

HYBRID ANALYSIS OF TRANSIENT NON-LINEAR CONVECTION–DIFFUSION PROBLEMS

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ABSTRACT

A hybrid numerical-analytical approach, based on recent developments in the generalized integral transform technique, is presented for the solution of a class of non-linear transient convection–diffusion problems. The original partial differential equation is integral transformed into a denumerable system of coupled non-linear ordinary differential equations, which is numerically solved for the transformed potentials. The hybrid analysis convergence is illustrated by considering the one-dimensional non-linear Burgers equation and numerical results are presented for increasing truncation orders of the infinite ODE system.

KEY WORDS Hybrid analysis Convection–diffusion problem Burgers equation

NOMENCLATURE

$A(t, y)$	coefficients matrix in system (7)
b	coefficient in non-linear convection term
$d(x)$	equation coefficient in linear dissipation term
$f(x)$	initial potential distribution
$k(x)$	equation coefficient in diffusion term
$P(x, t)$	equation source function
t	time variable
$T(x, t)$	potential distribution
$u(x, t, T)$	velocity vector in convection term
$u(T)$	velocity in Burgers equation
u_0	coefficient in linear convection term
$w(x)$	equation coefficient in transient term
x	position vector in general system (1)
x	space coordinate in Burgers equation (8)
$y(t)$	solution vector in system (7)

Greek symbols

$\alpha(x)$	boundary condition coefficient
$\beta(x)$	boundary condition coefficient
$\phi(x, t)$	boundary source function
ν	coefficient in diffusion term of Burgers equation (8a)

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Subscripts and Superscripts

i, j order of eigenvalue
 integral transformed quantity

INTRODUCTION

Heat and mass transfer problems are quite frequently modelled by transient convection–diffusion equations, when the convective and diffusive effects somehow compete to provide the final solution behaviour. Not less frequently, and particularly in the convection term, non-linearities are present which make the classical analytical approaches¹ not *a priori* applicable to this class of problem. Purely numerical approaches are then considered, either as fully or semi-discrete versions of the finite differences² or finite element method³. The discrete approximations can, however, experience an anomalous behaviour due to numerical dispersion or dissipation. Fortunately, alternative schemes were devised to overcome such difficulties to some extent, through backward spatial difference approximations ('upwind') for the convective term or by introducing some sort of artificial viscosity to damp the numerical oscillations^{2,3}. Nevertheless, it would be at least desirable to develop analytical solutions for non-linear transient convection–diffusion problems, which could serve benchmarking purposes for more involved situations, and eventually provide an alternative hybrid computational tool. In light of the various recent developments in the so-called generalized integral transform technique (GITT)^{4–16} for the analytical solution of *a priori* non-transformable diffusion problems, an extension of such ideas is here attempted. In fact, two important steps were already taken in this direction, in connection with linear convection–diffusion problems¹⁵ and with non-linear purely diffusive problems¹⁶. Therefore, by combining ideas^{15,16}, formal solutions are obtained for transient multidimensional convection–diffusion problems with non-linear convection terms, based on integral transformation of the spatial operators and reduction of the original partial differential system into an infinite system of coupled non-linear ordinary differential equations. Upon truncation to a sufficiently large finite order, the ODE system is numerically solved for the transformed potentials by making use of well-established algorithms for initial value problems¹⁷, readily available in scientific subroutines libraries⁸. The inversion formula is then trivially recalled to produce the desired original potential. The present hybrid numerical-analytical approach is illustrated by considering the one-dimensional Burgers equation^{17,19}, which typically represents the competition between convection and diffusion with a simple mathematical model. The convergence behaviour of the hybrid analysis is then investigated, for increasing truncated ODE system sizes, and critically compared against a semi-discrete solution for different values of the governing parameters.

