A Transmission Line Modelling (TLM) method for steady-state convection-diffusion

Alan Kennedy[1,*,†] and William J. O'Connor[2]

[1]*School of Mechanical and Manufacturing Engineering, Dublin City University, Glasnevin, Dublin 9, IRELAND*

[2]*Department of Mechanical Engineering, University College Dublin, Belfield, Dublin 4, Ireland*

SUMMARY

This paper describes how the lossy Transmission Line Modelling (TLM) method for diffusion can be extended to solve the convection-diffusion equation. The method is based on the correspondence between the convection-diffusion equation and the equation for the voltage on a lossy transmission line with properties varying exponentially over space. It is unconditionally stable and converges rapidly to highly accurate steady-state solutions for a wide range of Peclet numbers from low to high. The method solves the non-conservative form of the convection-diffusion equation but it is shown how it can be modified to solve the conservative form. Under transient conditions the TLM scheme exhibits significant numerical diffusion and numerical convection leading to poor accuracy, but both these errors go to zero as a solution approaches steady-state.

INTRODUCTION

Convection-diffusion (also called drift-diffusion or advection-diffusion) describes the situation where a diffusant (a chemical substance, heat, etc.) moves through space due to a combination of diffusion and transport phenomena. It arises, for example, in the modelling of semiconductors, in computational fluid dynamics (CFD), in systems with heat conduction and relative motion such as extrusion, and in air and groundwater transport of pollutants [1, 2]. This paper shows that, if the properties of a transmission line (TL) vary spatially in a specified way, the equation governing the voltage along the line under steady-state conditions is equivalent to the one-dimensional convection-diffusion equation. It demonstrates how the TLM method can be used to model such a transmission line. The accuracy of most alternative methods (including finite difference, finite volume, and finite element schemes) is significantly reduced when the cell Peclet number, Pe', is high (typically when $Pe' > 2$, where $Pe' = v\Delta x/D$, v being the convection velocity, D the diffusion coefficient, and Δx the node spacing) [1-3]. It will be shown below that this is not the case with the TLM method.

The simplest transmission line is just a pair of wires over which an electrical signal can be transmitted. A TL has distributed inductance and capacitance, and for that reason, a voltage applied to it at any point will cause voltage waves to propagate along it in both directions. The propagation velocity is dependent on the inductance and capacitance. In a numerical model of a TL the voltage is calculated at discrete points in both space (or "nodes") and in time. If the relationship between the propagation velocity and the space and time steps are such that signals leaving any node arrive at an adjacent node at the next time step, then the transmission line segments linking nodes can be treated simply as delay-lines of one time increment delay. The TLM method is an explicit time-domain scheme that, in one-dimension, keeps track of Dirac voltage pulses travelling to the left and to the right through a network of successive TL segments.

*Correspondence to: Alan Kennedy, School of Mechanical and Manufacturing Engineering, Dublin City University, Glasnevin, Dublin 9, IRELAND

†E-mail: alan.kennedy@dcu.ie

A lossy transmission line is a TL with resistance distributed along its length. The voltage on a uniform lossy line satisfies the Telegrapher's Equation [4, 5]

$$\frac{\partial V}{\partial t} = \frac{1}{R_d C_d}\frac{\partial^2 V}{\partial x^2} - \frac{L_d}{R_d}\frac{\partial^2 V}{\partial t^2} \tag{1}$$

where R_d, C_d, and L_d are the distributed resistance, capacitance, and inductance respectively. This is equivalent to the one-dimensional diffusion equation with one extra term (the third term in (1)). If this (wave-propagation) term is negligible then solving for the voltage on a lossy transmission line is equivalent to solving the diffusion equation [6-8]. This is the basis for the TLM method for modelling diffusion. It is unconditionally stable and has been successfully used to model both thermal and molecular diffusion problems [4, 9].

In lossy TLM a continuous transmission line is replaced by a network of discrete TL segments connected by lumped resistors. This network is then modelled exactly. Since it only contains passive components the method must be unconditionally stable [4]. It has been shown previously that the lossy TLM method can be extended to model the convection-diffusion equation through the inclusion of controlled current sources at each node [10] but the addition of these active components can lead to instability [4]. This paper shows how convection-diffusion can be modelled using a fully passive TL network.

It has been shown that, because it is stable with long time steps, lossy TLM can rapidly converge to a steady-state solution [11]. For any particular problem there exist optimum values for the TLM parameters that result in ultra-fast convergence. Too-long a time step leads to an increase in wave-like behaviour, thereby increasing the number of time steps required to reach steady-state.

THE METHOD

The differential equation governing the voltage on a lossy transmission line can be written as (see Appendix A)

$$\begin{aligned}\frac{\partial V}{\partial t} &= \frac{\partial}{\partial x}\left(\frac{1}{R_d(x)C_d(x)}\frac{\partial V}{\partial x}\right) - \frac{1}{R_d(x)}\frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right)\frac{\partial V}{\partial x} - \\ &\frac{L_d(x)}{R_d(x)}\frac{\partial^2 V}{\partial t^2} + \left[\frac{\partial}{\partial x}\left(\frac{L_d(x)}{R_d(x)C_d(x)}\right) - \frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right)\left(\frac{L_d(x)}{R_d(x)}\right)\right]\frac{\partial i}{\partial t}\end{aligned} \tag{2}$$

If the third and fourth terms are negligible this is equivalent to the non-conservative form of the convection-diffusion equation

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x}\right) - v\frac{\partial V}{\partial x} \tag{3}$$

if

$$D(x) = \frac{1}{R_d(x)C_d(x)} \tag{4}$$

and

$$v(x) = \frac{1}{R_d(x)}\frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right) = D(x)C_d(x)\frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right) \tag{5}$$

These conditions, Equations (4) and (5), can be expressed in terms of the Peclet number, *Pe*,

$$Pe(x) := \frac{v(x)}{D(x)} = C_d(x)\frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right) \tag{6}$$

This paper first considers the case where $Pe(x)$ is constant over space. A distributed capacitance given by

$$C_d(x) = c_1 \exp(-xPe + c_2) \tag{7}$$

where c_1 and c_2 are constants, will satisfy Equation (6). Combining Equations (4) and (7) then gives the required distributed resistance

$$R_d(x) = c_1^{-1} D(x)^{-1} \exp(xPe - c_2) \tag{8}$$

The propagation velocity on a transmission line is given by

$$u(x) = \frac{1}{\sqrt{L_d(x) C_d(x)}} \tag{9}$$

If the distributed inductance varies over space as

$$L_d(x) = c_3 \exp(xPe - c_2) \tag{10}$$

then $u(x)$ will be a constant

$$u = \frac{1}{\sqrt{c_3 c_1}} \tag{11}$$

If $L_d(x)$, $C_d(x)$, and $R_d(x)$ satisfy Equations (10), (7), and (8), then the fourth term in Equation (2) becomes

$$\left[\frac{\partial}{\partial x}\left(D(x) c_3 \exp(xPe - c_2)\right) - c_1 c_3 D(x) \frac{\partial}{\partial x}\left(c_1^{-1} \exp(xPe - c_2)\right) \right] \frac{\partial i}{\partial t} \tag{12}$$

which will equal zero if $D(x)$ is constant over space. This term will go to zero anyway as the voltage and current on the transmission line approach a steady-state.

