# Error analysis and reduction in lossy TLM

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SUMMARY

This paper presents a novel technique to analyze the lossy TLM method for diffusion. From the equations derived for the variance error, it also shows how adjusting the transmission coefficient for one time step can reduce the long-term variance error to zero and significantly increase the accuracy of transient results obtained.

## 1. INTRODUCTION

Initially developed by Johns in 1977 [1], the lossy Transmission Line Modelling (TLM) method has been applied to both thermal and particle diffusion. It is an explicit, time-domain technique that has been shown to produce accurate results, to be efficient when compared to traditional numerical schemes, and to be unconditionally stable [2, 3]. The code required is often shorter than that needed to implement more traditional solutions for a given problem [4] and the nature of the TLM method means that the modeller stays close to the physical process being modelled [5, 6]. There is no direct use of differential equations and this is particularly advantageous when modelling nonlinear problems.

The so-called "fundamental" solution of the one-dimensional diffusion equation

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2} \tag{1}$$

where $D$ is the diffusion coefficient and $\phi$ is the concentration of diffusing substance (diffusant), is the transient solution of the equation for a single instantaneous injection of a quantity of diffusant, $\Theta$, at time $t = 0$ at position $x = 0$ into an infinite medium with zero initial concentration at all other points. The solution for these conditions is [7]

$$\phi(x,t) = \frac{\Theta/A}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \tag{2}$$

where $A$ is the cross-sectional area represented in one dimension. The equation for a Gaussian distribution with mean position $\bar{x} = 0$, variance $s^2$, and integral $\varsigma$, is

$$P(x) = \frac{\varsigma}{\sqrt{2\pi s^2}}\exp\left(-\frac{x^2}{2s^2}\right) \tag{3}$$

It is clear from a comparison of Equations (2) and (3) that the fundamental solution is Gaussian-shaped with variance at time $t$ given by

$$s^2 = 2Dt \tag{4}$$

The variance increases at a constant rate over time as the diffusant spreads. When the TLM solution is implemented, it is found to be approximately Gaussian in shape, but the variance does not increase as expected over the initial time steps. This discrepancy leads to a significant error over these time

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steps and to a lesser long-term error that never reduces to zero. It has been shown that the first time step of the scheme is inconsistent with further time steps but that the method can be altered temporarily for that time step in such a way as to make it consistent [8]. An expression for the variance at each time step has been derived previously [9, 10]. This paper presents a novel technique for analysing TLM schemes which yields a more general expression that gives additional information. Arising from this analysis, a method for reducing the long-term variance error to zero is proposed and tested. It is shown that this adjustment to the standard lossy TLM method can significantly reduce the error in transient solutions for a variety of initial and boundary conditions.

## 2. THE METHOD

### *2.1 Link-resistor implementation*

The lossy TLM method for diffusion modelling is based on the fact that the differential equation for voltage on a lossy transmission line (i.e. one with distributed resistance) has the same form as the diffusion equation so long as the transmission line (TL) inductance is negligible [1]. This condition is satisfied in practice if $\Delta t/\Delta x$ is small where $\Delta t$ is the time step and $\Delta x$ is the distance between nodes. Further details of the lossy TLM method are given elsewhere [3]. There are two possible configurations as shown in Figure 1. This paper initially focuses on the link-resistor (LR) configuration but the analysis is also applied to the link-line (LL) scheme. Each element is composed of two lossless transmission line (TL) segments of impedance $Z$ (which essentially act as delay lines, a voltage pulse entering at one end arriving at the other end $\Delta t/2$ later) and two resistors. In the TLM method, the field variable, $\phi$, is represented by the voltages at the nodes.

The method is initialised with incident voltage pulses at each node, one from the left and one from the right. Figure 2a shows the incident pulses arriving at LR nodes $n$ and $n$+1 at time step $k$. The node voltage at node $n$ resulting from these incident pulses is

$$ {}_{k}Vn_{n} = {}_{k}Vil_{n} + {}_{k}Vir_{n} \tag{5} $$

At the same instant pulses are scattered back from the node into each TL section, one to the left

$$ {}_{k}Vsl_{n} = {}_{k}Vn_{n} - {}_{k}Vil_{n} \tag{6} $$

and one to the right

$$ {}_{k}Vsr_{n} = {}_{k}Vn_{n} - {}_{k}Vir_{n} \tag{7} $$

as shown in Figure 2b. Combining these equations gives

$$ {}_{k}Vsl_{n} = {}_{k}Vir_{n} \tag{8} $$

$$ {}_{k}Vsr_{n} = {}_{k}Vil_{n} \tag{9} $$

At time $\Delta t/2$ later, these pulses arrive at an impedance discontinuity due to the presence of the resistors and so only a fraction, $\tau$, (known as the transmission coefficient) of each scattered pulse is transmitted on, arriving at adjacent nodes $\Delta t/2$ later. The remaining fraction ($\rho = 1-\tau$) of the scattered pulses is reflected back, arriving $\Delta t/2$ later at the nodes from which they originated. The incident voltage pulses at time step $k$+1 are simply the sum of these reflected and transmitted pulses (as shown in Figure 2c)

$$ {}_{k+1}Vir_{n} = (1-\tau)\,{}_{k}Vsr_{n} + \tau\,{}_{k}Vsl_{n+1} \tag{10} $$

$$ {}_{k+1}Vil_{n} = (1-\tau)\,{}_{k}Vsl_{n} + \tau\,{}_{k}Vsr_{n-1} \tag{11} $$

The values of these incident voltage pulses can be used to calculate the node voltages at time step $k$+1 and the scattered pulses and so the procedure can be repeated. It can be shown that the node voltages over time approximate a transient solution of Equation (1), $\tau$ being related to the diffusion coefficient, $D$, by

$$ D' = \tfrac{1}{2}\tau/(1-\tau) \tag{12} $$

where $D'$ is the dimensionless cell diffusion coefficient, $D' = D\Delta t/\Delta x^2$.

Note that $\tau$ is related is equal to $Z/(R+Z)$ and must be between 0 and 1 for a physically realisable TL network with passive components. This restriction does not limit the value of $D'$ and so the scheme is unconditionally stable.

### *2.2 Initialisation*

In any transient diffusion problem, the initial concentration profile over space must be known in order to calculate a solution over time. In TLM the node voltage is analogous to the concentration and so the initial node voltages will be known. In order to calculate the scattered voltages the incident node voltages are required and so, in TLM, it is the incident pulses at each node that are initialised. From these, the node voltages are calculated using Equation (5). Since any diffusant injected at a single point is equally likely to move left as it is to move right, it is standard practice to set both incident pulses equal to half the desired initial node voltage. This leads to the pulses scattered to left and to right being equal and so is consistent with the physical system being modelled.

