



On the non-linear Maxwell–Cattaneo equation with non-constant diffusivity: Shock and discontinuity waves

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ABSTRACT

A numerical study on a non-linear hyperbolic diffusion equation is proposed. The Hartree hybrid method combining finite difference techniques with the method of characteristics is used in the presence of discontinuities between initial and boundary conditions. The technique proved to be a useful tool to overcome oscillation problems and spurious solutions in case of strong non-linearities related to both attractive or repulsive interactions between diffusing species. Two different expressions for the diffusion coefficient are used in order to compare our results with the ones obtained in previous studies relying upon the Laplace transform technique and the McCormack predictor–corrector method. Finally, an analytic approach based on the singular surface theory is proposed to motivate the numerical results and to clarify some controversial aspects concerning the penetration depth of a diffusive front in the presence of interactions.

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1. Introduction

It is widely recognized that the hyperbolic heat and mass transfer equations offer a promising tool to solve many physics and engineering problems when the classical Fourier or Fick approach are proven to be unsuccessful [1,2]. Among the most important applications, we remember the nano-fluid heat transport [3], the high-energy laser pulse technology [4], the chromatography [5], the single-molecule fluorescence spectroscopy [6] and the food engineering [7].

Heat and mass diffusion problems in time-delayed hyperbolic equations are generally cast into the following form [8,9]:

$$\gamma \frac{\partial u(\vec{r}, t)}{\partial t} + \nabla \cdot \vec{q}(\vec{r}, t) = 0 \quad (1)$$

$$\vec{q}(\vec{r}, t + \tau) = -k(u) \nabla u(\vec{r}, t) \quad (2)$$

where $u(\vec{r}, t)$ is temperature (γ is heat capacity per unit volume) or concentration (γ is unit) in case of heat or mass transfer, $k(u)$ is the thermal conductivity or mass diffusivity, \vec{r} is the position vector, t is the time and τ is a time lag connecting the flux \vec{q} with the gradient of u . Eq. (1) accounts for energy or mass conservation, while

Eq. (2) refers to a phenomenological transport law subject to a time relaxation process. The physical motivation of this approach is basically due to the need of overcoming the well-known “conduction paradox” [10,11], namely the onset of an unbounded propagation speed of a wave as an effect of a sudden perturbation of u in the embedding medium.

In one spatial dimension, a first-order Taylor expansion of (2) transforms the aforementioned system into:

$$\gamma \frac{\partial u(x, t)}{\partial t} + \frac{\partial q(x, t)}{\partial x} = 0 \quad (3)$$

$$\tau \frac{\partial q(x, t)}{\partial t} + q(x, t) = -k(u) \frac{\partial u(x, t)}{\partial x} \quad (4)$$

Combining (3) and (4) and eliminating q , we get the non-linear Maxwell–Cattaneo equation:

$$\frac{\partial u}{\partial t} + \tau \frac{\partial^2 u}{\partial t^2} = \frac{1}{\gamma} \frac{\partial}{\partial x} \left[k(u) \frac{\partial u}{\partial x} \right] \quad (5)$$

Eq. (5) with constant k was extensively studied in statistical physics to model inertial effects in particle walks where there is a preference for the walker to continue the prior direction of motion [12,13]. The Maxwell–Cattaneo equation allows to interpret systematic deviations from the classical heat diffusion approach in many experimental cases where τ assumes surprisingly high values as in biological tissues, polymeric and inhomogeneous materials [14,15]. In particular, the relaxation time for the mass flux is a crucial parameter as it triggers an onset of discontinuities in polymers structure [16]. Moreover, strong discrepancies between parabolic