Combining Equations (10) and (11) gives the distributed inductance in terms of u

$$L_d(x) = \frac{1}{c_1 u^2} \exp(xPe - c_2) \tag{13}$$

The impedance of a transmission line is

$$Z(x) = \sqrt{\frac{L_d(x)}{C_d(x)}} \tag{14}$$

Substituting for $L_d(x)$ and $C_d(x)$ using Equations (13) and (7) gives the impedance as

$$Z(x) = c_1^{-1} u^{-1} \exp(xPe - c_2) \tag{15}$$

Using Equations (8) and (13) to replace $R_d(x)$ and $L_d(x)$, the third term in Equation (2) can be rewritten in terms of $D(x)$ and u.

To summarise, if the properties of a non-uniform lossy transmission line vary according to Equations (10), (7), and (8), and if $Pe(x)$ and $D(x)$ (and, therefore, $v(x)$) are constant over space, then the propagation velocity will be constant along the line and the voltage will satisfy

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(D(x) \frac{\partial V}{\partial x} \right) - v(x) \frac{\partial V}{\partial x} - D(x) \frac{1}{u^2} \frac{\partial^2 V}{\partial t^2} \tag{16}$$

This is equivalent to the non-conservative form of the convection-diffusion equation (Equation (3)) with an added wave-propagation term that will go to zero as the voltage approaches a steady-state. The voltage on such a transmission line can be modelled using the TLM method, thus providing a numerical solution for Equation (16).

TRANSMISSION LINE MODELLING

In TLM the voltage on a transmission line is calculated at a series of nodes spaced Δx apart and at discrete time steps Δt apart. The non-uniform lossy transmission line between each pair of nodes is replaced by segments of uniform lossless (i.e. with zero resistance) transmission line of length $\Delta x/2$ separated by lumped resistors [4, 9]. Figure 1 illustrates two possible configurations, one in which the TL impedance and resistance values vary at the nodes and one in which they vary between nodes. Both represent “link-resistor” (LR) schemes since the elements are linked by resistors and the nodes are located between TL segments. Other, “link-line” (LL), configurations are possible [4, 12, 13] in which the nodes are located between resistors but this paper will only consider the configuration illustrated in Figure 1a.

A segment of lossless transmission line of length $\Delta x/2$ acts essentially as a delay line so that a voltage wave incident at one end will arrive at the other end $\Delta t/2$ later where Δx and Δt are related by the propagation velocity, $u = \Delta x/\Delta t$ [4]. The TLM method keeps track of Dirac voltage pulses (and associated current pulses) that pass through the network, each travelling a distance Δx during every time step. The method is initialised with incident pulses at each node, one from the left (denoted *Vil*) and one from the right (denoted *Vir*). These lead to voltages at the nodes (denoted *Vn*), the distribution of which, over space and time, represents the discretised solution of the PDE under consideration. The differences between these node voltages and the incident pulses lead instantaneously to pulses being scattered from the nodes, one to the left (*Vsl*) and one to the right (*Vsr*). The presence of resistors means that any pulse leaving a node at time step k meets an impedance discontinuity $\Delta t/2$ later. This leads to a fraction (τ, the “transmission coefficient”) of the pulse being transmitted onwards, arriving at the next node a further $\Delta t/2$ later (i.e. at time step k+1). The remaining fraction ($\rho = 1 - \tau$) of the pulse is reflected back, arriving at the node from which it originated, also at time step k+1. This process is repeated with these new incident pulses being used to calculate the node voltages at time step k+1 and so on.

The incident pulses arriving at nodes n and n+1 at time step k are illustrated in Figure 2a. Two rules can be used to calculate the resulting node voltages. The first rule is that, at the instant of scattering, the node voltage at any node is the sum of the incident and scattered pulses on each line connected to that node, so, for node n,

$$ {}_kVn_n = {}_kVil_n + {}_kVsl_n = {}_kVir_n + {}_kVsr_n \tag{17} $$

The second rule is that the current associated with the incident voltage pulses at node n must equal the current associated with the voltage pulses scattered from that node. Since the current impulse in a given direction is simply the corresponding voltage impulse travelling in that direction divided by the TL impedance

$$ \frac{{}_kVil_n}{Z_n} + \frac{{}_kVir_n}{Z_{n+1}} = \frac{{}_kVsl_n}{Z_n} + \frac{{}_kVsr_n}{Z_{n+1}} \tag{18} $$

Combining Equations (17) and (18) gives the node voltage in terms of the incident voltage pulses

$$ {}_kVn_n = \frac{2{}_kVil_n + 2P_n{}_kVir_n}{1 + P_n} \tag{19} $$

where P_n is the impedance ratio at node n defined by

$$ P_n = \frac{Z_n}{Z_{n+1}} \tag{20} $$

The scattered pulses (see Figure 2b) are, from Equation (17),

$$ {}_kVsl_n = {}_kVn_n - {}_kVil_n \tag{21} $$

$$ {}_kVsr_n = {}_kVn_n - {}_kVir_n \tag{22} $$

Each incident voltage pulse at node n at time step k+1 is the sum of the transmitted fraction of a pulse scattered from an adjacent node at time step k and the reflected fraction of a pulse scattered from the same node n, also at time step k (see Figure 2c), so

$$ {}_{k+1}Vir_n = \rho_{n+1}\, {}_kVsr_n + \tau_{n+1}\, {}_kVsl_{n+1} \tag{23} $$

and

$$ {}_{k+1}Vil_n = \rho_n\, {}_kVsl_n + \tau_n\, {}_kVsr_{n-1} \tag{24} $$

where τ_n is the transmission coefficient for the line connecting nodes n–1 and n and where $\rho_n = 1-\tau_n$. These incident voltages can be used to calculate the node voltage for time step k+1 and the scattered pulses and so the procedure can be repeated. It is clear that the TLM method is straightforward to implement and is a fully explicit time-domain scheme.