## 3. ANALYSIS

For modelling purposes the one-dimensional space must be divided up into finite sections of length $\Delta x$ with corresponding nodes numbered from 1 to $N$. The position $x_n$ and the dimensionless cell position $x'_n$ both give the location of node $n$ in space where $x'_n$ is defined as

$$x'_n = x_n / \Delta x \tag{13}$$

The set of values of a particular voltage constituent (either the node voltage itself, or voltage incident from the left, or voltage incident from the right, or one of the scattered voltages) over the nodes represents a discrete distribution with a number of measurable properties. If the voltage profile over space is Gaussian in shape then it can be defined by three parameters, the mean position, the variance, and the sum of the values. These parameters can also be evaluated for non-Gaussian distributions but they will not fully define such profiles. If ${}_kV_n$ is a voltage at node $n$ at time step $k$ then the sum of the voltage values at time step $k$, is simply

$${}_k\varsigma'_V = \sum_{n=1}^{N} {}_kV_n \tag{14}$$

The dimensionless mean position of the voltage distribution is

$${}_k\bar{x}'_V = \sum_{n=1}^{N} {}_kV_n x'_n \Big/ \sum_{n=1}^{N} {}_kV_n \tag{15}$$

and the dimensionless variance is

$${}_k s'^2_V = \sum_{n=1}^{N} {}_kV_n \left(x'_n - {}_k\bar{x}'_V\right)^2 \Big/ \sum_{n=1}^{N} {}_kV_n \tag{16}$$

The TLM method involves the addition and subtraction of voltage distributions. Let ${}_kV_1$ and ${}_kV_2$ represent two distributions at time step $k$ with properties ${}_k\varsigma'_{V_1}$, ${}_k\varsigma'_{V_2}$, ${}_k\bar{x}'_{V_1}$, ${}_k\bar{x}'_{V_2}$, ${}_k s'^2_{V_1}$, and ${}_k s'^2_{V_2}$ respectively. Adding the two distributions will result in a third distribution whose values sum to

$${}_k\varsigma'_{V_1+V_2} = {}_k\varsigma'_{V_1} + {}_k\varsigma'_{V_2} \tag{17}$$

and with mean position given by

$${}_k\bar{x}'_{V_1+V_2} = \left({}_k\varsigma'_{V_1}\,{}_k\bar{x}'_{V_1} + {}_k\varsigma'_{V_2}\,{}_k\bar{x}'_{V_2}\right) \Big/ \left({}_k\varsigma'_{V_1} + {}_k\varsigma'_{V_2}\right) \tag{18}$$

and variance [11]

$${}_k s'^2_{V_1+V_2} = \frac{{}_k s'^2_{V_1}\,{}_k\varsigma'^2_{V_1} + {}_k s'^2_{V_2}\,{}_k\varsigma'^2_{V_2} + {}_k\varsigma'_{V_1}\,{}_k\varsigma'_{V_2}\left({}_k s'^2_{V_1} + {}_k s'^2_{V_2} + \left({}_k\bar{x}'_{V_1} - {}_k\bar{x}'_{V_2}\right)^2\right)}{\left({}_k\varsigma'_{V_1} + {}_k\varsigma'_{V_2}\right)^2} \tag{19}$$

Note that these equations apply no matter what shapes the individual distributions have. In the special case where the two distributions have the same variance and sum, Equation (19) becomes

$$ {}_k s'^2_{V_1+V_2} = {}_k s'^2_{V_1} + \tfrac{1}{4}\left( {}_k \bar{x}'_{V_1} - {}_k \bar{x}'_{V_2} \right)^2 \tag{20} $$

*3.1 Distribution variance*

The following analysis applies to the LR configuration. A similar analysis of the LL scheme follows. Consider an infinite one-dimensional model with centre node located at $x' = 0$. If such a model is to be initialised with a node voltage ${}_0Vn_n$ at each node, then, using the standard initialisation method, the initial incident pulses are set to ${}_0Vil_n = {}_0Vir_n = {}_0Vn_n/2$. Thus the two incident voltage distributions have equal mean positions, variances, and sums of values. If this is the case then the symmetry of the method dictates that the two incident voltage distributions will be mirror images of each other at all subsequent time steps and will therefore have the same variance and sum of values. The notation can be simplified by letting

$$ {}_k \varsigma' = {}_k \varsigma'_{Vil} = {}_k \varsigma'_{Vir} \tag{21} $$

$$ {}_k s'^2 = {}_k s'^2_{Vil} = {}_k s'^2_{Vir} \tag{22} $$

If the mean position of the node voltage profile ${}_0Vn_n$ is initially at $x' = 0$ then it will remain at that location and the mean positions of the two incident voltage profiles will satisfy at all time steps

$$ {}_k \bar{x}' = -{}_k \bar{x}'_{Vil} = {}_k \bar{x}'_{Vir} \tag{23} $$

The node voltage distribution is the sum of the ${}_kVil$ and ${}_kVir$ distributions so the variance of the ${}_kVn$ distribution, from Equation (20), is

$$ {}_k s'^2_{Vn} = {}_k s'^2_{Vil} + \tfrac{1}{4}\left( {}_k \bar{x}'_{Vil} - {}_k \bar{x}'_{Vir} \right)^2 = {}_k s'^2 + \left( {}_k \bar{x}' \right)^2 \tag{24} $$

From Equations (8) and (9) the properties of the scattered voltage pulse two distributions are simply

$$ {}_k s'^2_{Vsl} = {}_k s'^2_{Vsr} = {}_k s'^2 \tag{25} $$

$$ {}_k \varsigma'_{Vsl} = {}_k \varsigma'_{Vsr} = {}_k \varsigma' \tag{26} $$

$$ {}_k \bar{x}'_{Vsl} = -{}_k \bar{x}'_{Vsr} = {}_k \bar{x}' \tag{27} $$

The two incident voltage pulse distributions at the next time step are the sum of reflected and transmitted pulse distributions as given by Equations (10) and (11). The ${}_{k+1}Vil$ distribution is $(1-\tau)$ times the ${}_kVsl$ distribution added to $\tau$ times the ${}_kVsr$ distribution shifted 1 node to the right. The mean position of the ${}_{k+1}Vil$ distribution is therefore

$$ {}_{k+1}\bar{x}'_{Vil} = \frac{\rho_k \varsigma'_{Vsl\,k} \bar{x}'_{Vsl} + \tau_k \varsigma'_{Vsr} \left( {}_k \bar{x}'_{Vsr} + 1 \right)}{\rho_k \varsigma'_{Vsl} + \tau_k \varsigma'_{Vsr}} = \frac{\rho_k \varsigma'_k \bar{x}' + \tau_k \varsigma' \left( -{}_k \bar{x}' + 1 \right)}{\rho_k \varsigma' + \tau_k \varsigma'} = {}_k \bar{x}' - 2\tau_k \bar{x}' + \tau \tag{28} $$