ANALYSIS

We proceed by considering a sufficiently general formulation, for our purposes here, of a transient convection–diffusion problem defined in the region V with boundary surface S , and including non-linear effects in the convective term, as follows:

$$w(\mathbf{x}) \frac{\partial T(\mathbf{x}, t)}{\partial t} + \mathbf{u}(\mathbf{x}, t, T) \cdot \nabla T(\mathbf{x}, t) + LT(\mathbf{x}, t) = P(\mathbf{x}, t), \quad \mathbf{x} \in V, t > 0 \quad (1a)$$

with initial and boundary conditions given, respectively, by

$$T(\mathbf{x}, 0) = f(\mathbf{x}) \quad \mathbf{x} \in V \quad (1b)$$

$$BT(\mathbf{x}, t) = \phi(\mathbf{x}, t) \quad \mathbf{x} \in S, \quad t > 0 \quad (1c)$$

where the equation and boundary operators are written as:

$$L \equiv -\nabla \cdot k(\mathbf{x})\nabla + d(\mathbf{x}) \quad (1d)$$

$$B \equiv \left[\alpha(\mathbf{x}) + \beta(\mathbf{x})k(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \right] \tag{1e}$$

and \mathbf{n} denotes the outward drawn normal to the surface S .

Without the convection term, i.e. $\mathbf{u}(\mathbf{x}, t, T) \equiv 0$, problem (1) becomes a class I linear diffusion problem according to an earlier classification¹, for which exact analytical solutions were obtained through the classical integral transform technique¹. For a non-zero vector \mathbf{u} , problem (1) is not *a priori* transformable, and the ideas in the generalized integral transform technique⁴⁻¹⁶ can be utilized to develop a hybrid numerical-analytical solution to this class of problems. Following the formalisms previously established for linear convection-diffusion problems¹⁵ and for purely diffusive non-linear problems¹⁶, the appropriate auxiliary problem is taken as:

$$L\psi_i(\mathbf{x}) = \mu_i^2 w(\mathbf{x})\psi_i(\mathbf{x}) \quad \mathbf{x} \in V \tag{2a}$$

with boundary condition

$$B\psi_i(\mathbf{x}) = 0 \quad \mathbf{x} \in S \tag{2b}$$

where the eigenvalues, μ_i 's, and related eigenfunctions, $\psi_i(\mathbf{x})$, are here assumed to be known from application of also recently advanced computational methods for Sturm-Liouville type problems¹. Problem (2) then allows, through the associated orthogonality property of the eigenfunctions, definition of the integral transform pair below:

$$\bar{T}_i(t) = \int_V w(\mathbf{x}) \mathbb{K}_i(\mathbf{x}) T(\mathbf{x}, t) dv \quad \text{transform} \tag{3a}$$

$$T(\mathbf{x}, t) = \sum_{i=1}^{\infty} \mathbb{K}_i(\mathbf{x}) \bar{T}_i(t) \quad \text{inverse} \tag{3b}$$

where the symmetric kernel $\mathbb{K}_i(\mathbf{x})$ is given by:

$$\mathbb{K}_i(\mathbf{x}) = \frac{\psi_i(\mathbf{x})}{N_i^{1/2}} \tag{3c}$$

and the normalization integral as:

$$N_i = \int_V w(\mathbf{x}) \psi_i^2(\mathbf{x}) dv \tag{3d}$$

The integral transformation of (1a) is now attempted by applying the operator

$$\int_V \mathbb{K}_i(\mathbf{x}) dv$$

to yield, after utilizing the boundary conditions (1c) and (2b):

$$\frac{d\bar{T}_i(t)}{dt} + \int_V \mathbb{K}_i(\mathbf{x}) [\mathbf{u}(\mathbf{x}, t, T) \cdot \nabla T(\mathbf{x}, t)] dv + \mu_i^2 \bar{T}_i(t) = \bar{g}_i(t) \quad i = 1, 2, \dots, t > 0 \tag{4a}$$