Impedance ratio

To calculate the node voltages the impedance ratios must be known. For node n, P_n is the ratio of the impedances of the connecting lines (i.e. lines connecting pairs of nodes) to the left and to the right. Let x_n be the location of node n so $x_n + \Delta x$ is the location of node n+1. The impedance of the connecting line TL segments linking these nodes, Z_{n+1}, is the average impedance of the equivalent segment of the non-uniform lossy transmission line with $Z(x)$ varying according to Equation (15). If $Pe(x)$ is constant then

$$ Z_{n+1} = \frac{1}{\Delta x}\int_{x_n}^{x_n+\Delta x} u^{-1}c_1^{-1}\exp\left(xPe - c_2\right)dx = u^{-1}c_1^{-1}\frac{\left(\exp\left(\Delta xPe\right)-1\right)\exp\left(x_nPe\right)}{Pe\Delta x\exp\left(c_2\right)} \tag{25} $$

or

$$ Z_{n+1} = c_4\exp\left(x_nPe\right) \tag{26} $$

where

$$ c_4 = u^{-1}c_1^{-1}\frac{\left(\exp\left(\Delta xPe\right)-1\right)}{Pe\Delta x\exp\left(c_2\right)} \tag{27} $$

The impedance of the connecting line TL segments to the left of node n is

$$ Z_n = c_4\exp\left(\left(x_n - \Delta x\right)Pe\right) \tag{28} $$

if c_4 is constant over space (which it will be if $Pe(x)$ and Δx are constant). Now $P_n = Z_n/Z_{n+1}$ so

$$ P_n = \frac{c_4\exp\left(\left(x_n - \Delta x\right)Pe\right)}{c_4\exp\left(x_nPe\right)} \tag{29} $$

which simplifies to

$$ P_n = \exp\left(-\Delta xPe\right) = \exp\left(-Pe'\right) \tag{30} $$

where Pe' is the dimensionless cell Peclet number, $Pe' = v'/D'$, D' being the dimensionless cell diffusion coefficient (or diffusion number), $D' = D\Delta t/\Delta x^2$, and v' being the dimensionless cell convection velocity (or convection number), $v' = v\Delta t/\Delta x$.

It is clear from Equation (30) that the impedance ratio is less than 1 for positive v values and greater than one for negative v values. This is physically reasonable since if $Z_{n+1} < Z_n$ for all nodes then the current scattered from each node to the right will be greater than that scattered to the left. The current in a TLM diffusion model is equivalent to diffusant flux [4] but there is no such straightforward equivalence with the convection-diffusion models described here.

Transmission coefficients

The transmission coefficient for a connecting line composed of two TL segments of impedance Z separated by two resistors of resistance R is [4]

$$\tau_{ZRRZ} = Z/(Z+R) \tag{31}$$

The transmission coefficient for the connecting line linking nodes n and n+1, τ_{n+1}, is therefore

$$\tau_{n+1} = Z_{n+1}/(Z_{n+1}+R_{n+1}) \tag{32}$$

where Z_{n+1} is the impedance of the TL segments and R_{n+1} is half the resistance of the connecting line. If the distributed resistance varies according to Equation (8) then half the resistance of the connecting line is

$$R_{n+1} = \frac{1}{2}\int_{x_n}^{x_n+\Delta x} R_d(x)dx = \frac{\exp(x_n Pe)(\exp(\Delta x Pe)-1)}{2c_1 PeD\exp(c_2)} = \frac{c_4 u\Delta x}{2D}\exp(x_n Pe) \tag{33}$$

Substituting for Z_{n+1} and R_{n+1} in Equation (32) using Equations (26) and (33) gives

$$\tau_{n+1} = \frac{c_4\exp(x_n Pe)}{c_4\exp(x_n Pe)+\dfrac{c_4 uPe\Delta x}{2D}\exp(x_n Pe)} = \frac{1}{1+\dfrac{u\Delta x}{2D}} \tag{34}$$

Since $u = \Delta x/\Delta t$ this can be rewritten as

$$\tau_{n+1} = \frac{2D\Delta t\Delta x^{-2}}{2D\Delta t\Delta x^{-2}+1} = \frac{2D'}{2D'+1} \tag{35}$$

The transmission coefficient will be the same for all connecting lines if D is constant over space. Since the impedance and resistance must be positive then, from Equation (32), all τ values must be between 0 and 1. From Equation (35) the only limit on D is, therefore, $D > 0$.

Initialisation

For any particular problem, the closer the initial node voltages are to the steady-state solution, the fewer the time steps that will be required. It is not possible to start the TLM method simply by setting the initial node voltages since, to allow the algorithm to advance, incident pulse values are required to calculate scattered pulses. It is, therefore, necessary to initialise the scheme by setting the incident pulse values in such a way as to produce the desired initial node voltages. It is standard practice in lossy TLM modelling to set the two initial pulses at each node to half the desired node voltage [4], i.e.

$$_0Vil_n + {_0Vir_n} = \tfrac{1}{2}\,{_0Vn_n} \tag{36}$$

Boundary conditions

This section shows how a Dirichlet boundary condition can be implemented. The standard method for implementing a constant boundary voltage for a link-resistor diffusion model (equivalent to a convection-diffusion model but with v = 0) is illustrated in Figure 3a [4]. To set the voltage at the boundary to a value V_C, a voltage source is connected as shown. The incident voltage from the left at time step k+1 is then

$$_{k+1}Vil_1 = \tau V_C + (1-2\tau)\,{_kVsl_1} \tag{37}$$

The same method can be used to impose a concentration at a boundary in a convection-diffusion model. The boundary is located between nodes in this scheme and hence it is referred to here as the element boundary method.

The impedance of the single TL segment to the left of node 1 in Figure 3a, Z_1, must equal the average of $Z(x)$ between x_1–½Δx and x_1. The impedance Z_2 is the average of $Z(x)$ between x_1 and

x_1+Δx. If $v(x)$ and $D(x)$ are both constant over space (i.e. if $Z(x)$ is given by Equation (15)), the impedance ratio at node 1, $P_1 = Z_1/Z_2$, is

$$P_1 = \left[2 - 2\exp\left(-\tfrac{1}{2}Pe'\right)\right] / \left[\exp\left(Pe'\right) - 1\right] \tag{38}$$

Similarly the impedance ratio at node N with a boundary ½Δx to the right of the node is

$$P_N = \left[\tfrac{1}{2} - \tfrac{1}{2}\exp\left(-Pe'\right)\right] / \left[\exp\left(\tfrac{1}{2}Pe'\right) - 1\right] \tag{39}$$

In the node boundary method the boundary corresponds with a node but the transmission line extends beyond the boundary (as shown in Figure 3b) and is terminated with an open circuit. An open circuit termination means that the voltage pulses scattered towards to the boundary are reflected back so

$$_{k+1}Vil_1 = {}_kVsl_1 \tag{40}$$

and the current source provides a current so as to ensure that

$$_kVn_1 = V_C \tag{41}$$

The method then proceeds as before. Note that it is not necessary to know the transmission coefficient for the line beyond the boundary or the impedance ratio for the boundary node.

Testing has shown that the choice of boundary implementation has no significant effect on the rate of convergence of the method or on the accuracy of the solution obtained.