Now ${}_{k+1}\bar{x}'_{Vil} = -{}_{k+1}\bar{x}'$ so this can be rewritten as

$$ {}_{k+1}\bar{x}' = \left(2\tau - 1\right)_k \bar{x}' - \tau \tag{29} $$

From symmetry

$$ {}_{k+1}\bar{x}'_{Vir} = -{}_{k+1}\bar{x}'_{Vil} = {}_{k+1}\ \bar{x}' \tag{30} $$

so Equation (29) gives the mean position of the two incident voltage distributions over time if the initial mean positions are known. If the standard initialisation method is used then the initial mean positions of the two incident pulse distributions are equal, but this need not be the case. Equation (29) can be solved using Z-transforms to get an equation for ${}_k\bar{x}'$ in terms of $\tau$ and $k$ as will be shown below.

Now the variance of the ${}_{k+1}Vil$ distribution is, from Equation (19),

$$ {}_{k+1}s'^2_{Vil} = \frac{ {}_k s'^2_{Vsl}\left(\rho_k \varsigma'_{Vsl}\right)^2 + {}_k s'^2_{Vsr}\left(\tau_k \varsigma'_{Vsr}\right)^2 + \rho_k \varsigma'_{Vsl}\tau_k \varsigma'_{Vsr}\left( {}_k s'^2_{Vsl} + {}_k s'^2_{Vsr} + \left( {}_k \bar{x}'_{Vsl} - \left( {}_k \bar{x}'_{Vsr} + 1\right)\right)^2\right)}{\left(\rho_k \varsigma'_{Vsl} + \tau_k \varsigma'_{Vsr}\right)^2} \quad (31) $$

Replacing terms using Equations (25), (26), and (27), and simplifying gives

$$ {}_{k+1}s'^2 = \left(4\,{}_k\bar{x}'^2 - 4\,{}_k\bar{x}' + 1\right)\left(\tau - \tau^2\right) + {}_k s'^2 \quad (32) $$

where ${}_{k+1}s'^2 = {}_{k+1}s'^2_{Vil} = {}_{k+1}s'^2_{Vir}$. From Equation (20), the variance of the node voltage distribution at time step $k$+1 is

$$ {}_{k+1}s'^2_{Vn} = {}_{k+1}s'^2_{Vil} + \tfrac{1}{4}\left( {}_{k+1}\bar{x}'_{Vil} - {}_{k+1}\bar{x}'_{Vir}\right)^2 \quad (33) $$

Substituting for terms using Equations (32), (29), and (30), and simplifying gives

$$ {}_{k+1}s'^2_{Vn} = {}_k s'^2 - 2\tau\,{}_k\bar{x}' + \tau + {}_k\bar{x}'^2 \quad (34) $$

The variance should increase with time as per Equation (4). Substituting dimensionless terms for $s^2$, $D$, and $t$, and rearranging gives

$$ s'^2 = 2D'k \quad (35) $$

i.e. $s'^2$ should increase by $2D'$ per time step. In practice it is found that the variance does not increase by a constant amount per time step. The model cell diffusion coefficient is therefore defined here for time step $k$ as

$$ {}_k D' = \tfrac{1}{2}\left( {}_{k+1}s'^2_{Vn} - {}_k s'^2_{Vn}\right) \quad (36) $$

Substituting for ${}_k s'^2_{Vn}$ and ${}_{k+1}s'^2_{Vn}$ using Equations (24) and (34) and simplifying gives

$$ {}_k D' = \tfrac{1}{2}\tau - \tau\,{}_k\bar{x}' \quad (37) $$

It is clear that ${}_kD'$ will only be constant over time if ${}_k\bar{x}'$ is a constant, $\bar{x}'_C$. From Equation (29), this is

$$ \bar{x}'_C = -\tfrac{1}{2}\tau/\left(1-\tau\right) \quad (38) $$

If the model is initialised with incident pulse distributions having mean positions ${}_0\bar{x}'_{Vir} = -{}_0\bar{x}'_{Vil} = \bar{x}'_C$ then the distribution spacing will remain constant as the model progresses and so will the model cell diffusion coefficient. For any other initial distribution spacing, these values will vary over time. Since the standard method for initialising a TLM diffusion model has ${}_0\bar{x}'_{Vir} = {}_0\bar{x}'_{Vil}$, the model cell diffusion coefficient varies with $k$.

As can be seen from Equation (37), in order to derive an equation for ${}_kD'$, it is first necessary to derive an equation for ${}_k\bar{x}'$. Taking the Z-transform of Equation (29) gives [12]

$$ zZ\left( {}_k\bar{x}'\right) - z_0\bar{x}' = \left(2\tau - 1\right)Z\left( {}_k\bar{x}'\right) - \tau z/\left(z-1\right) \quad (39) $$

which can be rearranged to give

$$ Z\left( {}_k\bar{x}'\right) = -\frac{z\tau}{\left(z-1\right)\left(z-2\tau+1\right)} + \frac{z_0\bar{x}'}{\left(z-2\tau+1\right)} \quad (40) $$

Applying the inverse Z-transform gives

$$ {}_k\bar{x}' = \left(\frac{\tau}{2\tau-2}\right)\left[1-\left(2\tau-1\right)^k\right] + {}_0\bar{x}'\left(2\tau-1\right)^k \quad (41) $$

This is an equation for the mean position of the incident pulse distributions over time. Since $|2\tau - 1| < 1$ for $0 < \tau < 1$, the limit as $k$ goes to infinity is

$$ \lim_{k\to\infty}\left( {}_k\bar{x}'\right) = -\tfrac{1}{2}\tau/\left(1-\tau\right) \quad (42) $$

which is equal to $\bar{x}'_C$ as derived above. As $k$ increases, therefore, the mean positions of the two incident voltage distributions approach values for which ${}_kD'$ is constant, no matter what ${}_0\bar{x}'$ is.