where

$$\bar{g}_i(t) = \int_V \mathbb{K}_i(\mathbf{x}) P(\mathbf{x}, t) dv + \int_S k(\mathbf{x}) \left[\mathbb{K}_i(\mathbf{x}) \frac{\partial T(\mathbf{x}, t)}{\partial \mathbf{n}} - T(\mathbf{x}, t) \frac{\partial \mathbb{K}_i(\mathbf{x})}{\partial \mathbf{n}} \right] ds \tag{4b}$$

while the untransformed term in (4a) above can be rewritten, after application of the inversion formula (3b), as:

$$\int_V \mathbb{K}_i(\mathbf{x}) [\mathbf{u}(\mathbf{x}, t, T) \cdot \nabla T(\mathbf{x}, t)] dv = \sum_{j=1}^{\infty} a_{ij}^*(t, T) \bar{T}_j(t) \tag{5a}$$

where

$$a_{ij}^*(t, T) = \int_V \mathbb{K}_i(\mathbf{x}) [\mathbf{u}(\mathbf{x}, t, T) \cdot \nabla \mathbb{K}_i(\mathbf{x})] dv \quad (5b)$$

Equation (4a) is then written more compactly as

$$\frac{d\bar{T}_i(t)}{dt} + \sum_{j=1}^{\infty} a_{ij}(t, T) \bar{T}_j(t) = \bar{g}_i(t) \quad i = 1, 2, \dots, t > 0 \quad (6a)$$

where

$$a_{ij}(t, T) = \delta_{ij} \mu_i^2 + a_{ij}^*(t, T) \quad (6b)$$

with

$$\delta_{ij} = \begin{cases} 0, & \text{for } i \neq j \\ 1, & \text{for } i = j \end{cases} \quad (6c)$$

The initial condition, (1b), is also integral transformed through the operator $\int_V w(\mathbf{x}) \mathbb{K}_i(\mathbf{x}) dv$, to provide:

$$\bar{T}_i(0) = \bar{f}_i \equiv \int_V w(\mathbf{x}) \mathbb{K}_i(\mathbf{x}) f(\mathbf{x}) dv \quad (6d)$$

Equations (6) form an infinite system of coupled non-linear ordinary differential equations for the transformed potentials, \bar{T}_i 's. For computation purposes, system (6) is truncated at the N th row and column, with N sufficiently large for the required convergence. The formal aspects behind the convergence to the infinite system solution as the truncation order, N , is increased, have been investigated elsewhere^{14,16}, and repeating such analysis is here avoided. The truncated system is then written in matrix form as:

$$\mathbf{y}'(t) + \mathbf{A}(t, \mathbf{y})\mathbf{y}(t) = \mathbf{g}(t) \quad t > 0 \quad (7a)$$

$$\mathbf{y}(0) = \mathbf{f} \quad (7b)$$

where

$$\mathbf{y}(t) = \{\bar{T}_1(t), \bar{T}_2(t), \dots, \bar{T}_N(t)\}^T \quad (7c)$$

$$\mathbf{A}(t, \mathbf{y}) = \{a_{ij}(t, T)\} \quad (7d)$$

$$\mathbf{g}(t) = \{\bar{g}_1(t), \bar{g}_2(t), \dots, \bar{g}_N(t)\}^T \quad (7e)$$

$$\mathbf{f} = \{\bar{f}_1, \bar{f}_2, \dots, \bar{f}_N\}^T \quad (7f)$$

The non-linear initial value problem defined by (7) is likely to belong to a class of stiff ordinary differential systems, specially for increasing values of N , while the transformed solutions, $\bar{T}_i(t)$, decay at increasingly different rates in t . Fortunately, various special numerical integrators have been designed within the last two decades, to this class of systems¹⁷. For instance, subroutine DIVPAG from the IMSL library¹⁸ is an extremely reliable stiff system integrator, which implements Gear's method of backward differentiation with variable order, and is widely available in most computer centres.

Once the transformed potentials have been computed from numerical solution of system (7), the inversion formula (3b) is recalled to reconstruct the original potential, $T(x, t)$, in explicit form.