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Nomenclature

$F_{1,2}$	dimensionless characteristic velocity.
$G_{1,2}$	dimensionless factors in characteristic equations
$H_{1,2}$	dimensionless factors in characteristic equations
I_1	modified Bessel function of the first kind
k	thermal conductivity (W/m K) or mass diffusivity (m^2/s)
k_0	reference thermal conductivity (W/m K) or reference mass diffusivity (m^2/s)
k^*	dimensionless temperature or concentration θ -dependent function
q	heat flux ($\text{J}/\text{m}^2 \text{s}$) or mass flux ($\text{mol}/\text{m}^2 \text{s}$)
Q	dimensionless heat or mass flux
r	space variable vector (m)
R	vector of dependent variables in the p -system
t	time (s)
T	vector of dependent variables in the p -system
u	temperature (K) or concentration (mol/m^3)
u_0	initial temperature (K) or concentration (mol/m^3)
u_1	wall temperature (K) or concentration (mol/m^3)
U	wave speed (m/s)
w	local dimensionless wave speed
w_0	reference wave speed
x	space variable (m)

Greek symbols

β	dimensionless parameter modelling the θ -dependence in $k^*(\theta)$
γ	heat capacity per unit volume ($\text{J}/\text{m}^3 \text{K}$) or unit in mass transport
η	dimensionless space variable
θ	dimensionless temperature or concentration
v	vector of dependent variables in the p -system
ξ	dimensionless time
τ	relaxation time (s)
Ω	heaviside unit step function

Subscripts

r	rightward
l	leftward

Superscripts

+	value of a generic variable at the front wave
–	value of a generic variable behind the front wave

and hyperbolic heat and mass transfer models were observed during drying processes of thin layers at high energy surface flux [17,18].

From a computational point of view, common efforts are directed to overcome convergence and stability problems in the neighbourhood of the travelling discontinuities [19]. To this purpose, several finite difference techniques rely upon the use of the MacCormack predictor–corrector scheme both in linear and non-linear diffusion models [20,21]. High resolution schemes combine high-order discretizations and oscillation-free techniques, as in the total-variation diminishing flux-limited methods (TVD), where a feedback mechanism extracts information from the approximate solution and uses this information to ascertain where in the solution domain the accuracy can be improved [22]. In this context, very promising results have been obtained using Van Leer's monotone upstream scheme for conservation laws (MUSCL) [23,24]. However, TVD schemes have a crucial drawback in that they degenerate to a lower order at the extrema of the solution [25]. Compact finite differences [26] are reminiscent of spectral methods, where the approximation to a derivative at one grid point involves all the nodal values. However, the presence of discontinuities between initial and boundary conditions produces spurious numerical results in spectral methods provided a proper regularizing technique is adopted. These oscillations, the Gibbs phenomena, may not even decay in magnitude by mesh refining in non-linear problems. The same drawback is suffered by the most recent non-standard finite difference (NSFD) techniques [27].

In this work, we use the Hartree hybrid method to numerically solve Eq. (3) where $k(u)$ depends on a parameter accounting for interactions between diffusing species [28] or modelling different responses of substrate to thermal transport in case of mass or heat transfer, respectively. This choice is also motivated by the need of clarifying some controversial aspects of diffusion in case of attractive interactions [29], namely when $dk/du < 0$. The paper is divided as follows. In Section 2, we outline the essentials of the numerical method here adopted. In Section 3, we discuss the results and we compare the solution with the ones presented in previous studies. In Section 4, we motivate our numerical results using an analytical approach based on the singular or discontinuity surface theory [30]. Finally, in Section 5 we draw the conclusions.

2. Model and algorithm

It is convenient, in order to compare our results with the ones presented in other works [21,29,31], to write the system of Eqs. (3) and (4) in a dimensionless form. We assume that:

$$u(\infty, t) = u_0; \quad u(0, t) = u_1$$

$$\eta = \frac{x}{2(\tau k_0/\gamma)^{1/2}}; \quad \xi = \frac{t}{2\tau}; \quad Q = \frac{q}{(u_1 - u_0)(\gamma k_0/\tau)^{1/2}}; \quad \theta = \frac{u - u_0}{u_1 - u_0} \quad (6)$$

The thermal conductivity or mass diffusivity is expressed as:

$$k(u) = k_0 k^*(u) \quad (7)$$

where k_0 is a reference value of k and $k^*(u)$ is an arbitrary function of u which, in terms of θ , will be chosen in the following according to a specific expression of linear or non-linear θ -dependence, that is $k^*(\theta) = 1 + \beta\theta$ or $k^*(\theta) = e^{\beta\theta}$. It should be noted that, in case of linear approximation, $\beta < 0$ for many substances [32].