Using Equation (41) to substitute for ${}_k\bar{x}'$ in Equation (37) gives the model cell diffusion coefficient for time step $k$ as a function of $\tau$, $k$, and ${}_0\bar{x}'$

$$ {}_kD' = \tfrac{1}{2}\tau + \tfrac{1}{2}\tau^2\left(1-(2\tau-1)^k\right)/(1-\tau) - \tau\,{}_0\bar{x}'(2\tau-1)^k \tag{43} $$

Knowing the model cell diffusion coefficient for each time step and the initial variance of the node voltage distribution, it is now possible to calculate the variance at each time step. Rearranging Equation (36) gives

$$ {}_{k+1}s'^2_{Vn} - {}_ks'^2_{Vn} = 2\,{}_kD' \tag{44} $$

so the cell variance of the node voltage distribution after $k$ time steps is

$$ {}_ks'^2_{Vn} = {}_ks'^0_{Vn} + 2\sum_{i=0}^{k-1} {}_iD' \tag{45} $$

Replacing ${}_iD'$ using Equation (43) and summing using MAPLE® gives

$$ {}_ks'^2_{Vn} = {}_os'^2_{Vn} + k\tau/(1-\tau) + \left[\tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 + {}_0\bar{x}'\,\tau/(1-\tau)\right]\left[(2\tau-1)^k - 1\right] \tag{46} $$

Note that if ${}_0\bar{x}' = 0$ and ${}_0s'^2_{Vn} = 0$, then this is equivalent to the equation for cell variance derived by Chardaire and de Cogan [9, 10, 13]. Equation (46) applies to the link-resistor TLM formulation and gives the cell variance at any time step no matter what the initial conditions are. The third term represents an error in the cell variance

$$ {}_kEs'^2_{Vn} = \left[\tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 + {}_0\bar{x}'\,\tau/(1-\tau)\right]\left[(2\tau-1)^k - 1\right] \tag{47} $$

As expected, setting ${}_0\bar{x}' = -\tfrac{1}{2}\tau/(1-\tau)$ gives ${}_kEs'^2_{Vn} = 0$. If a model is initialised in the standard manner with ${}_0\bar{x}' = 0$ then Equation (47) becomes

$$ {}_kEs'^2_{Vn} = \tfrac{1}{2}\left[\tau/(1-\tau)\right]^2\left[(2\tau-1)^k - 1\right] \tag{48} $$

Since $\lim_{k\to\infty}(2\tau-1)^k = 0$, the error in the cell variance approaches the limit

$$ \lim_{k\to\infty}\left({}_kEs'^2_{Vn}\right) = -\tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 \tag{49} $$

While equations for the variance at any time step have been established previously for a number of lossy TLM networks [9, 10, 13], the relationship between the variance and the mean positions of the initial incident voltage distributions has not. It will be shown that the equations derived above can be used to improve the accuracy of the LR lossy TLM algorithm under some circumstances by reducing the long-term variance error to zero for models initialised using the standard method. It will also be shown that the same is true for the LL configuration.

## 4. ERROR REDUCTION

In general, given a desired initial concentration profile, it is not possible to set the mean positions of the initial incident voltage distributions to ${}_0\bar{x}'_{Vir} = -{}_0\bar{x}'_{Vil} = -\tfrac{1}{2}\tau/(1-\tau)$. For example consider the case where there is to be a single initial injection. If the cell diffusion coefficient is such that $\tau = 0.9$, then the mean positions of ${}_0Vil$ and ${}_0Vir$ would have to be 9 nodes apart for zero error in the node voltage variance over time. It is clearly impossible to achieve this with the standard initialisation while maintaining the desired initial concentration profile. If the desired initial node voltage distribution is spread over more than 9 nodes then it may be possible to calculate initial incident pulse profiles that produce this profile while having correctly spaced mean positions but that would not be a trivial problem. It may, however, be possible to temporarily adjust the transmission

coefficient over one or more time steps so that the long-term variance error is zero even if the model is initialised in the standard way. Since the initial time step in a TLM model is not consistent with the other time steps [8], altering that time step in order to achieve more accurate results will not reduce the consistency of the method.

Equation (46) can be rewritten to give the variance at time step $k$ in terms of the node voltage variance and the incident pulse distribution mean positions at any previous time step $j$

$$ {}_k s'^2_{Vn} = {}_j s'^2_{Vn} + (k-j)\tau/(1-\tau) + \left[\tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 + {}_j\bar{x}'\,\tau/(1-\tau)\right]\left[(2\tau-1)^{(k-j)} - 1\right] \tag{50} $$

If the transmission coefficient is ${}_1\tau$ for the first time step and if ${}_0\bar{x}' = 0$ (i.e. model initialised with standard method) then Equation (50) becomes simply

$$ {}_1 s'^2_{Vn} = {}_0 s'^2_{Vn} + {}_1\tau \tag{51} $$

and Equation (29) gives the incident pulse distribution mean positions for the second time step

$$ {}_1\bar{x}' = -{}_1\tau \tag{52} $$

If the transmission coefficient is changed to $\tau$ for all subsequent time steps, then Equation (50) gives the cell variance at time step $k$

$$ {}_k s'^2_{Vn} = {}_0 s'^2_{Vn} + {}_1\tau + (k-1)\tau/(1-\tau) + \left[\tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 - {}_1\tau\,\tau/(1-\tau)\right]\left[(2\tau-1)^{(k-1)} - 1\right] \tag{53} $$

Setting $(2\tau-1)^{(k-1)}$ to zero and rearranging this gives the long-term cell variance

$$ \lim_{k\to\infty}\left({}_k s'^2_{Vn}\right) = {}_0 s'^2_{Vn} + k\,\tau/(1-\tau) + {}_1\tau + ({}_1\tau - 1)\tau/(1-\tau) - \tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 \tag{54} $$

The third, fourth, and fifth terms in this equation represent errors in the node voltage variance. If the transmission coefficient for the first time step is set to ${}_1\tau^*$, a value which causes these error terms to cancel, then the long-term variance error will be zero. This requires that

$$ {}_1\tau^* + ({}_1\tau^* - 1)\tau/(1-\tau) - \tfrac{1}{2}\left[\tau/(1-\tau)\right]^2 = 0 \tag{55} $$

or

$$ {}_1\tau^* = \left(2\tau - \tau^2\right)/(2-2\tau) \tag{56} $$

If the transmission coefficient is changed to this value for the first time step then the cell variance error should approach zero as $k$ increases. Results for such an adjustment are shown in Figure 3 confirming that the variance error rapidly approaches zero after the first few time steps.

For values of $\tau > 0.586$ the value of ${}_1\tau^*$ is greater than 1. Such a value is achievable in a physical network if negative resistors are used but then stability is no longer guaranteed.

Using a similar procedure to that shown above, the long term variance error can be calculated for the situation where $\tau$ is changed to a different value for the second time step only. If this adjusted value is ${}_2\tau^*$ as given by

$$ {}_2\tau^* = \frac{2\tau + 3\tau^2 - 4\tau^3}{2 + 2\tau - 4\tau^2} \tag{57} $$

then the long-term variance error will again be zero [11]. This is also confirmed in Figure 3. It has been found that if the second time step is adjusted instead of the first then a transmission coefficient greater than one is required for $\tau > 0.685$ and so stability is guaranteed for higher values of the cell diffusion coefficient. It may be beneficial to adjust the third time step instead but this has not been examined.

