a}$$

Taking the derivative of eq. (8.a), it is possible to achieve an ODE system for $\mu_i(z)$, in the form:

$$\frac{d\mu_i}{dz}=\frac{Sh_w\gamma\cos(\mu_i(z))\dfrac{\partial C(1,z)}{\partial z}}{sin(\mu_i(z))+\mu_i(z)\cos(\mu_i(z))+Sh(C(1,z))sin(\mu_i(z))},\quad i=1,2,3,... \tag{8.b}$$

where:

$$\frac{\partial C(1,z)}{\partial z}=\sum_{j=1}^{\infty}\frac{1}{N_j^2(z)}\left[\left(\frac{d\Psi_j(1;z)}{dz}N_j(z)-\Psi_j(1;z)\frac{dN_j(z)}{dz}\right)\bar{C}_j(z)+\Psi_j(1;z)N_j(z)\frac{d\bar{C}_j(z)}{dz}\right] \tag{8.c}$$

The inlet boundary conditions for this ODE system, eqs. (8.b-c), can be obtained by the evaluation of equation (8.a) at z = 0. It can also be highlighted that at z = 0, there is a prescribed concentration inlet condition, but when computing the eigenvalues for this inlet condition, the inverse formula for the concentration should be employed in eq.(8.a), to be consistent with the substitution performed in deriving eq.(8.c) for its derivative evaluation.

Nonlinear Filter Solution

As an alternative to the nonlinear eigenvalue problem methodology, the GITT can be directly applied, as usual, to the original problem defined by eqs. (1), considering a linear eigenvalue problem, as first proposed by [Cardoso et al. 2009]. However, this approach requires a large amount of terms in the series solution, especially if no convergence enhancement scheme is adopted, since the eigenvalue problem does not include the nonlinear boundary condition term, which reappears as a source term in the transformed system. Employing a nonlinear (or implicit) filter solution can be a very effective alternative strategy to account for the nonlinear source term and avoid a slower convergence behavior of the eigenfunction expansion [Cotta & Mikhailov 1997]. In order to remove the nonlinearity of the boundary condition (Eq. 4.c), the following nonlinear filter solution has been proposed:

$$C(r,z) = C_h(r,z) + C_f(r;z) \tag{9}$$

where $C_h(r,z)$ is the homogeneous potential solution and $C_f(r;z)$ is the nonlinear filter solution. The filter solution is then obtained from the following problem formulation:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_f(r;z)}{\partial r}\right) = 0 \tag{10.a}$$

$$\left.\frac{\partial C_f(r;z)}{\partial r}\right|_{r=0} = 0 \tag{10.b}$$

$$\left.\frac{\partial C_f(r;z)}{\partial r}\right|_{r=1} + Sh_w C_f(1;z) = -Sh_w\gamma\left[C_h^2(1,z) + 2C_h(1,z)C_f(1;z) + C_f^2(1;z)\right] \tag{10.c}$$

The problem defined by Eqs (10) has analytical solution given by:

$$C_f(z) = \frac{-\left[1+2\gamma C_h(1,z)\right] \pm \sqrt{1+4\gamma C_h(1,z)}}{2\gamma} \tag{11}$$

Eq. (11) establishes an explicit nonlinear relationship between the filter and the homogeneous concentration at $r=1$, for the particular form of the boundary source term here analyzed. Note that there will be a real solution corresponding to the filter only if $1+4\gamma C_h(1,z) \geq 0$.