Whatever the expression of $k^*(\beta, \theta)$, the condition

$$k^*(\beta = 0, \theta) = 1 \quad (8)$$

must be fulfilled to ensure that, in the absence of interactions, k tends to the reference value k_0 typical of the linear case.

From (3), (4), (6) and (7), we get:

$$\frac{\partial \theta}{\partial \xi} + \frac{\partial Q}{\partial \eta} = 0$$

$$\frac{\partial Q}{\partial \xi} + k^*(\theta) \frac{\partial \theta}{\partial \eta} + 2Q = 0 \quad (9)$$

If we consider a diffusion process in a semi-infinite medium with a sudden change in the wall temperature or concentration, the initial and boundary conditions for all the present simulations are taken as:

$$\theta(\eta, 0) = 0 \quad \eta > 0$$

$$Q(\eta, 0) = 0 \quad \eta > 0 \quad (10)$$

$$\theta(0, \xi) = 1$$

We recall now briefly some features of the Hartree hybrid method here adopted, which uses a combination of finite differences with the method of characteristics [33].

From (9), we derive the expressions of the two families of characteristic curves $F_1(\theta)$ and $F_2(\theta)$, namely:

$$\frac{\partial \eta}{\partial \xi} \Big|_1 = F_1(\theta) = \sqrt{k^*(\theta)}; \quad \frac{\partial \eta}{\partial \xi} \Big|_2 = F_2(\theta) = -\sqrt{k^*(\theta)} \quad (11)$$

Along the characteristics, the solution of system (9) must satisfy the following conditions:

$$\begin{aligned} dQ + G_1 d\theta + H_1 d\xi &= 0 \\ dQ + G_2 d\theta + H_2 d\xi &= 0 \end{aligned} \quad (12)$$

where

$$G_{1,2} = F_{1,2} \pm \sqrt{k^*(\theta)}; \quad H_{1,2} = 2Q \quad (13)$$

From a Taylor expansion of Eq. (9) and assuming that points P and S belong to the characteristic curves F_1 and F_2 respectively, we can write:

$$\begin{aligned} \eta_D - \eta_P &= \frac{1}{2} [F_1(D) + F_1(P)] \Delta \xi \\ \eta_D - \eta_S &= \frac{1}{2} [F_2(D) + F_2(S)] \Delta \xi \\ Q_D - Q_P + \frac{1}{2} [G_1(D) + G_1(P)] (\theta_D - \theta_P) + \frac{1}{2} [H_1(D) + H_1(P)] \Delta \xi &= 0 \\ Q_D - Q_S + \frac{1}{2} [G_2(D) + G_2(S)] (\theta_D - \theta_S) + \frac{1}{2} [H_2(D) + H_2(S)] \Delta \xi &= 0 \end{aligned} \quad (14)$$

In Fig. 1, a point A with coordinates $(i\Delta\eta, j\Delta\xi)$ belongs to a line where the solution is supposed to be determined. The solution at the point D on the line corresponding to the following time step $(j+1)\Delta\xi$ can be found by iterative solution of the previous system in the unknowns $\eta_P, \eta_S, \theta_P, \theta_S$. The values of $\theta_P, \theta_S, Q_P, Q_S$ are guessed at the beginning of the iterative cycle and are sequentially updated by interpolation once the η -coordinate of the points P and S are determined. Many interpolation strategies can be adopted; among them, the upwind-downwind schemes proved to be the most reliable trade-off between accuracy and stability. On the opposite, the Lagrange schemes do not allow to avoid the onset of spurious oscillations. In its essence, the method requires the solution of a non-linear algebraic system with four unknowns at each grid point. This scheme has a second-order truncation error and it is more accurate, though more time consuming, than the simpler Courant–Isaacson–Rees discretization technique [33].