In practice a value of $\tau$ greater than 1 for one time step does not lead to instability. It has been shown previously that oscillations occur in the output of LR and LL models with single initial injections and high transmission coefficients [14, 15]. A rise in the value of $\tau$ for even one time step can lead to an increased level of oscillation in the output (as illustrated in Figure 4 which has results for a single initial injection with $\tau = 0.7$) and so the results obtained by adjusting ${}_2\tau$ can be more accurate than those obtained by adjusting ${}_1\tau$. Figure 5 shows, however, that this is not the case when the initial

voltage profile is smooth. Also, such high $\tau$ values will normally be avoided if accurate transient results are required.

It should be noted from Figure 5b (and Figure 4) that the adjusted schemes produce less accurate results for $\tau = 0.7$ while Figure 5a shows that a significant improvement is obtained when $\tau = 0.25$. This dependency on $\tau$ is explored further below.

## 5. LINK-LINE CONFIGURATION

In the link-line scheme [3, 14, 15] (Figure 1a) the node voltage is again given by Equation (5). The scattered voltages are

$$ {}_kVsl_n = \tau\, {}_kVir_n + (1-\tau)\, {}_kVil_n \tag{58} $$

$$ {}_kVsr_n = \tau\, {}_kVil_n + (1-\tau)\, {}_kVir_n \tag{59} $$

and the new incident voltages are

$$ {}_{k+1}Vir_n = {}_kVsl_{n+1} \tag{60} $$

$$ {}_{k+1}Vil_n = {}_kVsr_{n-1} \tag{61} $$

This scheme can be analysed as above. The mean position of the ${}_kVir$ distribution is found to be

$$ {}_{k+1}\bar{x}' = (2\tau - 1)\, {}_k\bar{x}' - 1 \tag{62} $$

Using Z-transforms gives the mean position at time step $k$ as

$$ {}_k\bar{x}' = \tfrac{1}{2}\left[1/(\tau-1)\right]\left[1-(2\tau-1)^k\right] + {}_0\bar{x}'(2\tau-1)^k \tag{63} $$

which converges to $1/(2\tau - 2)$ over time for $0 < \tau < 1$. The cell variance of the node voltage distributions at time steps $k$ and $k$+1 are

$$ {}_k s'^2_{Vn} = {}_k s'^2 + {}_k\bar{x}'^2 \tag{64} $$

$$ {}_{k+1}s'^2_{Vn} = {}_k s'^2 - 4\tau\, {}_k\bar{x}' + 1 + {}_k\bar{x}'^2 + 2\, {}_k\bar{x}' \tag{65} $$

giving a model cell diffusion coefficient of

$$ {}_kD' = \tfrac{1}{2} - (2\tau - 1)\, {}_k\bar{x}' \tag{66} $$

Substituting for ${}_k\bar{x}'$ using Equation (63) gives

$$ {}_kD' = \tfrac{1}{2} - \left[(2\tau-1)^k (2\tau\, {}_0\bar{x}' - 2\, {}_0\bar{x}' - 1) + 1\right](2\tau-1)/(2\tau-2) \tag{67} $$

From this, the cell variance of the node voltage at time step $k$ can be calculated as before

$$ {}_k s'^2_{Vn} = {}_0 s'^2_{Vn} + \frac{\tau}{1-\tau}k + \frac{\left[(6\tau - 4\tau^2 - 2)\, {}_0\bar{x}' + 2\tau - 1\right]\left[(2\tau-1)^k - 1\right]}{2(\tau-1)^2} \tag{68} $$

If ${}_0\bar{x}' = 0$ (i.e. standard initialisation) then the cell variance at the next time step is ${}_1s'^2_{Vn} = {}_0s'^2_{Vn} + 1$ and the mean position of the incident voltage distributions is given by ${}_1\bar{x}' = -1$. Since both of these are independent of $\tau$, changing its value for the first time step has no effect on the long-term cell variance. If, instead, the transmission coefficient is altered to ${}_2\tau$ for the second time step, then the long-term node voltage cell variance becomes

$$ {}_\infty s'^2_{Vn} = {}_0 s'^2_{Vn} + k\tau/(1-\tau) - 2\tau/(1-\tau) + 4\, {}_2\tau + \tfrac{1}{2}\left[(6\tau - 4\tau^2 - 2)(2\, {}_2\tau) - 2\tau + 1\right]/(\tau-1)^2 \tag{69} $$

If the value is adjusted to

$$ {}_2\tau^* = \left(\tau^2 - \tfrac{3}{2}\tau + \tfrac{1}{4}\right)/(\tau-1) \tag{70} $$

then the long-term variance error will be zero.

The LL scheme can exhibit significant oscillations depending on the initial excitation and boundary conditions [3, 14, 15]. In such circumstances, it is normal practice to average the node voltages over consecutive pairs of time steps.

## 6. TESTING

This error reduction method has been tested for a variety of initial and boundary conditions and the results are presented in this section.

### *6.1 Infinite medium with Gaussian-shaped initial concentration profile*

Adjusting the transmission coefficient for the second time step in the manner described above results in zero long-term variance error. If the initial node voltage distribution is Gaussian-shaped then the analytical solution is a Gaussian distribution with a variance that increases over time. Since the mean position of ${}_kVn$ does not change and since the sum of the node voltage values remains constant in an infinite TLM model, then, if the variance of the node voltage is correct, the model output should be perfectly accurate but this is only true if the node voltage distribution remains Gaussian-shaped over time. If it deviates from a Gaussian shape, then the model output may be inaccurate even if ${}_k\varsigma'_{Vn}$, ${}_k\bar{x}'_{Vn}$, and ${}_k s'^2_{Vn}$, are exactly what they should be at each time step.

A LR model with $D = 1$ and $\Delta x = 1$ was run with an initial Gaussian node voltage distribution of cell variance 50 until $t = 100$ for a range of $\Delta t$ values. In each case a measurement was made of how far the result deviated from a Gaussian shape. To do this, the variance, mean position, and the sum of the values of the node voltage distribution were measured and a Gaussian function calculated with these properties. The maximum difference between the node voltage and this function was then measured. The results are plotted against $\Delta t$ in Figure 6a and against $\tau$ in Figure 6b. Similar results were obtained for the equivalent LL scheme. It is clear that when $\Delta t \approx 0.285$ (corresponding to $\tau \approx 0.36$), the model output is almost exactly Gaussian in shape and so the only errors in the results are due to the error in the node voltage distribution variance. Reducing the variance error to zero should therefore significantly increase the accuracy of the results.