TESTING

The steady-state solution of the convection-diffusion equation

$$\frac{\partial V}{\partial t} = D\frac{\partial^2 V}{\partial x^2} - v\frac{\partial V}{\partial x} \tag{42}$$

with boundary conditions $V(0,t) = 0$ and $V(\lambda,t) = 100$ is [14]

$$V(x,\infty) = 100\frac{\exp(xPe) - 1}{\exp(\lambda Pe) - 1} \tag{43}$$

If D and v are both constant over space then so will be the impedance ratio, P_n, and the transmission coefficient τ_n. A model with N = 21 nodes, Δx = 1, boundary conditions $_kVn_1 = 0$ and $_kVn_N = 100$ implemented using the node boundary method, and initial node voltages $_0Vn_n = 100(n-1)/(N-1)$, was tested and the results after 5000 time steps compared with the analytical solution given by Equation (43) (see Figure 4). The relative errors (defined at node n as $(V(x_n,\infty) - {}_{5000}Vn_n)/V(x_n,\infty)$ where x_n is the location of node n) are consistently of the same order as the computer storage precision. The method, like the TLM method for diffusion, is unconditionally stable. It is highly accurate and produces physically consistent results even for high cell Peclet numbers. The accuracy of the results obtained is not significantly affected by the number of nodes used (see Figure 5). If the upwind boundary voltage is higher than that at the downwind boundary then instability can occur with high Pe' and v' values, but testing has shown that this is a result of round-off errors and is not inherent in the method.

The results shown above are for D and v constant over space. Now v is made variable. Using symbolic maths software, the steady-state solution for the non-conservative form of the convection-diffusion equation

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial V}{\partial x}\right) - v(x)\frac{\partial V}{\partial x} \tag{44}$$

with $D(x)$ constant , $v(x) = a + bx$, $V(0,t) = 0$, and $V(\lambda,t) = 100$ is found to be

$$V(x,\infty)=100\frac{\operatorname{erf}\left((a+bx)D^{-1}(-2b/D)^{-\frac{1}{2}}\right)-\operatorname{erf}\left(aD^{-1}(-2b/D)^{-\frac{1}{2}}\right)}{\operatorname{erf}\left((a+b\lambda)D^{-1}(-2b/D)^{-\frac{1}{2}}\right)-\operatorname{erf}\left(aD^{-1}(-2b/D)^{-\frac{1}{2}}\right)} \tag{45}$$

With $D(x)$ constant and $v(x) = a + bx$ Equation (6) becomes

$$\frac{a+bx}{D}=C_d(x)\frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right) \tag{46}$$

which can be solved giving

$$C_d(x)=c_5\exp\left(\frac{-x(2a+bx)}{2D}\right) \tag{47}$$

where c_5 is a constant. Combining Equations (4) and (47) gives an equation for the distributed resistance

$$R_d(x)=(c_5D)^{-1}\exp\left(\frac{x(2a+bx)}{2D}\right) \tag{48}$$

Combining Equations (9) and (14) and replacing the propagation velocity, u, with $\Delta x/\Delta t$ gives

$$Z(x)=\frac{\Delta t}{\Delta x C_d(x)} \tag{49}$$

or, in this case,

$$Z(x)=\frac{\Delta t}{\Delta x}c_5^{-1}\exp\left(\frac{x(2a+bx)}{2D}\right) \tag{50}$$

The impedance of the connecting line joining nodes n and n+1, Z_{n+1}, is the average impedance of the non-uniform lossy transmission line between x_n and $x_n + \Delta x$

$$Z_{n+1}=\frac{1}{\Delta x}\int_{x_n}^{x_n+\Delta x}Z(x)dx \tag{51}$$

Substituting for $Z(x)$ using Equation (50) and integrating gives

$$Z_{n+1}=\frac{\Delta t}{\Delta x^2}c_5^{-1}\exp\left(-\frac{a^2}{2Db}\right)\sqrt{-\pi\frac{D}{2b}}\left(\operatorname{erf}\left(\frac{a+bx_n}{\sqrt{-2bD}}\right)-\operatorname{erf}\left(\frac{a+b(x_n+\Delta x)}{\sqrt{-2bD}}\right)\right) \tag{52}$$

Similarly the impedance for the line connecting nodes $n-1$ and n is

$$Z_n=\frac{\Delta t}{\Delta x^2}c_5^{-1}\exp\left(-\frac{a^2}{2Db}\right)\sqrt{-\pi\frac{D}{2b}}\left(\operatorname{erf}\left(\frac{a+b(x_n-\Delta x)}{\sqrt{-2bD}}\right)-\operatorname{erf}\left(\frac{a+bx_n}{\sqrt{-2bD}}\right)\right) \tag{53}$$

and so the impedance ratio at node n is, on substituting for Z_n and Z_{n+1} in Equation (20),

$$P_n=\frac{\left(\operatorname{erf}\left(\frac{a+b(x_n-\Delta x)}{\sqrt{-2bD}}\right)-\operatorname{erf}\left(\frac{a+bx_n}{\sqrt{-2bD}}\right)\right)}{\left(\operatorname{erf}\left(\frac{a+bx_n}{\sqrt{-2bD}}\right)-\operatorname{erf}\left(\frac{a+b(x_n+\Delta x)}{\sqrt{-2bD}}\right)\right)} \tag{54}$$

Now the value of each resistor between nodes n and n+1 is half the resistance of the equivalent length of non-uniform transmission line, i.e.

$$R_{n+1} = \frac{1}{2}\int_{x_n}^{x_n+\Delta x} R_d\left(x\right)dx \tag{55}$$

Substituting for $R_d(x)$ using Equation (48) and integrating gives

$$R_{n+1} = \frac{\left(c_5 D\right)^{-1}}{2}\exp\left(-\frac{a^2}{2Db}\right)\sqrt{-\pi\frac{D}{2b}}\left(\operatorname{erf}\left(\frac{a+bx_n}{\sqrt{-2bD}}\right)-\operatorname{erf}\left(\frac{a+b\left(x_n+\Delta x\right)}{\sqrt{-2bD}}\right)\right) \tag{56}$$

Now substituting for Z_{n+1} and R_{n+1} in Equation (32) using Equations (52) and (56) and simplifying gives, as when $v(x)$ is constant,

$$\tau_{n+1} = \frac{2D'}{2D'+1} \tag{57}$$

It should be noted that the constant c_5 does not appear in the equations for the model parameters, P_n and τ_n, and can, therefore, be chosen arbitrarily. Once P_n is calculated for each node and τ_n is calculated for each connecting line the method can be implemented as described above. As when $v(x)$ is constant over space, the accuracy appears, from testing, to be limited only by the storage precision. Typical results are given in Figure 6.