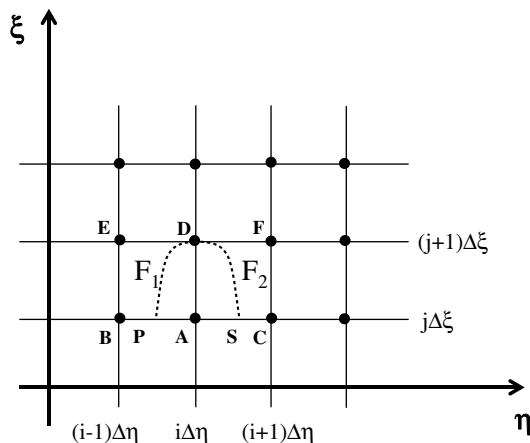


Fig. 1. Scheme of the discretization technique adopted by the Hartree hybrid method.

3. Results and discussion

In Fig. 2, we have tested the previously described method in case of constant diffusivity k^* . In this case, the analytical solution of (9) with boundary an initial conditions (10) and $k^*(\theta) = 1 + \beta\theta$ with $\beta = 0$ is the following [34,35]:

$$\theta(\eta, \xi) = \Omega(\xi - \eta) \left[e^{-\eta} + \eta \int_{\eta}^{\xi} e^{-z} \frac{I_1(\sqrt{z^2 - \eta^2})}{\sqrt{z^2 - \eta^2}} dz \right] \quad (15)$$

where $\Omega(\xi - \eta)$ is the Heaviside unit step function and I_1 is the modified Bessel function of the first kind. The dashed line corresponds to the solution calculated according to (15), while the solid one has been numerically obtained by the Hartree hybrid method. A satisfactory agreement is obtained for different values of the dimensionless time despite the absence of regularizing or damping criteria aiming at smoothing the oscillations in the vicinity of the wave front.

In Figs. 3 and 4, we have reported the solution θ versus the space variable with $k^*(\theta) = 1 + \beta\theta$ for a single fixed value of $\beta < 0$ and $\beta > 0$, respectively. Firstly, we observe that the advancing part of the travelling wave for $\beta < 0$ seems to behave as in the linear case. Besides, the front slope is a decreasing function of time and it has a trend consistent with the one of a discontinuity wave. By the way, Glass et al. [21] considered an analogous situation for weaker attractive interactions ($\beta = -0.25$) and concluded that the local speed of the leading portion was not significantly different from that of the $\beta = 0$ wave. The case for $\beta > 0$, as visualized in Fig. 4, is characterized by the presence of a steep profile, highly suggestive of a shock wave, keeping its verticality for all times and moving with a higher speed with respect to the linear case.

Heuristically, the onset of a discontinuity wave or a genuine shock wave for attractive ($dk^*/d\theta < 0$) or repulsive ($dk^*/d\theta > 0$) interactions can be visualized in Fig. 5. For $dk^*/d\theta < 0$, the profile close to the point A tends to diffuse with a lower speed than the one located at the point B , namely: $\theta_A > \theta_B \rightarrow k_A^* < k_B^* \rightarrow w_A < w_B$, where $w = w_0 \sqrt{k^*(\theta)}$ is the local wave speed [21]. An opposite situation occurs for $dk^*/d\theta > 0$, where the same starting configuration evolves producing a vertical profile between A and B with the onset of a shock wave. In the following paragraph, we will explain with a more rigorous discussion that, for $dk^*/d\theta < 0$, we cannot have a shock wave but only a discontinuity wave travelling at a speed independent of the tuning parameter β .

In Fig. 6, we report some profiles of θ versus η at constant ξ for several values of $\beta < 0$. It can be seen that the penetration distance of the wave front does not vary for different values of β , including