A LR model with an initial Gaussian-shaped concentration distribution was run with $\tau$ constant and the error in the result was calculated after 10 time steps. The same model was also run with the adjustment ${}_2\tau = {}_2\tau^*$ and again the error was calculated. This was repeated for different $\tau$ values and the results are shown in Figure 7. In all cases shown adjusting the transmission coefficient for the second time step reduced the error in the node voltage after 10 time steps. The most significant reduction shown occurred with $\tau = 0.35$ (as expected from the results in Figure 6). For higher $\tau$ values adjusting ${}_2\tau$ can reduce the accuracy of the method as was seen in Figure 5b.

It is clear from Figure 7 that the error in the result after 10 time steps can be significantly reduced by altering ${}_2\tau$ and that the level of reduction depends on the value of $\tau$. What is not clear is whether this improvement is sustained over longer numbers of time steps. In order to answer this question, the models were run for 1000 time steps and the maximum absolute relative error in ${}_kVn$ was calculated at each time step using the formula [11]

$$ {}_kMARE = \max_{n=1}^{N}\left(\left|{}_kVn_n^{ANAL} - {}_kVn_n\right|\right) \Big/ \max_{n=1}^{N}\left({}_kVn_n^{ANAL}\right) \tag{71} $$

where ${}_kVn_n^{ANAL}$ is the analytical solution at node $n$ and time step $k$. This error value is plotted against $k$ for $\tau = 0.35$ in Figure 8 for a LR model. It is clear that adjusting ${}_2\tau$ gives improved results at every time step with the sole exception of time step 2. The same is true for the LL scheme.

In a typical transient modelling scenario the diffusion coefficient is set and a result is required for a particular point or points in time. In order to test the effect of adjusting ${}_2\tau$, standard and adjusted LR models were run with a diffusion coefficient of $D = 1$ and a node-spacing of $\Delta x = 1$ for a range of $\Delta t$ values and the maximum relative error at time $t = 20$ measured. The one model setting, $\tau$, is dependent on both $\Delta t$ and $D$ so, instead of plotting the error values against $\Delta t$, they are plotted against $\tau$. Similar results measured at $t = 100$ are presented in Figure 9b. While the error in the standard model reduces to a minimum as $\Delta t$ approaches zero, the error for the adjusted model

reaches a minimum for a time step corresponding to a transmission coefficient of approximately 0.35. Similar results were obtained from an equivalent LL model.

These results suggest that for a given node-spacing, the output obtained from an adjusted model with a time step giving $\tau \approx 0.35$ is more accurate than that obtained from a standard model with smaller time steps. This method, therefore, has the potential to deliver high accuracy with a reduced number of calculations.

So far the adjusted method has only been tested where the initial distribution is Gaussian in shape and the medium is infinite. Similar comparisons of the standard and adjusted models are made below for other initial and boundary conditions for which analytical solutions are available.

### *6.2 Infinite medium with step input*

The solution of the diffusion equation with initial conditions $\phi = 1$, $x < 0$; $\phi = 0$, $x > 0$; $t = 0$, over an infinite medium is [7]

$$\phi(x,t) = \tfrac{1}{2}\operatorname{erfc}\left(\tfrac{1}{2}x/\sqrt{Dt}\right) \tag{72}$$

where erfc is the error-function complement. A LR model was set up with 300 nodes, nodes 1 to 150 having an initial node voltage of 1 and nodes 151 to 300 set initially with ${}_0Vn = 0$, $x = 0$ corresponding to midway between nodes 150 and 151. Figure 10a shows a typical result obtained for a setting of $D = 2$ after 100 seconds with $\Delta x = \Delta t = 1$. At that time there is no variation in the concentration at the boundary so it can be assumed that the model represents an infinite system. Figure 10b shows the maximum relative error after 5 seconds for models with $D = 2$ over a range of $\Delta t$ (and, therefore, of $\tau$) values. As for an initial Gaussian-shaped distribution, the adjusted model gives more accurate results over a range of $\tau$ values. The minimum error for the adjusted model corresponds to $\tau \approx 0.4$. The same is true for the errors after 100 seconds. The same is also true for similar LL models if the nodes voltages are averaged over consecutive pairs of time steps.

The analysis method used above to obtain the formula for ${}_2\tau^*$ was based on the assumption that the solution was Gaussian-shaped. This is true for a single initial injection and for a Gaussian-shaped initial distribution in an infinite medium. It is not surprising that the adjustment of ${}_2\tau$ also increases the accuracy of the results obtained for an initial step input since the solution is the sum of a series of Gaussian-shaped distributions. This is not the case if the medium has a finite length.

### *6.3 Finite medium*

The analytical solution of the diffusion equation for a one-dimensional system of length $\lambda$ with boundary conditions $\phi(0,t) = \phi(\lambda,t) = 0$ and initial condition $\phi(x,0) = \sin(\pi x/\lambda) + 3\sin(2\pi x/\lambda)$ is [8]

$$\phi(x,t) = e^{-\left(D\pi^2/\lambda^2\right)t}\sin(\pi x/\lambda) + 3e^{-\left(4D\pi^2/\lambda^2\right)t}\sin(2\pi x/\lambda) \tag{73}$$

A LR model was set up with 21 nodes and $\Delta x = \Delta t = 1$. The fixed boundary concentrations were implemented using the standard method for the link-resistor scheme [3]. As before, the model was run with a fixed diffusion coefficient, $D = 2$, and a range of time step lengths with and without adjustment of the transmission coefficient for the second time step. The maximum relative errors calculated at $t = 5$ and $t = 200$ are plotted against $\tau$ in Figure 11. The optimum $\tau$ value for the adjusted model is approximately 0.35. The same is true for a similar LL model. It is interesting to note that as time progresses in this case (i.e. as the solution approaches a steady-state) the accuracy of the unadjusted model approaches that of the adjusted model (Figure 11b).

### *6.4 2-D modelling*

The analysis performed above for the one-dimensional lossy TLM method could be extended to two and three-dimensional schemes. It has been found, however, that if the same adjustment is made to the transmission coefficient in two-dimensional LR models as in the one-dimensional models then the long-term variance error is again reduced to zero. This is not the case for equivalent LL models.

The analytical solution of the two-dimensional diffusion equation with zero concentration at all points initially and boundary conditions $\phi(0,y,t) = \phi(\lambda,y,t) = \phi(x,0,t) = \phi(x,\lambda,t) = 100$ for $t > 0$, is [16]

$$\phi(x,y,t) = 100 - 100 \sum_{a,b=odd} \frac{16}{ab\pi^2} \sin\left(a\pi\frac{x}{\lambda}\right)\sin\left(b\pi\frac{y}{\lambda}\right)\exp\left(-\frac{\left(a^2+b^2\right)\pi^2}{\lambda^2}Dt\right) \qquad (74)$$

A LR model was used for comparison with 31×31 nodes, $D$ = 1 and $\Delta x$ = 1. The maximum relative error at time $t$ = 20 is plotted in Figure 12 against the transmission coefficient for the standard and adjusted model. The improvement due to the transmission coefficient adjustment is, once again, significant over a range of $\tau$ values. It should be noted that the optimum $\tau$ value is higher than for the one-dimensional case.