In most modelling situations equations for $v(x)$ and $D(x)$ will not be available; instead their values will be known at discrete points in space. If piece-wise equations for $v(x)$ and $D(x)$ can be obtained (by spline-fitting for example) then a piece-wise solution of Equation (6) can be found and that is sufficient to determine equations for $R_d(x)$ and $Z(x)$ for each connecting line which can be integrated as above to calculate P_n and τ_n for each node.

An alternative is to use Equation (30), derived for the situation where $v(x)$ is constant over space, even if $v(x)$ varies. The impedance ratio at node n is then simply

$$P_n = \exp\left(-\Delta x Pe_n\right) \tag{58}$$

where Pe_n, the Peclet number at node n, is $v(x_n)/D(x_n)$. The errors resulting from this simplification will depend on how $v(x)$ and $D(x)$ vary over space and on the node spacing. For the example illustrated in Figure 6, using this simplified method gives a solution with a maximum relative error of 7.5×10^{-3}. A significant advantage of explicit numerical schemes is the fact that nonlinear problems can be modelled with relative ease [15]. If $v(x)$ and/or $D(x)$ vary with $V(x, t)$ then Equation (58) could be used to recalculate the impedance ratios at each time step without significantly increasing the model run-time.

MODIFIED METHOD FOR CONSERVATIVE FORM

The conservative form of the convection-diffusion equation can be written as

$$\frac{\partial V}{\partial t} = D\frac{\partial^2 V}{\partial x^2} - v\frac{\partial V}{\partial x} - V\frac{\partial v}{\partial x} \tag{59}$$

which has one extra term in comparison with the non-conservative form. Such a term can be modelled in TLM by adding current sources at each node controlled so as to alter the rate of change of the node voltage [10]. The required additional rate of increase of Vn at node n at time step k is proportional to the node voltage Vn and to $\partial v/\partial x$ which can be approximated at node n by

$$\left.\frac{\partial v}{\partial x}\right|_n = \frac{v_{n+1}-v_{n-1}}{2\Delta x} = \frac{v'_{n+1}-v'_{n-1}}{2\Delta t} \tag{60}$$

To increase the rate of change of voltage by $V\partial v/\partial x$ the voltage at each time step must be adjusted by $\Delta t V\partial v/\partial x$ so, in the TLM method, the node voltage must be adjusted by $-\tfrac{1}{2}Vn_n^k\left(v'_{n+1}-v'_{n-1}\right)$.

Raising a node voltage in TLM by a value ΔV will cause each of the scattered pulses from the node also to be each increased by ΔV. Considering, for example, the case where $\tau = 0$, it is clear that at the next time step the node voltage will be raised by $2\Delta V$. Instead of raising the node voltage by ΔV, therefore, it must be increased by $\Delta V/2$.

There are two options for modifying the method: the added $V\partial v/\partial x$ term can be approximated using the node voltage values either from the current time step or from the previous time step. In the first case the node voltage equation for the modified scheme is

$$ {}_kVn_n = \left(\frac{2{}_kVil_n + 2P_n{}_kVir_n}{1+P_n} \right) \left(1 - \frac{v'_{n+1} - v'_{n-1}}{4} \right) \tag{61} $$

while in the second case it is

$$ {}_kVn_n = \left(\frac{2{}_kVil_n + 2P_n{}_kVir_n}{1+P_n} \right) - {}_{k-1}Vn_n \left(\frac{v'_{n+1} - v'_{n-1}}{4} \right) \tag{62} $$

TESTING OF MODIFIED METHOD

The steady-state solution of the conservative one-dimensional convection-diffusion equation with boundary conditions $V(0,t) = 0$ and $V(\lambda,t) = 100$, and with the convection velocity varying over space as $v = a + bx$ is (as obtained using symbolic maths software)

$$ V(x) = 100 \exp\left[\frac{\frac{1}{2}(x-\lambda)(2a+bx+b\lambda)}{D} \right] \left[\frac{\operatorname{erf}\left(\frac{a}{\sqrt{2bD}}\right) - \operatorname{erf}\left(\frac{(a+bx)}{\sqrt{2bD}}\right)}{\operatorname{erf}\left(\frac{a}{\sqrt{2bD}}\right) - \operatorname{erf}\left(\frac{(a+b\lambda)}{\sqrt{2bD}}\right)} \right] \tag{63} $$

The results presented below are for $b > 0$ but Equation (54) can only be evaluated if $b < 0$. This problem is solved by replacing b with $-b$ and x with $-x$ in Equation (54) and calculating P_n as before.

It was found during testing that, for Dirichlet boundary conditions, if Equation (62) is used then the steady-state result is largely independent of Δt but the scheme becomes unstable if the wave propagation term is significant (i.e. if $D(\Delta t/\Delta x)^2$ is large). This may limit the ability of the method to reach a steady-state solution rapidly since it limits Δt. It was found that if Equation (61) is used then the scheme appears to be unconditionally stable but the accuracy of the solution varies significantly with Δt (see Figure 7). These findings are illustrated in Figure 9 in the next section. In both schemes the errors increase with Δx and with $\partial v/\partial x$.

CONVERGENCE

The unmodified method is unconditionally stable and so large Δt values can be used for which the solution should rapidly approach steady state. To test whether this is true in practice, models with boundary conditions $V(0,t) = 0$ and $V(\lambda,t) = 100$, initial condition $V(x,0) = 100x/\lambda$, $\lambda = 20$, and with 21 nodes, were run until a steady-state was reached. The number of time steps required to reach convergence, $k_{Convergence}$, defined as the minimum k for which $\max_{n=1}^{N} \left| Vn_n^k - Vn_n^{k-1} \right| < 1\times10^{-5}$, was measured.

Figure 8 shows results for models with velocity constant over space. For any model, the number of time steps required to satisfy the convergence condition drops as expected as Δt increases but then rises again above an optimum time step length. This behaviour has been noted previously in TLM diffusion models [11]. The increase is associated with the wave-propagation term in the differential equation for the lossy transmission line which becomes significant at higher Δt values and leads to wave-like behaviour which takes time to settle down. It can be seen from Figure 8 that the minimum number of time steps required to reach steady state decreases as Pe' increases. This is true whether the increase is due to an increase in v, a reduction in D, or an increase in Δx. Testing has shown that as Pe' increases the optimum Δt setting, $\Delta t_{optimum}$, decreases towards $\Delta x^2/2D$, i.e. the value for which τ_n = 0.5 (see Figure 8), and the minimum value of $k_{Convergence}$ decreases towards $N - 1$, the least number of time steps required for each node to 'know' the boundary conditions.

At present there is no direct method for determining $\Delta t_{optimum}$ for a particular model: experimental running of the model over a range of settings is the only option. It has been suggested however, that if the optimum value is found in this manner for a similar model with a reduced number of nodes, then it should be possible from this to determine the $\Delta t_{optimum}$ value for the original model [11].