After finding the filter solution, the problem to determine the homogeneous potential can be analysed, which is defined by the following equations:

$$U(r)\frac{\partial C_h(r,z)}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_h(r,z)}{\partial r}\right) + P\left(r,z,C_h(1,z)\right) \tag{12.a}$$

$$C_h(r,0) = 1 - C_f(r;0) \tag{12.b}$$

$$\left.\frac{\partial C_h(r,z)}{\partial r}\right|_{r=0} = 0;\quad \left.\frac{\partial C_h(r,z)}{\partial r}\right|_{r=1} + Sh_w C_h(1,z) = 0 = 0 \tag{12.c-d}$$

where

$$P\left(r,z,C_h(1,z)\right) = -U(r)\frac{dC_f(z)}{dz} \tag{12.e}$$

As it can be observed from eqs.(12), application of the nonlinear filter results in a linear and homogeneous boundary condition, while a nonlinear source term is created in the partial differential equation (12.a). The traditional GITT methodology can now be applied to this homogeneous problem with a linear boundary condition at $r=1$. For this purpose, the following eigenvalue problem was chosen in order to provide the basis for the expansion of the homogeneous potential in terms of orthogonal eigenfunctions.

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\Psi_i}{dr}\right)+\mu_i^2 U(r)\Psi_i(r)=0 \tag{13.a}$$

$$\left.\frac{d\Psi_i}{dr}\right|_{r=0}=0;\quad \left.\frac{d\Psi_i}{dr}\right|_{r=1}+Sh_w\Psi_i(1)=0 \tag{13.b-c}$$

The eigenvalue problem above defined has the analytical solution in terms of Laguerre polynomials:

$$\Psi_i(r)=e^{-\frac{r^2\mu_i}{\sqrt{2}}}L_{\frac{1}{4}\left(-2+\sqrt{2}\mu_i\right)}\left(\sqrt{2}r^2\mu_i\right) \tag{14}$$

However, the Laguerre polynomial leads to some difficulty in obtaining analytical expressions for the integrals that appear due to the integral transformation of Eq. (12.a). Therefore, as in the previous section, the GITT itself can be applied to obtain a solution to the original eigenvalue problem, when the eigenfuctions can be expressed by eigenfunction expansions based on a simpler auxiliary eigenvalue problem, for which exact analytic solutions are readily available. Thus, the following simpler auxiliary eigenvalue problem is proposed:

$$\frac{d^2\Omega_l}{dr^2}+\nu_l^2\Omega_l(r)=0 \tag{15.a}$$

$$\left.\frac{d\Omega_l}{dr}\right|_{r=0}=0;\quad \left.\frac{d\Omega_l}{dr}\right|_{r=1}+Sh_w\Omega_l(1)=0 \tag{15.b-c}$$

The analytical solution for $\Omega_l(r)$ is given as:

$$\Omega_l(r)=\cos\left(\nu_l r\right) \tag{16.a}$$

The eigenvalues ν_l can be calculated from the transcendental equation obtained by substituting the eigenfunction in the boundary condition (15.c):

$$-\sin\left(\nu_l\right)\nu_l+Sh_w\cos\left(\nu_l\right)=0 \tag{16.b}$$

From the orthogonality property of the eigenfunctions, the transform and inverse formulae for the original eigenfunctions Ψ can be written as:

$$\bar{\Psi}_{il}=\int_0^1\tilde{\Omega}_l\left(r\right)\Psi_i\left(r\right)dr \tag{17.a}$$

$$\Psi_i\left(r\right)=\sum_{l=1}^{\infty}\tilde{\Omega}_l\left(r\right)\bar{\Psi}_{il} \tag{17.b}$$

where $\bar{\Psi}_{il}$ are eigenvectors that will be obtained from the integral transform solution of the eigenvalue problem defined in Eqs. (13), and $\tilde{\Omega}_l(r)$ is the normalized eigenfunction:

$$\tilde{\Omega}_l(r) = \frac{\Omega_l(r)}{\sqrt{N_{\Omega l}}} \; ; \; N_{\Omega l} = \int_0^1 \Omega_l^2(r)dr \tag{17.c-d}$$

Eq. (13a) is now operated on with $\int_0^1 \tilde{\Omega}_l(r)(.)dr$, to yield the transformed algebraic eigenvalue system:

$$\left[-A_{lm} + \mu_i^2 B_{lm}\right]\bar{\Psi}_{im} = 0 \tag{18.a}$$

where

$$A_{lm} = \int_0^1 r \frac{d\Omega_l}{dr}\frac{d\Omega_m}{dr} dr \; ; \; B_{lm} = \int_0^1 rU(r)\Omega_l(r)\Omega_m(r)dr \tag{18.b-c}$$