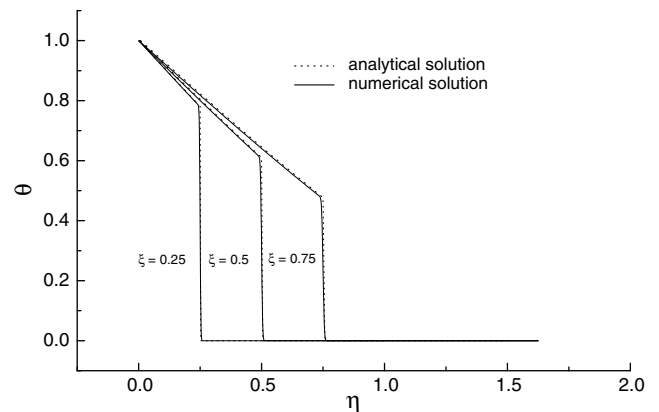


Fig. 2. Solid line: Plot of the solution θ versus the space variable η at three different times ξ for $\beta = 0$. Dashed line: plot of the analytic solution obtained by Eq. (15). $\Delta \xi = 2.5 \times 10^{-4}$; $\Delta \eta = 1. \times 10^{-4}$.

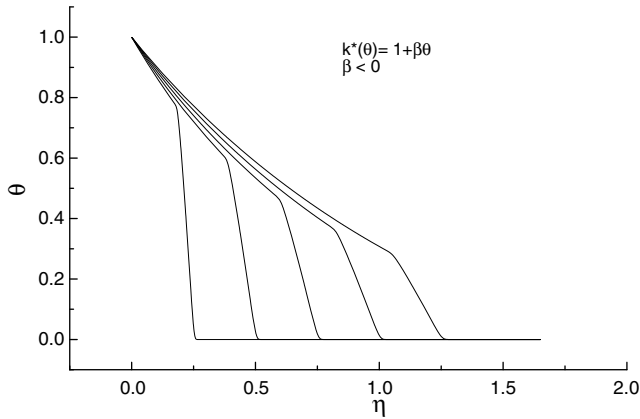


Fig. 3. Plot of the solution θ versus the space variable η at different times $\zeta = 0.25; 0.5; 0.75; 1.0; 1.25$ for $k^*(\theta) = 1 + \beta\theta$ and $\beta = -0.5$. $\Delta\zeta$ and $\Delta\eta$ as in Fig. 2.

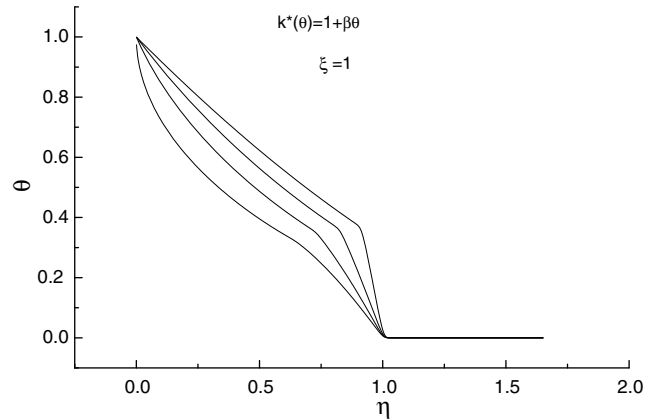


Fig. 6. Plot of the solution θ versus the space variable η at fixed time. From left to right, $\beta = -1; -0.75; -0.5; -0.25$. $\Delta\zeta$ and $\Delta\eta$ as in Fig. 2.

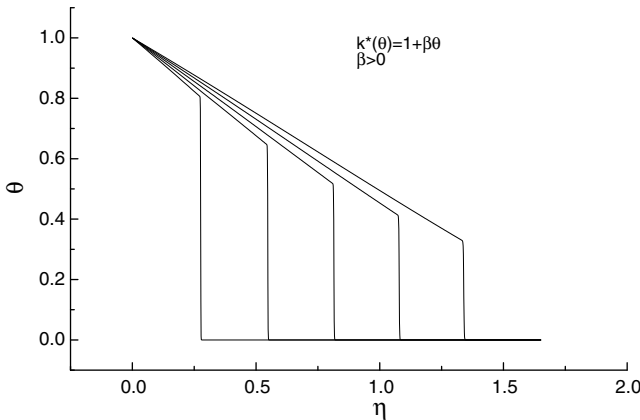


Fig. 4. Plot of the solution θ versus the space variable η at different times $\zeta = 0.25; 0.5; 0.75; 1.0; 1.25$ for $k^*(\theta) = 1 + \beta\theta$ and $\beta = 0.5$. $\Delta\zeta$ and $\Delta\eta$ as in Fig. 2.