Figure 9a shows equivalent results for models with spatially varying velocity values using the two versions of the modified method. As noted above, if Equation (62) is used then the method is not unconditionally stable but it has been found that a minimum $k_{Convergence}$ value is reached within the stability limits for all D' and v' settings tested and that this value is comparable with that for a similar model with constant convection velocity. If Equation (61) is used then the method appears to be unconditionally stable and $k_{Convergence}$ is significantly less sensitive to the value of Δt. Figure 9b shows that if Equation (62) is used then the maximum relative error in the solution is largely independent of Δt but using Equation (61) gives more accurate results over a wide range of time step lengths. In both cases the errors can be reduced by decreasing Δx.

TRANSIENT RESULTS

From Equations (35) and (30), for a model with constant v' and D' under steady-state conditions, v' and D' are related to τ and P_n according to the following equations

$$D' = \frac{\tau}{2(1-\tau)} \tag{64}$$

and

$$v' = -D' \ln(P_n) \tag{65}$$

It has been found analytically [16] that under purely transient conditions (i.e. for convection-diffusion in an infinite medium) the relationships are

$$D' = \left(\frac{\tau(2\tau P_n - P_n - 1)(P_n - 2\tau + 1)}{2(\tau - 1)^3 (1 + P_n)^2} \right) \tag{66}$$

and

$$v' = \frac{\tau}{1-\tau} \left(\frac{1 - P_n}{1 + P_n} \right) \tag{67}$$

If P_n = 1 then v' = 0 and the two sets of equations are equal. Otherwise the difference between the equations represents numerical diffusion and convection exhibited by the scheme under transient conditions but which go to zero as a solution approaches steady state.

DISCUSSION AND CONCLUDING REMARKS

A novel TLM method has been described for the solution of the non-conservative form of the steady-state one-dimensional convection-diffusion equation. It is unconditionally stable and produces highly accurate results even for high cell Peclet numbers. If v and D are known over space then the accuracy of the method is independent of the element length.

If v and/or D vary over space then an ODE must be solved and the solution integrated between pairs of nodes in order to obtain an optimum solution. A simplified scheme avoids these steps but produces less accurate results, the accuracy depending on the node spacing.

It has been shown previously that the TLM method for diffusion converges rapidly to a steady-state solution when an optimum Δt setting is used [11]. The addition of convection leads to a faster rate of convergence. In general the optimum time step length is not known but it approaches the value for which $\tau = 0.5$ as Pe' is increased (by, for example, an increase in Δx). Although a time-domain scheme, and therefore not an obvious choice for obtaining steady-state solutions, the accuracy of the results suggests that TLM may be significantly more efficient than other methods, especially when the Peclet number is high.

The method can be modified to solve the conservative form of the convection-diffusion equation by using current sources at each node that raise the node voltages at each time step by an amount proportional to the node voltage, measured either at the current time step or at the previous time step. If values from the current time step are used then the modified method appears to be unconditionally stable and more accurate (for most Δt values) but the error in the solution is highly dependent on Δt. The reasons for this are not clear at present.

Central to the new method is the idea of exponential variation of impedance over space. Note however that in deriving and using the TLM algorithm, only local impedance ratios between adjacent TL segments are required. There are therefore no concerns regarding the numerical accuracy of exponentially varying impedance terms over the entire modelling space.

Reaction-diffusion can be modelled using the TLM method by including leakage resistors in the TL network connecting each node to ground [10, 17]. There would appear to no reason why the convection-diffusion method described in this paper could not be extended to solve reaction-convection-diffusion equations in a similar manner. Since the difference between the non-conservative and conservative forms of the convection-diffusion equation is also essentially a reaction term, it may be possible to solve the conservative form using a different method than that described above.

As with other TLM schemes, the method described here is straightforward to implement, requires a relatively small amount of code, and, since it is explicit and in the time domain, is easily extended to the solution of non-linear problems.

This paper considers only one-dimensional problems with Dirichlet boundary conditions. Future papers will look at the extension of the method to multi-dimensional problems and to the implementation of other boundary condition types.

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APPENDIX A

Let $C_d(x)$, $L_d(x)$, and $R_d(x)$ be the distributed capacitance, inductance, and resistance respectively of a non-uniform lossy transmission line at any point *x*. Over a short length, Δx, these can be represented by lumped components as shown in Figure 10. If the current and voltage are *i* and *V* at one end of a short TL segment then they can be approximated by truncated Taylor series at the other end.

The voltage across the inductor is then $\frac{\partial V}{\partial x}\Delta x + iR_d(x)\Delta x$. Since the voltage across an inductance *L* with current *i* flowing through it is $V = L\frac{di}{dt}$, then for the distributed TL inductance

$$\frac{\partial V}{\partial x}\Delta x + iR_d(x)\Delta x = -L_d(x)\Delta x\frac{\partial i}{\partial t} \tag{68}$$

the minus sign arising because the voltage is such as to oppose the current flow. Dividing across by $R_d(x)C_d(x)\Delta x$ gives

$$\frac{1}{R_d(x)C_d(x)}\frac{\partial V}{\partial x} + i\frac{1}{C_d(x)} = -\frac{L_d(x)}{R_d(x)C_d(x)}\frac{\partial i}{\partial t} \tag{69}$$

and rearranging Equation (68) gives

$$-i = \frac{1}{R_d(x)}\frac{\partial V}{\partial x} + \frac{L_d(x)}{R_d(x)}\frac{\partial i}{\partial t} \tag{70}$$

The currents at the ends of the TL segment are different. The difference, $-\frac{\partial i}{\partial x}\Delta x$, is the current charging the capacitor. Since, for a capacitor, $i = C\frac{dV}{dt}$, then for the TL segment

$$-\frac{\partial i}{\partial x}\Delta x = C_d(x)\Delta x\frac{\partial V}{\partial t} \tag{71}$$

Differentiating Equation (69) with respect to *x* and partially expanding the result gives

$$\begin{aligned}&\frac{\partial}{\partial x}\left(\frac{1}{R_d(x)C_d(x)}\frac{\partial V}{\partial x}\right) + \frac{1}{C_d(x)}\frac{\partial i}{\partial x} + \frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right)i = \\ &-\frac{L_d(x)}{R_d(x)C_d(x)}\frac{\partial^2 i}{\partial x\partial t} - \frac{\partial}{\partial x}\left(\frac{L_d(x)}{R_d(x)C_d(x)}\right)\frac{\partial i}{\partial t}\end{aligned} \tag{72}$$

Differentiating Equation (71) with respect to *t* gives

$$-\frac{\partial^2 i}{\partial x\partial t} = C_d(x)\frac{\partial^2 V}{\partial t^2} \tag{73}$$

Now using Equations (70), (71), and (73), to replace terms in Equation (72) and rearranging yields