Equations (18) form an infinite algebraic system that can be numerically solved for a sufficiently large truncation order MT to ensure the desired accuracy for the eigenvalues μ_i. The norms of the eigenfunctions $\Psi_i(r)$ are then computed as:

$$Norm_{\Psi,i} = \int_0^1 rU(r)\Psi_i^2(r)dr = \sum_{l=1}^{MT}\sum_{m=1}^{MT} \left(B_{lm}\bar{\Psi}_{im}\right)\bar{\Psi}_{il} \tag{18.d}$$

After the eigenvalue problem solution, the transform and inverse formulae for the homogeneous concentration can be defined, as:

$$\bar{C}_{h_i}(r) = \int_0^1 rU(r)\tilde{\Psi}_i(r)C_h(r,z)dr \tag{19.a}$$

$$C_h(r,z) = \sum_{i=1}^{\infty} \tilde{\Psi}_i(r)\bar{C}_{h_i}(z) \tag{19.b}$$

where $\tilde{\Psi}_i(Y,Z)$ is the normalized eigenfunction defined as:

$$\tilde{\Psi}_i(r) = \frac{\Psi_i(r)}{\sqrt{Norm_{\Psi,i}}} \tag{19.c}$$

The integral transformation of Eq. (12.a) is accomplished by applying the operator $\int_0^1 \tilde{\Psi}_i(r)(.)dr$ and making use of the boundary conditions given by Eqs. (12.c-d) and (13.b-c), yielding the transformed system of ordinary differential equations:

$$\frac{d\bar{C}_{h,i}}{dz} + \mu_i^2 \bar{C}_{h,i}(z) = \bar{P}_i\left(z, C_h(1,z)\right) \tag{20.a}$$

where

$$\bar{P}_i\left(z, C_h(1,z)\right) = -\int_0^1 r\tilde{\Psi}_i(r)U(r)dr\,\frac{dC_f(z)}{dz} \quad (20.b)$$

The inlet boundary conditions given by eq. (12.b) are transformed through the operator $\int_0^1 rU(r)\tilde{\Psi}_i(r)(.)dr$, to provide:

$$\bar{C}_{h,i}(0) = \int_0^1 r\tilde{\Psi}_i(r)U(r)\left(1 - C_f(r;0)\right)dr \quad (20.c)$$

Equations (20) form a nonlinear and coupled system of ordinary differential equations that must be solved numerically by appropriate computational routines, such as the NDSolve intrinsic function of the *Mathematica* system [Wolfram, 2015]. After the numerical solution procedure is concluded, the concentration profile is built through its respective inversion formulae and the proposed nonlinear filter solution.

After the solution of the concentration field is available, the average solute concentration along the channel can be analytically derived through the following relation:

$$C_{av}(z) = \frac{\int_0^1 rU(r)C(r,z)\,dr}{\int_0^1 rU(r)dr} \quad (20.d)$$

RESULTS

The results presented in this section were obtained through a mixed symbolic-numerical computational routine built on the *Mathematica* v.10 platform, and employing the subroutine *NDSolve* for the solution of the nonlinear transformed ODEs systems, eqs.(7) and eqs.(20). Numerical results were generated through the two solution schemes explored in this work and are compared with results available in the literature as a way of numerically verifying the developed computational code.