## 7. DISCUSSION AND CONCLUDING REMARKS

A novel technique has been developed for analysing TLM diffusion networks and has been successfully applied to both the LR and LL schemes. There is no reason why it cannot be similarly applied to more complex TL networks [11]. It can be used for parameterisation and can also yield equations for node voltage distribution variance errors.

The technique of state-space analysis has been used previously for parameterisation in TLM but this is limited to networks with a single scattering event per time step such as the LL diffusion scheme with constant TL impedance and cannot be applied to the LR TLM method [17-19]. Other techniques [9, 10, 13] have yielded equations for the node voltage variance over time after a single initial injection in the LL and LR diffusion schemes but these are more difficult to apply and provide less information. To date the new method has only been applied to a one-dimensional network but there would appear to be no reason why it could not be used to analyse multi-dimensional lossy TLM schemes.

One significant advantage of the new technique is that the equations derived at each step of the analysis can easily be checked against results obtained from a model since the mean positions, sums, and variances of all voltage distributions can be measured at each time step.

In an infinite medium after a single initial injection of diffusant the variance of the concentration distribution should increase over time at a constant rate related to the diffusion coefficient. When the increase in variance per time step is measured for standard diffusion models it is found that it initially varies over time before settling down at the correct value. This transient leads to significant errors over the first few time steps and to a constant long-term error in the variance of the node voltage distribution. An error in the variance will result in errors in the concentrations at each node. Testing has shown that for the TLM scheme the node voltage distribution is not Gaussian-shaped so the variance error is not the only source of concentration errors at each node. How close the shape is to Gaussian depends on the value of $\tau$, the transmission coefficient.

It has been shown that the variance error can be removed by initialising a model with *Vil* and *Vir* distributions that have mean positions separated by a certain distance related to $\tau$. Such an initialisation is not, however, consistent with the physical problem being modelled and is not, in general, possible for a given desired initial node voltage profile.

Analysis of the one-dimensional lossy TLM scheme has shown that the long-term variance error can also be reduced to zero simply by adjusting the transmission coefficient for one time step. Testing has shown that this can reduce the concentration errors in transient results, the level of reduction depending on $\tau$. Maximum accuracy occurs when $\tau$ is approximately equal to 0.35. For a constant diffusion coefficient, $D$, and a specified node-spacing, an adjusted model with $\Delta t$ selected so as to give a close to optimal value of $\tau$ will yield more accurate results than a standard model, even with a significantly shorter time step length.

The adjusted scheme is at least as accurate as the standard scheme for $\tau < 0.35$ in all cases tested. The optimum value of $\tau$ depends on the initial and boundary conditions but the testing performed to date indicates that, for a setting of $\tau \approx 0.35$, the results obtained from an adjusted model are consistently more accurate that those obtainable using the standard lossy TLM scheme.

In practical modelling situations $D$ may vary over time and space and it may also be desirable, for the sake of efficiency, to vary the node-spacing over space and $\Delta t$ over time. The fact that the method of error reduction proposed here only gives significant increases in accuracy over a small range of $\tau$ values may limit its advantages under such circumstances but further testing is required.

It has been found experimentally that the adjustment of $\tau$ required in a one-dimensional LR model in order to reduce the long-term variance error to zero is the same as that required in a 2-D LR model. It is assumed that it is the same in a 3-D model but this has not been tested here. The same is not true for the link-line configuration. Analysis of a 2-D LL network has not been performed to date.

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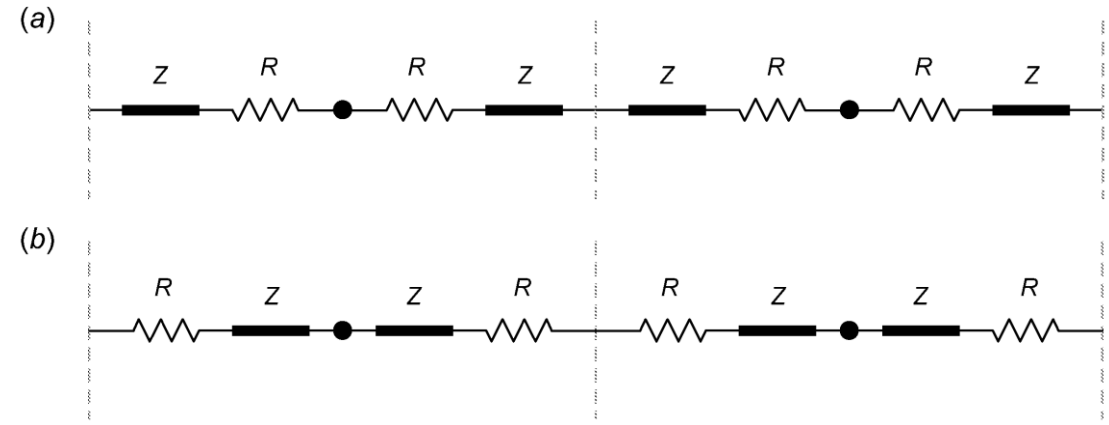


Figure 1: Link-line configuration with nodes located between resistor pairs (a) and link-resistor configuration with nodes located between TL segments (b).