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{R_d(x)C_d(x)}\frac{\partial V}{\partial x}\right) - \frac{1}{R_d(x)}\frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right)\frac{\partial V}{\partial x} - \frac{L_d(x)}{R_d(x)}\frac{\partial^2 V}{\partial t^2} + \left[\frac{\partial}{\partial x}\left(\frac{L_d(x)}{R_d(x)C_d(x)}\right) - \frac{\partial}{\partial x}\left(\frac{1}{C_d(x)}\right)\left(\frac{L_d(x)}{R_d(x)}\right)\right]\frac{\partial i}{\partial t} \tag{74}$$

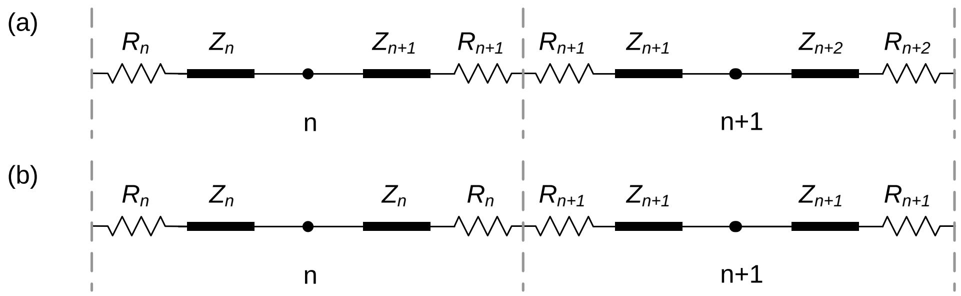


Figure 1: Two link-resistor configurations with resistance and impedance values varying at nodes (a) and between nodes (b). The thicker lines represent segments of transmission line. Note that a TL must be composed of two conductors, but, since the second, return conductor must always exist, it is standard practice not to show it in TLM network diagrams.

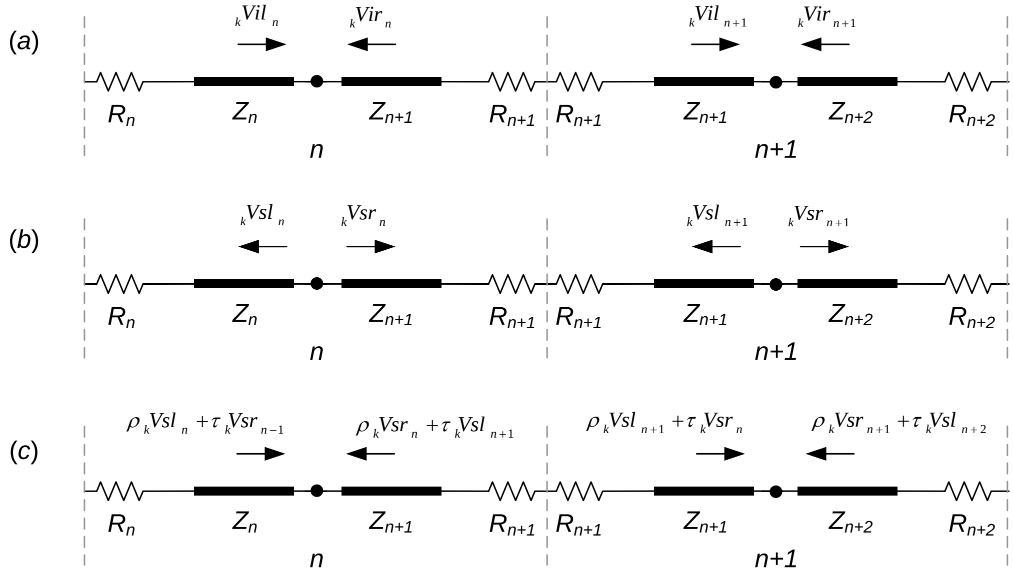


Figure 2: Nodes with incident pulses at time step *k* (a), scattered pulses (b), and incident pulses at time step *k*+1 (c).

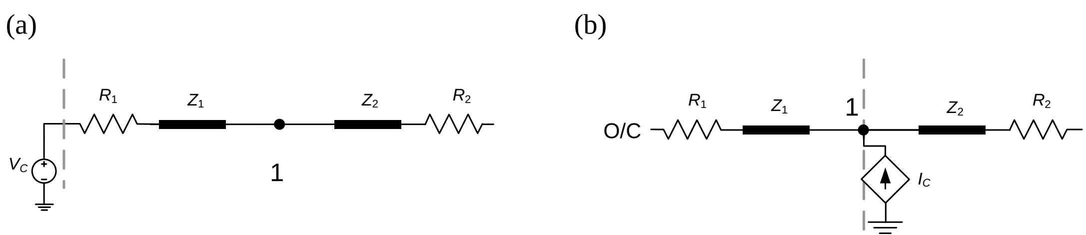


Figure 3 : Fixed voltage boundaries for link-resistor diffusion/convection-diffusion models using the element boundary method (a) and using the node boundary method (b). The location of the boundary in both cases is indicated by a dashed line. With the node boundary method the network extends beyond the boundary.

(a) (b)

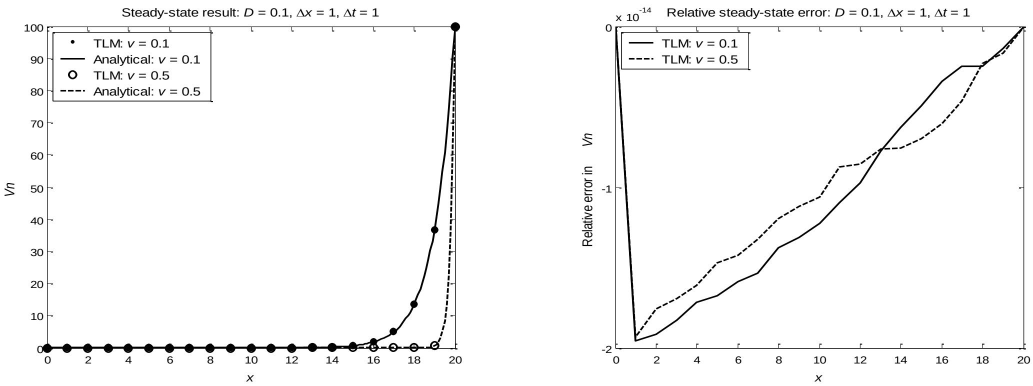


Figure 4: Results from the TLM method after 5000 time steps with *Pe*' = 1 and *Pe*' = 5 and the corresponding analytical solutions (a) and the relative errors in the TLM solutions (b). Note that while the two relative error plots are similar in this case, this is not true in general.