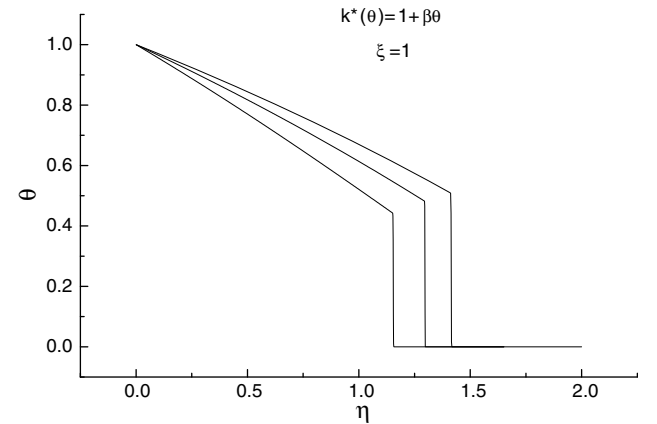


Fig. 7. Plot of the solution θ versus the space variable η at fixed time. From left to right, $\beta = 1; 2; 3$. $\Delta\zeta$ and $\Delta\eta$ as in Fig. 2.

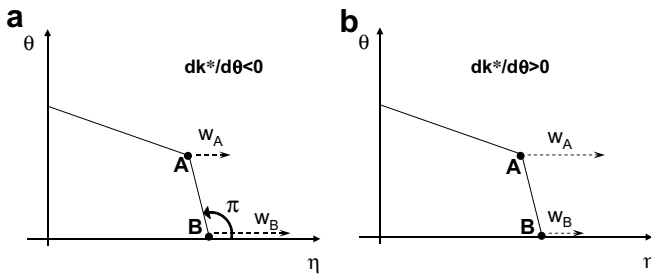


Fig. 5. Sketch of two different situations for an initial profile evolution in case of $dk^*/d\theta < 0$ (panel (a)) and $dk^*/d\theta > 0$ (panel (b)). In panel (a), the angle π tends to increase at the following time step, while in panel (b) the line joining the points A and B evolves towards a vertical configuration typical of a shock wave.

$\beta = -0.25$. As previously stated, this result is consistent with Glass et al. study [21], but it is in contrast with the more recent observations of Liu [29]. Liu investigated a case of thermal diffusion governed by the same equations here adopted and criticized the previous papers of Glass et al. and of Chen and Lin [31] explicitly claiming that the penetration distance of a thermal wave for $\beta = -0.25$ at fixed $\zeta = 1$ should be different from that of $\beta = 0$.

As in Fig. 6, the plots of Fig. 7 are realized at constant time for several values of $\beta > 0$. The distance travelled by the advancing front is now clearly an increasing function of β . As generally pointed out in analogous studies, the cases for $\beta > 0$ are highly cru-

cial for many numerical methods owing to the appearance of numerical instabilities and oscillations in the vicinity of the moving front. It should be noted that this method is not affected by the aforementioned spurious results even for high values of β .

Besides, to further motivate our last observations, we have also plotted the solution of system (9) subject to (10) in Fig. 8 using an exponential expression $k^*(\theta) = e^{\beta\theta}$ that Liu proposed in order to test

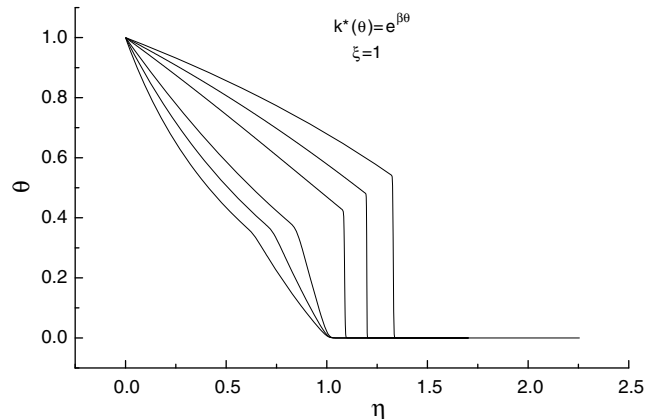


Fig. 8. Plot of the solution θ versus the space variable η at fixed time for $k^*(\theta) = e^{\beta\theta}$. From left to right, $\beta = -1.5; -1; -0.5; 0.5; 1; 1.5$. $\Delta\zeta$ and $\Delta\eta$ as in Fig. 2.