Tables 1.a,b present the convergence behavior of the dimensionless average solute concentration at different positions along the z direction and for different truncation orders NT of the concentration eigenfunction expansion, with different values of the governing parameters, $Sh_w = 0.1$ and $\gamma = 10$, and $Sh_w = 10$ and $\gamma = 1$, respectively. The truncation order of the transformed ODE system was kept at the larger value of N=NT+20, so as to warrant that the transformed concentrations were fully converged while the present convergence analysis was undertaken for the average concentration behavior. At the last line, the numerical results obtained through the GITT without filtering or any convergence enhancement scheme [Cardoso et al. 2009], but with very high truncation orders (NT up to 1000), are also presented. The present solution with nonlinear eigenvalue problem provides a quite considerable convergence improvement over the previous GITT implementation [Cardoso et al. 2009], yielding at least six fully converged significant digits in the axial variable range analyzed and with truncation orders as low as NT=40. Also, the present solution with a nonlinear eigenvalue problem was chosen to be carried out without applying a filter, so as to analyze only the relative gain of incorporating the full nonlinear boundary condition into the eigenvalue problem formulation. The solution obtained through the GITT with nonlinear filter has also achieved an impressive convergence rate, reaching 4 to 6 converged significant digits up to this maximum truncation order of NT=60 terms. It should be recalled that a simpler auxiliary eigenvalue problem, typical of a diffusion problem in the Cartesian coordinates system has been considered, and its truncation order was kept at the larger value of N=NT+20, so as to warrant that the eigenvalues were fully converged while the present convergence analysis was undertaken for the average concentration behavior. Both sets of results are in excellent agreement with the previous GITT results with large truncation orders [Cardoso et al. 2009].

Table 1.a

Convergence behaviour of the average concentration $C_{av}(z)$ for $Sh_w = 0.1$ and $\gamma = 10$.

GITT with Nonlinear Eigenvalue Problem						
NT	***z* = 0.01**	***z* = 0.1**	***z* = 0.2**	***z* = 0.5**	***z* = 1**	***z* = 2**
10	0.983595	0.877728	0.787327	0.590917	0.397553	0.218047
20	0.983595	0.877728	0.787327	0.590917	0.397552	0.218047
30	0.983595	0.877727	0.787327	0.590917	0.397552	0.218047
40	0.983594	0.877727	0.787327	0.590917	0.397552	0.218047
50	0.983594	0.877727	0.787327	0.590917	0.397552	0.218047
60	0.983594	0.877727	0.787327	0.590917	0.397552	0.218047
GITT with Nonlinear Filter						
NT	***z* = 0.01**	***z* = 0.1**	***z* = 0.2**	***z* = 0.5**	***z* = 1**	***z* = 2**
10	0.983645	0.877751	0.787343	0.590924	0.397554	0.218046
20	0.983602	0.877731	0.787329	0.590918	0.397552	0.218046
30	0.983597	0.877729	0.787328	0.590917	0.397552	0.218046
40	0.983595	0.877728	0.787327	0.590917	0.397552	0.218046
50	0.983595	0.877728	0.787327	0.590917	0.397552	0.218046
60	0.983595	0.877727	0.787327	0.590917	0.397552	0.218046
Ref.*	0.9835	0.8774	0.7869	0.5903	0.3970	0.2177

Table 1.b

Convergence behaviour of the average concentration $C_{av}(z)$ for $Sh_w = 10$ and $\gamma = 1$.

GITT with Nonlinear Eigenvalue Problem						
NT	***z* = 0.01**	***z* = 0.1**	***z* = 0.2**	***z* = 0.5**	***z* = 1**	***z* = 2**
10	0.922803	0.636375	0.455896	0.174963	0.035826	0.001508
20	0.922804	0.636375	0.455895	0.174963	0.035826	0.001508
30	0.922803	0.636374	0.455895	0.174963	0.035826	0.001508
40	0.922802	0.636374	0.455895	0.174963	0.035826	0.001508
50	0.922802	0.636374	0.455895	0.174963	0.035826	0.001508
60	0.922802	0.636374	0.455895	0.174963	0.035826	0.001508
GITT with Nonlinear Filter						
NT	***z* = 0.01**	***z* = 0.1**	***z* = 0.2**	***z* = 0.5**	***z* = 1**	***z* = 2**
10	0.923158	0.636510	0.455985	0.174997	0.035833	0.001509
20	0.922889	0.636408	0.455918	0.174971	0.035828	0.001509
30	0.922838	0.636388	0.455904	0.174966	0.035827	0.001508
40	0.922822	0.636382	0.455900	0.174965	0.035826	0.001508
50	0.922814	0.636379	0.455898	0.174964	0.035826	0.001508
60	0.922810	0.636377	0.455897	0.174964	0.035826	0.001508
Ref.*	0.9227	0.6363	0.4558	0.1749	0.0358	0.00150