APPLICATION

The hybrid solution here presented is now illustrated through consideration of the one-dimensional non-linear Burgers equation^{17,19}, which is a frequently employed model equation

for transient convection-diffusion phenomena, and used for development and validation of numerical schemes. The mathematical formulation of the problem here considered is:

$$\frac{\partial T(x,t)}{\partial t} + u(T) \frac{\partial T(x,t)}{\partial x} = v \frac{\partial^2 T(x,t)}{\partial x^2} \quad 0 < x < 1, \quad t > 0 \quad (8a)$$

with initial and boundary conditions given, respectively, by

$$T(x,0) = 1 \quad 0 \leq x \leq 1 \quad (8b)$$

$$T(0,t) = 1 \quad T(1,t) = 0 \quad t > 0 \quad (8c,d)$$

and for the present application the non-linear function $u(T)$ is taken as:

$$u(T) = u_0 + bT \quad (8e)$$

For best computational performance, the boundary conditions (8c,d) are made homogeneous through the simple transformation:

$$T(x,t) = T_\infty(x) + T^*(x,t) \quad (9a)$$

where $T_\infty(x)$ is the solution of the linear steady-state problem:

$$u_0 \frac{dT_\infty(x)}{dx} = v \frac{d^2 T_\infty(x)}{dx^2} \quad (9b)$$

$$T_\infty(0) = 1 \quad T_\infty(1) = 0 \quad (9c)$$

which is readily solved as:

$$T_\infty(x) = \frac{1 - \exp\left[\frac{u_0}{v}(x-1)\right]}{1 - \exp\left[-\frac{u_0}{v}\right]} \quad (9d)$$

The resulting problem for $T^*(x,t)$ becomes:

$$\frac{\partial T^*(x,t)}{\partial t} + u^*(x, T^*) \frac{\partial T^*(x,t)}{\partial x} = v \frac{\partial^2 T^*(x,t)}{\partial x^2} - d(x)T^*(x,t) + P(x) \quad 0 < x < 1 \quad t > 0 \quad (10a)$$

where

$$u^*(x, T^*) = u_0 + b(T^* + T_\infty(x)) \quad (10b)$$

$$d(x) = b \frac{dT_\infty(x)}{dx} \quad (10c)$$

$$P(x) = -bT_\infty \frac{dT_\infty(x)}{dx} \quad (10d)$$

with initial and boundary conditions:

$$T^*(x,0) = f^*(x) = 1 - T_\infty(x) \quad 0 \leq x \leq 1 \quad (10e)$$

$$T^*(0,t) = 0 \quad T^*(1,t) = 0 \quad t > 0 \quad (10f,g)$$

For $b=0$ (linearized Burgers equation), the expressions obtained in Reference 15 are readily recovered and a purely analytical solution is reached.

RESULTS AND DISCUSSIONS

Numerical results were obtained for typical values of the parameters that govern the relative importance of convection (linear and non-linear terms) and diffusion, u_0 , b , and v . Truncated systems of order $N \leq 30$, with automatic order control, were solved through IMSL subroutine DIVPAG, with sufficient accuracy requirement in terms of relative error, in order to demonstrate the convergence characteristics of the hybrid solution. *Table 1* presents the potential distributions, at different values of $t=0.1$ and 0.5 , for increasing values of N , but fixed at each run. The excellent convergence behaviour is easily noticeable throughout *Table 1*, but it is interesting to note the behaviour with respect to the governing parameters. As usual in eigenfunction expansion techniques, convergence becomes slower for decreasing t ; also, as the importance of convection increases, either through the linear (u_0) or non-linear (b) contributions, larger systems are required to provide the same relative accuracy. For instances, with $b=0.01$ and $u_0=1.0$, convergence to five digits is achieved with $N \approx 15$, with $b=0.5$ and $u_0=1.0$, 15 to 20 terms are required, while for $b=5.0$ and $u_0=1.0$ convergence is reached for $N \approx 25$. For validation purposes, a semi-discrete scheme based on the combined use of spatial collocation and the method of lines was employed, which is readily available in subroutine DMOLCH from the IMSL library¹⁸, for one-dimensional parabolic problems. The results from this well-established routine are in excellent agreement with those here presented, for 31 grid points in the spatial discretization. A fully discrete finite-differences approach was also utilized, based on MacCormack's explicit predictor-corrector scheme², which is a second-order accurate scheme both in time and space. Again, with 31 grid points in the spatial discretization, a reasonably good agreement to three significant digits was achieved.