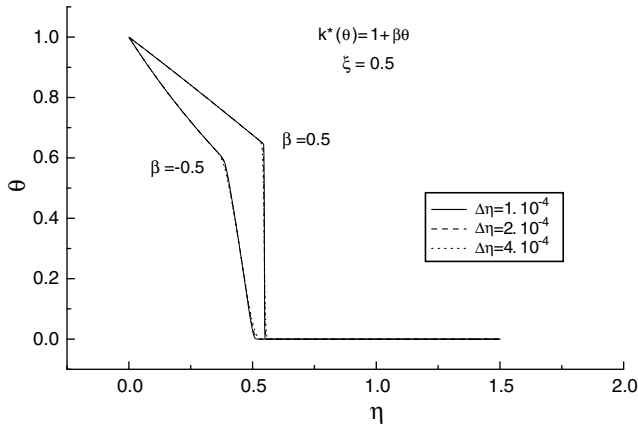


Fig. 9. Effect of discretization on the solution θ for different values of β when $k^*(\theta) = 1 + \beta\theta$. $\Delta\xi$ as in Fig. 2.

the reliability of his method in case of strong non-linearities. No numerical oscillation is produced by the present method for all choices of β and, in particular, for those values of β giving slightly spurious results with the Laplace transform method of Liu [29].

Finally, in Fig. 9 we show the independence of our results with respect to the discretization. The data collapse onto a single curve for decreasing values of $\Delta\eta$.

4. An analytical approach to the problem

We transform system (9) into the following form to better visualize its belonging to the class of the inhomogeneous p -systems [36]:

$$\frac{\partial \mathbf{v}}{\partial \xi} + \frac{\partial}{\partial \eta} R(\mathbf{v}) = T(\mathbf{v}); \quad \mathbf{v} = \begin{Bmatrix} \theta \\ Q \end{Bmatrix}; \quad R = \begin{Bmatrix} Q \\ \int_0^\eta k^*(z) dz \end{Bmatrix}; \quad T = \begin{Bmatrix} 0 \\ -2Q \end{Bmatrix} \quad (16)$$

Eq. (11) gives the characteristic velocities related to Eq. (16). In the following, we will consider only the expression $F_1 = \sqrt{k^*(\theta)}$, as we treat rightwards moving waves. The Lax entropy conditions to be fulfilled in order to have a shock [36] travelling with velocity U are:

$$F_1(\theta_r) < U < F_1(\theta_l) \quad (17)$$

where the subscripts “r” and “l” stay for “rightward” and “leftward” respectively. Remembering that the wave moves towards the unperturbed zone where $\theta_r = 0 < \theta_l$ and considering a general function $k^*(\beta, \theta)$, we notice that the aforementioned inequality cannot be fulfilled when $\frac{\partial k^*}{\partial \theta} < 0$.

Besides, taking into account that, in a p -system with a linear inhomogeneous term T , only genuine shocks or discontinuity (acceleration) waves are allowed [37], we deduce that only discontinuity waves may exist for $k^*(\theta) = 1 + \beta\theta$ or $k^*(\theta) = e^{\beta\theta}$ when $\beta < 0$. These waves are also known as “temperature-rate waves” in case of heat transfer [38].

To quantitatively motivate the previous numerical results for $\beta < 0$, we will recall briefly here some features of the singular surface analysis, a technique successfully used by Jordan et al. in dealing with travelling perturbations in hyperbolic systems [39,40].