(*) [Cardoso et al. 2009]

Table 2 presents a comparison of the dimensionless average concentration values between the two hybrid solution schemes explored in this work with available literature data [Urtiaga et al. 1992], for different values of Sh_w, γ and *z*. The GITT results here reported were obtained with a fixed truncation order of NT=60, while the truncation order for the transformed system and for the eigenvalue problem solutions were held at the fixed value of N=80. One may observe the expected excellent agreement between the two converged GITT solutions, which provide a verification of the numerical results of [Urtiaga et al.

1992], with an adherence to at least two significant digits in all positions and parameter values considered.

Table 2

z	$Sh_w = 0.1$ and $\gamma = 0$			$Sh_w = 0.1$ and $\gamma = 0.1$		
	Urtiaga et al. (1992)	Nonlinear Filter	Nonlinear Eigenvalue Problem	Urtiaga et al. (1992)	Nonlinear Filter	Nonlinear Eigenvalue Problem
0.01	0.997937	0.998034	0.998034	0.997739	0.997844	0.997844
0.1	0.980597	0.980814	0.980814	0.978829	0.979062	0.979062
0.2	0.961899	0.962186	0.962185	0.958534	0.958842	0.958842
0.5	0.908104	0.908536	0.908536	0.900555	0.901012	0.901012
1.0	0.825084	0.825714	0.825714	0.812170	0.812824	0.812824
2.0	0.682032	0.682032	0.682032	0.660485	0.662879	0.662879
z	$Sh_w = 0.1$ and $\gamma = 1$			$Sh_w = 1$ and $\gamma = 0$		
	Urtiaga et al. (1992)	Nonlinear Filter	Nonlinear Eigenvalue Problem	Urtiaga et al. (1992)	Nonlinear Filter	Nonlinear Eigenvalue Problem
0.01	0.995759	0.996195	0.996195	0.982283	0.982961	0.982961
0.1	0.963544	0.964428	0.964428	0.859620	0.860585	0.860585
0.2	0.933780	0.931542	0.931542	0.748813	0.749808	0.749808
0.5	0.840861	0.842418	0.842418	0.499920	0.500057	0.500057
1.0	0.716369	0.718403	0.718403	0.254408	0.255004	0.255004
2.0	0.532879	0.535389	0.535389	0.066080	0.066316	0.066316
z	$Sh_w = 1$ and $\gamma = 0.1$			$Sh_w = 1$ and $\gamma = 1$		
	Urtiaga et al. (1992)	Nonlinear Filter	Nonlinear Eigenvalue Problem	Urtiaga et al. (1992)	Nonlinear Filter	Nonlinear Eigenvalue Problem
0.01	0.980048	0.981756	0.981756	0.971118	0.973046	0.973046
0.1	0.851779	0.854148	0.854148	0.811091	0.813065	0.813065
0.2	0.738177	0.740630	0.740630	0.682304	0.684142	0.684142
0.5	0.486580	0.488829	0.488829	0.421381	0.422825	0.422824
1.0	0.245085	0.246757	0.246757	0.198930	0.199924	0.199923
2.0	0.063000	0.063670	0.063670	0.048622	0.049018	0.049018