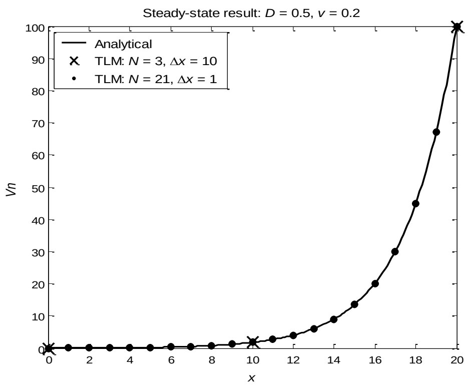


Figure 5: Results obtained after 5000 time steps with Δt = 1 from two models with *Pe* = 0.4: one with 21 nodes and *Pe*' = 0.4, and one with 3 nodes and *Pe*' = 4. The estimates of *V*(10) obtained from the two models differ by only 2×10^{-14}.

(a) (b)

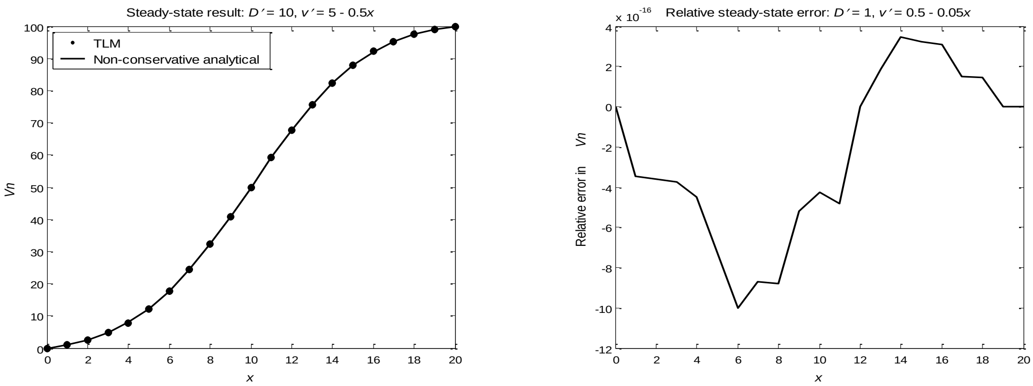
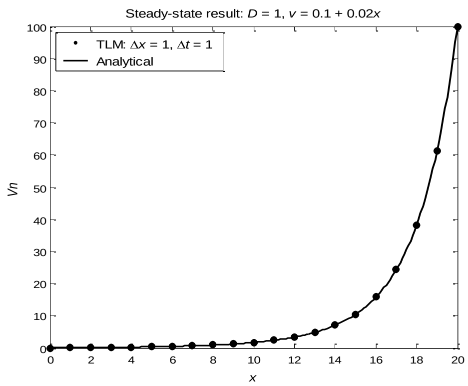


Figure 6: Results from the TLM method after 5000 time steps and the corresponding analytical solution for model with *v*(*x*) varying linearly over space (a) and the relative errors in the TLM solution (b).

(a)



(b)

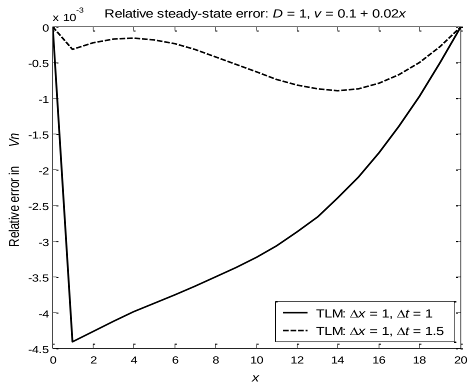


Figure 7: Results from the modified TLM method (using Equation (62) with Δt = 1) after 5000 time steps and the corresponding analytical solution of the conservative convection-diffusion equation for a situation where v varies linearly over space (a) and the relative errors in the TLM solutions obtained with two different time increments, Δt = 1 and Δt = 1.5 (b).

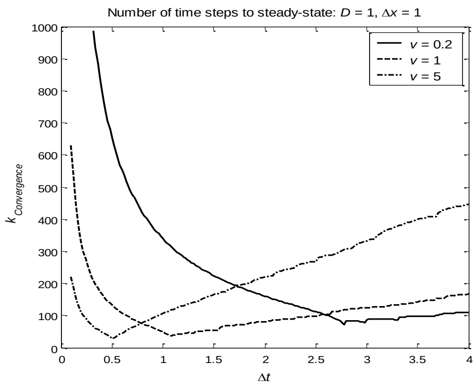
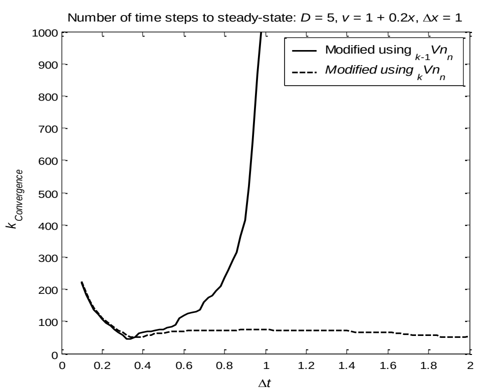


Figure 8: The number of time steps required for convergence plotted against Δt for models with Pe' = 0.2, Pe' = 1, and Pe' = 5. With D = 1 and Δx = 1, τ = 0.5 corresponds to Δt = 0.5.

(a)



(b)

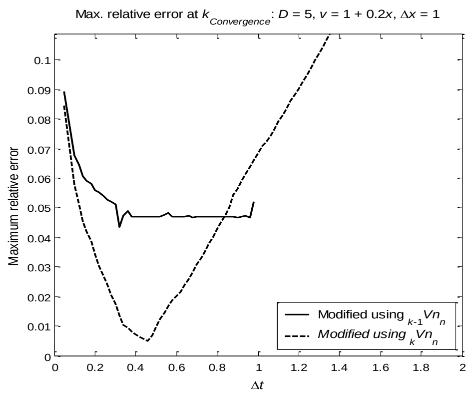


Figure 9: The number of time steps required for convergence plotted against Δt for models with spatially varying velocity modified using Equation (61) (i.e. using the values of $_{k-1}Vn_n$) and Equation (62) (i.e. using the values of $_kVn_n$) (a) and the maximum relative errors in the solutions (b).

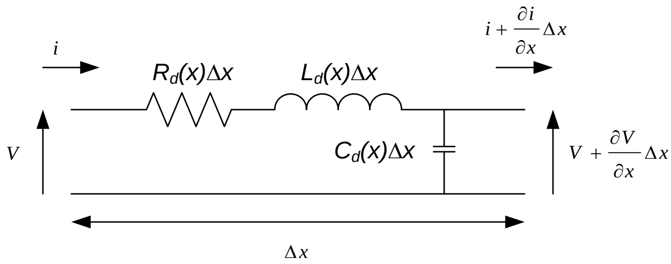


Figure 10: Lossy transmission line segment with spatially varying parameters.