It should be noted that although the numerical results in *Table 1* were produced with a fixed number of ordinary differential equations for each run, in order to demonstrate the convergence behaviour for increasing N , the basic computational algorithm for this approach²⁰, proceeds in a more efficient way, by automatically controlling the order of truncation N at each time step. The analytical part of the solution, represented by the inversion formula (3b), provides a local error estimator at almost no cost, given by the maximum relative error estimator at almost no cost, given by the maximum relative error of partial sums with respect to the total sum of (3b). Therefore, computation is started at $t=0$ with an initial N estimated, for instances, from a lowest order solution of system (7), when non-diagonal elements of the coefficients matrices are completely neglected. By examining the convergence of the inversion formula at each subsequent time step, the value of N is adaptatively changed, so as to satisfy the required accuracy and reduce computational costs. A typical run of this problem for a required tolerance of 10^{-4} (4 digits accuracy), takes about 50sec of CPU time on a CYBER 180/840.

Table 1 Convergence of hybrid solution and comparison with numerical solution

x/N	5	10	15	20	30	Numerical*
$t=0.1 (u_0=0.1; b=0.01; v=1.0)$						
0.1	0.97123	0.97117	0.97118	0.97118	0.97118	0.97115
0.3	0.89035	0.89035	0.89036	0.89036	0.89036	0.89028
0.5	0.74422	0.74420	0.74420	0.74420	0.74420	0.74410
0.7	0.50578	0.50576	0.50576	0.50576	0.50576	0.50566
0.9	0.18123	0.18128	0.18128	0.18127	0.18127	0.18123
$t=0.5 (u_0=0.1; b=0.01; v=1.0)$						
0.1	0.90607	0.90607	0.90607	0.90607	0.90607	0.90607
0.3	0.71460	0.71460	0.71460	0.71460	0.71460	0.71459
0.5	0.51760	0.51760	0.51760	0.51760	0.51760	0.51759
0.7	0.31469	0.31469	0.31469	0.31469	0.31469	0.31469
0.9	0.10614	0.10614	0.10614	0.10614	0.10614	0.10614

Table 1 (continued)