This comparative analysis is complemented through Figures 2-4, which provide the profiles of the dimensionless average solute concentration along the length of the hollow fiber membrane, for different values of Sh_w and γ**.** These GITT results were obtained with a truncation order of NT=60 with a truncation order for the transformed system and for the eigenvalue problem of N=80. To the graphical scale, it is quite clear that the two hybrid solution schemes here employed are in excellent agreement with the previously reported results [Urtiaga et al. 1992]. It is evident that the average concentration of the solute is strongly influenced by the values of both Sh_w and γ, but it is also observable that for larger values of Sh_w the variable distribution coefficient plays a less significant role. It should be noted that the nonlinear filtering solution here adopted leads to a complex domain solution for values of γ less than zero. For this reason, in the following graphs, there are no curves of the nonlinear filter solution for negative values of γ. The solution scheme with the nonlinear eigenvalue problem does not have this sort of limitation, being valid for any value of γ**.**

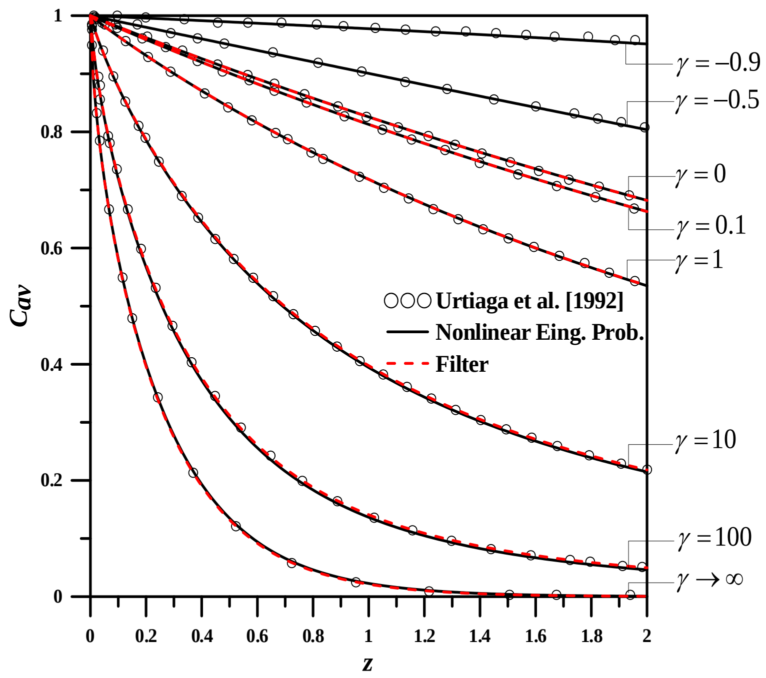

Figure 2. Effect of variable distribution coefficient on dimensionless average solute concentration for $Sh_w = 0.1$.

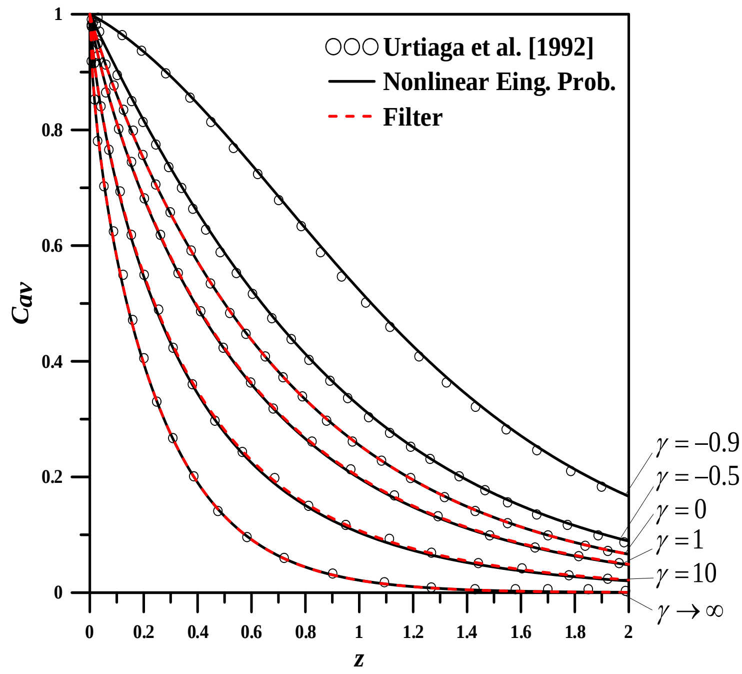

Figure 3. Effect of variable distribution coefficient on dimensionless average solute concentration for $Sh_w = 1$.