We will let F^+ and F^- denote the values of a generic variable, F , ahead of and behind, respectively, the wavefront $\Sigma(\xi)$, which is advancing in the positive η -direction. The amplitude $[F]$ of the jump in the function $F(\xi, \eta)$ across the wave is:

$$[F] = [F^-] - [F^+] \quad (18)$$

According to Hadamard’s lemma [39], where the subscript k in F_k refers to the derivative of F with respect to k , we have:

$$\frac{d[F]}{d\xi} = [F_\xi] + U[F_\eta] \quad (19)$$

In a discontinuity wave, θ and Q are continuous functions across Σ while θ_ξ , θ_η , Q_ξ and Q_η are not. Therefore,

$$[\theta] = 0 \quad \forall \xi \rightarrow \frac{d[\theta]}{d\xi} = 0 \quad (20)$$

$$[Q] = 0 \quad \forall \xi \rightarrow \frac{d[Q]}{d\xi} = 0 \quad (21)$$

Combining Eqs. (19)–(21) we obtain:

$$[\theta_\xi] + U[\theta_\eta] = 0 \quad (22)$$

$$[Q_\xi] + U[Q_\eta] = 0 \quad (23)$$

Applying the operator $[\]$ to both sides of equations in system (9), we get:

$$[\theta_\xi] + [Q_\eta] = 0 \quad (24)$$

$$[Q_\xi] + [k^*(\theta)\theta_\eta] + 2[Q] = 0 \quad (25)$$

The jump of a product is now developed according to the Lindsay and Straughan jump rule [41], namely:

$$[k^*(\theta)\theta_\eta] = k^*(\theta)^+[\theta_\eta] + \theta_\eta^+[k^*(\theta)] + [k^*(\theta)][\theta_\eta] \quad (26)$$

Remembering that $k^*(\theta)^+ = k^*(\theta_r) = 1$ and $[k^*(\theta)] = 0$ for $k^*(\theta) = 1 + \beta\theta$ or $k^*(\theta) = e^{\beta\theta}$, we can write Eq. (25) in final form:

$$[Q_\xi] + [\theta_\eta] = 0 \quad (27)$$

The system of Eqs. (22)–(24) and (27), here better represented in matrix notation

$$\begin{pmatrix} 1 & U & 0 & 0 \\ 0 & 0 & 1 & U \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} [\theta_\xi] \\ [\theta_\eta] \\ [Q_\xi] \\ [Q_\eta] \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (28)$$

gives a solution provided the matrix of coefficients has $\det = 0$, whence $U = \pm 1$. Only the value $U = 1$ will be considered here, as we have $\Sigma(\xi)$ travelling in the positive η -direction.

Thus, we conclude that the discontinuity wave has a penetration depth independent of β , for $\beta < 0$, for all choices of $k^*(\beta, \theta)$ investigated by Liu [29]. This result motivates both our numerical results of Figs. 3, 6 and 8 and the ones of Glass et al. [21] and Chen and Lin [31], while it disagrees from Liu’s criticism.

We tried to apply the same approach to the case $\beta > 0$ in order to describe the shock waves, but our attempts were unfruitful. In fact, to the best of our knowledge, the singular surface analysis method does not allow one to obtain an ODE describing a genuine shock amplitude evolution in case of a non-linear hyperbolic system [42].

5. Conclusions

In this paper, we have presented a numerical solution of a hyperbolic non-linear telegrapher-type equation accounting for heat or mass diffusion when the diffusivity depends on temperature or concentration, respectively.

The most important results can be summarized in the following points:

- The Hartree hybrid method proved to be a satisfactory trade-off between computational simplicity and reliability of results. In fact, no numerical oscillations were found despite the absence of regularizing criteria, the presence of a discontinuity between initial and boundary conditions and in a wide range of the

parameter β tuning the expression of diffusivity. For these reasons, we could analyze stronger non-linearities with respect to the ones considered in previous works.

- From a methodological point of view, the paper gives a contribution to the discussion concerning the dynamics of a diffusion front in hyperbolic partial differential equations when the diffusivity is a decreasing function of the dependent variable. This case has been object of previous numerical investigations but the conclusions were, up to now, controversial. In this context, the singular surface theory allows to give some answers that the numerical methods cannot supply.

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