x/N	5	10	15	20	30	Numerical*
$t=0.1 (u_0=0.1; b=0.5; v=1.0)$						
0.1	0.97611	0.97609	0.97609	0.97609	0.97609	0.97607
0.3	0.90430	0.90428	0.90428	0.90428	0.90428	0.90422
0.5	0.76546	0.76541	0.76540	0.76540	0.76540	0.76531
0.7	0.52682	0.52680	0.52679	0.52679	0.52679	0.52670
0.9	0.19035	0.19038	0.19037	0.19037	0.19037	0.19033
$t=0.5 (u_0=0.1; b=0.5; v=1.0)$						
0.1	0.91932	0.91952	0.91949	0.91947	0.91948	0.91948
0.3	0.74414	0.74417	0.74416	0.74415	0.74416	0.74415
0.5	0.55017	0.55014	0.55013	0.55013	0.55013	0.55013
0.7	0.33919	0.33926	0.33926	0.33926	0.33926	0.33926
0.9	0.11533	0.11528	0.11527	0.11527	0.11527	0.11527
$t=0.1 (u_0=1.0; b=0.01; v=1.0)$						
0.1	0.98152	0.98108	0.98111	0.98113	0.98112	0.98111
0.3	0.92128	0.92131	0.92132	0.92132	0.92132	0.92126
0.5	0.79882	0.79863	0.79861	0.79861	0.79861	0.79853
0.7	0.57269	0.57254	0.57250	0.57249	0.57250	0.57241
0.9	0.22014	0.22054	0.22047	0.22043	0.22045	0.22041
$t=0.5 (u_0=1.0; b=0.01; v=1.0)$						
0.1	0.93980	0.93979	0.93979	0.93979	0.93979	0.93979
0.3	0.79919	0.79919	0.79919	0.79919	0.79919	0.79919
0.5	0.62622	0.62621	0.62621	0.62621	0.62621	0.62621
0.7	0.41335	0.41334	0.41334	0.41334	0.41334	0.41334
0.9	0.15194	0.15194	0.15194	0.15194	0.15194	0.15194
$t=0.1 (u_0=1.0; b=0.5; v=1.0)$						
0.1	0.98507	0.98458	0.98461	0.98463	0.98462	0.98461
0.3	0.93240	0.93243	0.93244	0.93243	0.93243	0.93238
0.5	0.81800	0.81774	0.81772	0.81772	0.81772	0.81764
0.7	0.59425	0.59409	0.59404	0.59403	0.59403	0.59395
0.9	0.23064	0.23110	0.23100	0.23097	0.23099	0.23095
$t=0.5 (u_0=1.0; b=0.5; v=1.0)$						
0.1	0.95031	0.95034	0.95032	0.95032	0.95032	0.95032
0.3	0.82591	0.82594	0.82594	0.82593	0.82593	0.82593
0.5	0.66018	0.66014	0.66014	0.66014	0.66014	0.66014
0.7	0.44271	0.44274	0.44273	0.44273	0.44273	0.44273
0.9	0.16424	0.16431	0.16429	0.16428	0.16429	0.16429
$t=0.1 (u_0=1.0; b=5.0; v=1.0)$						
0.1	1.0004	0.99846	0.99849	0.99852	0.99851	0.99851
0.3	0.98887	0.98897	0.98900	0.98897	0.98897	0.98896
0.5	0.94953	0.94774	0.94771	0.94770	0.94771	0.94769
0.7	0.79457	0.79337	0.79330	0.79325	0.79328	0.79324
0.9	0.35350	0.35452	0.35430	0.35420	0.35426	0.35423
$t=0.5 (u_0=1.0; b=5.0; v=1.0)$						
0.1	0.99799	0.99653	0.99655	0.99658	0.99657	0.99657
0.3	0.97866	0.97903	0.97904	0.97901	0.97901	0.97901
0.5	0.92319	0.92232	0.92226	0.92226	0.92227	0.92226
0.7	0.75150	0.75122	0.75111	0.75108	0.75110	0.75109
0.9	0.32549	0.32671	0.32649	0.32641	0.32646	0.32645

*Subroutine DMOLCH/IMSL¹⁸ (31 grid points).

The present approach is sufficiently straightforward and computationally efficient to offer an interesting alternative to purely numerical approaches, specially under high accuracy requirements such as for benchmarking purposes. Also, approximate solutions at low truncation orders are sufficiently accurate for most practical purposes, and computational effort is then kept to a minimum. Extension of such computations to multidimensional situations readily follow from the general solution here provided. The related eigenvalue problem (2) is then solved by standard approaches for Sturm–Liouville systems^{1,20}, after application of separation of variables on this auxiliary partial differential system. Also, the associated volume integrals for determination of the ODE system coefficients, are evaluated as multiple integrals (double or triple), and all of the remaining steps for the one-dimensional case are essentially the same. A number of multidimensional linear problems were previously handled by the present approach^{12,13,20}, including the computational implementation that is practically unaffected by the non-linear terms here introduced. It should be recognized that one major advantage of this method lies in the fact that the original potential is analytically and explicitly expressed by the inversion formula in all but one independent variable, t , and a numerical discretization procedure is required only for integration in this coordinate, which allows one to employ well-established algorithms for ODE systems with automatic accuracy control, widely available in subroutines libraries, yielding an overall robust and reliable tool.

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