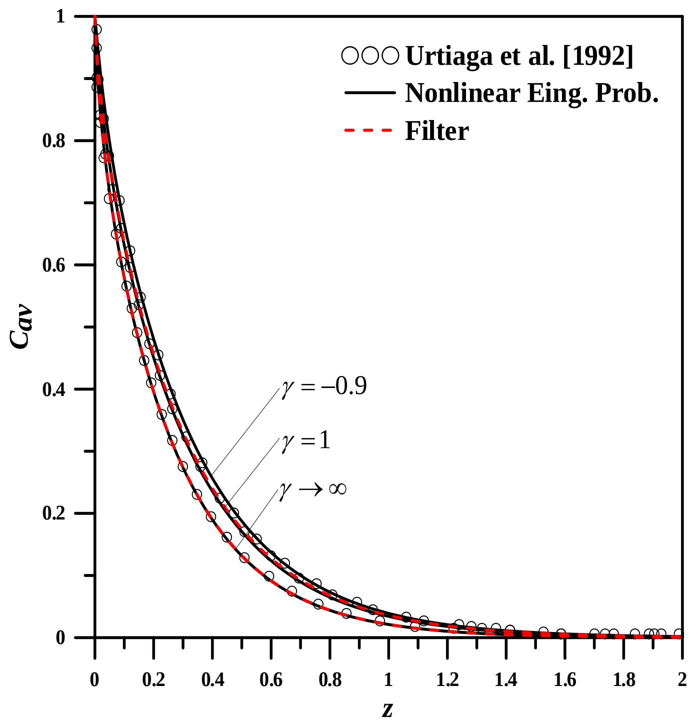

Figure 4. Effect of variable distribution coefficient on dimensionless average solute concentration for $Sh_w = 10$.

CONCLUSION

The integral transform analysis of nonlinear convection-diffusion problems is here considered, further advancing a recently introduced alternative approach through the adoption of a nonlinear eigenvalue problem in the proposition of the eigenfunction expansions. A mass transfer model related to metals extraction with polymeric hollow fiber membranes is examined more closely. The nonlinear boundary condition source term is introduced into the eigenvalue problem and simultaneously solved with the set of ordinary differential equations for the transformed concentration field. The adopted nonlinear eigenvalue problem is in fact a simpler version, typical of diffusion problems in Cartesian coordinates, so as to achieve analytical integrations throughout the solution procedure. A second hybrid solution through GITT is also implemented in the particular situation here considered, for critical comparisons, based on the proposition of a nonlinear filter that eliminates the nonlinearity in the boundary condition of the filtered problem, moving this effect to the convection-diffusion equation itself. The use of filtering solutions is an important tool in the convergence enhancement of eigenfunction expansions, especially when the boundary conditions are made homogeneous by the filter. Both hybrid solution schemes, either with the nonlinear eigenvalue problem or with the nonlinear filter, have markedly improved convergence rates with respect to the plain GITT solution with a linear eigenvalue problem and without any filter, previously implemented with very high truncation orders. The proposed solution with a nonlinear eigenvalue problem reaches six significant digits convergence with truncation orders as low as 40 terms. The agreement among all three GITT solutions is remarkable, for different values of the governing parameters, as well as with another available purely numerical solution of the same problem.

The proposed GITT approach with nonlinear eigenvalue problem then provides a general methodology for convection-diffusion problems with nonlinear boundary conditions. It may even be further improved in terms of convergence rate, by either considering an eigenvalue problem that incorporates all the original spatial operators of the partial differential equation and/or by considering complementary convergence enhancement techniques, such as an analytical filtering solution to reduce the importance of the source terms.

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