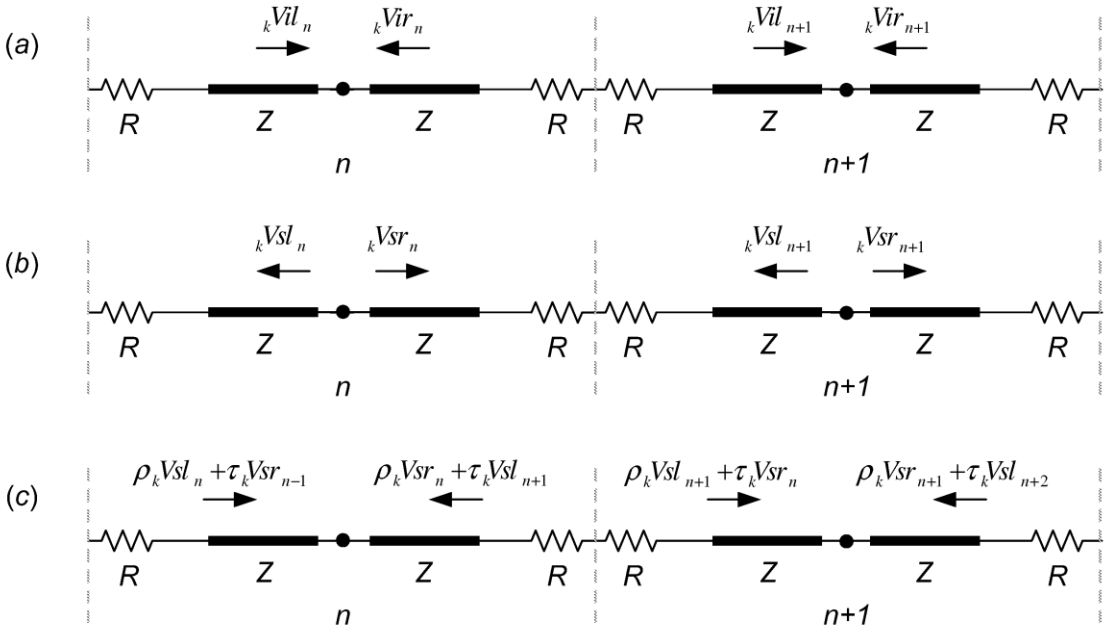


Figure 2: LR nodes with incident pulses (a), scattered pulses (b), and new incident pulses (c).

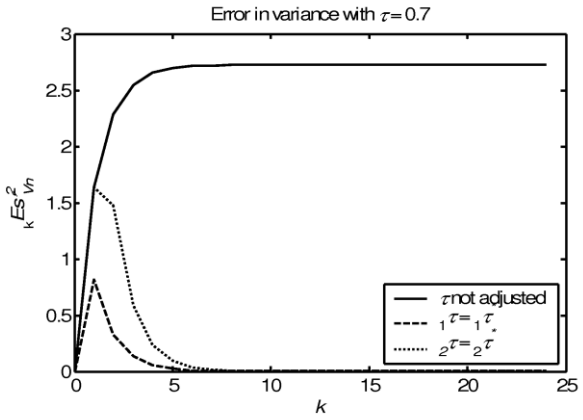


Figure 3: Error in variance for infinite models with single initial injections. Results are shown for three models, one standard model, one with $_1\tau$ adjusted, and one with $_2\tau$ adjusted. It can be seen that the long-term variance error for the adjusted models is 0.

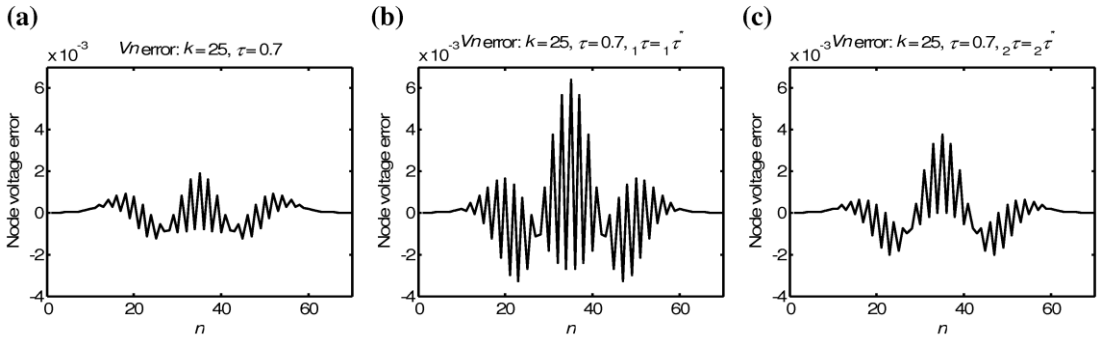


Figure 4: Errors in results from models with an initial injection at node 50 after 25 time steps with no adjustment (a), with the first time step adjusted, (b) and with the second time step adjusted (c).

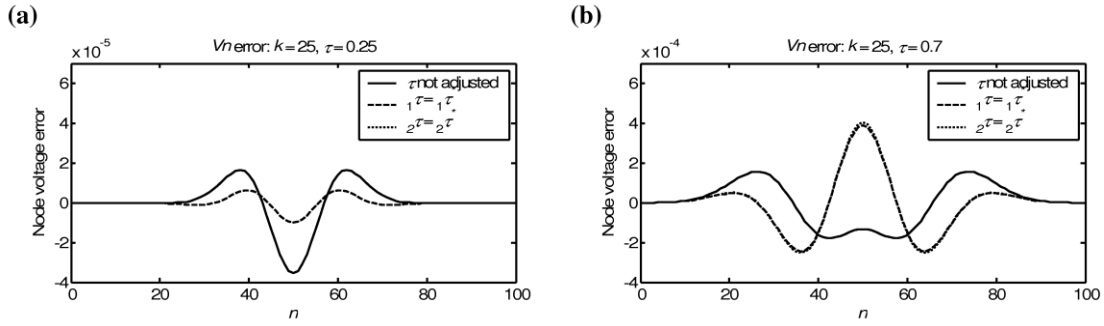


Figure 5: Errors in results from models with an initial Gaussian-shaped node voltage distribution with $\tau = 0.25$ (a) and $\tau = 0.7$ (b). The errors for the two adjusted models are similar in each case.

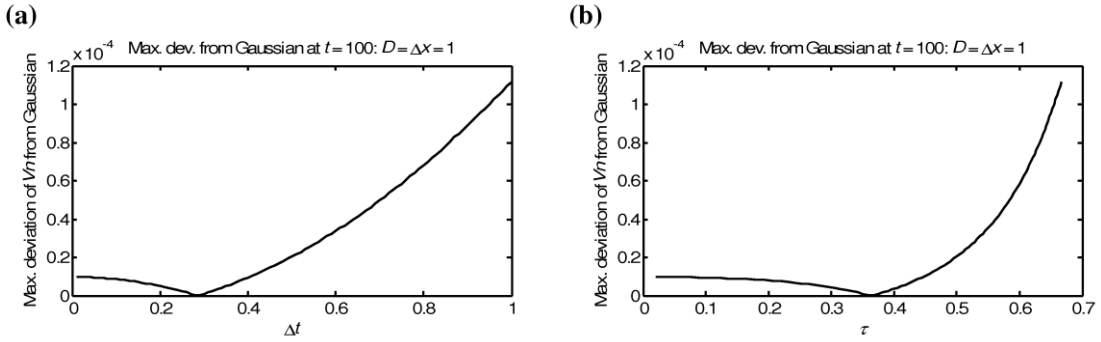


Figure 6: Maximum difference between the node voltages at $t$ = 100 for a model initialised with a Gaussian-shaped concentration distribution, and a Gaussian distribution with the same mean position, variance, and sum of values.

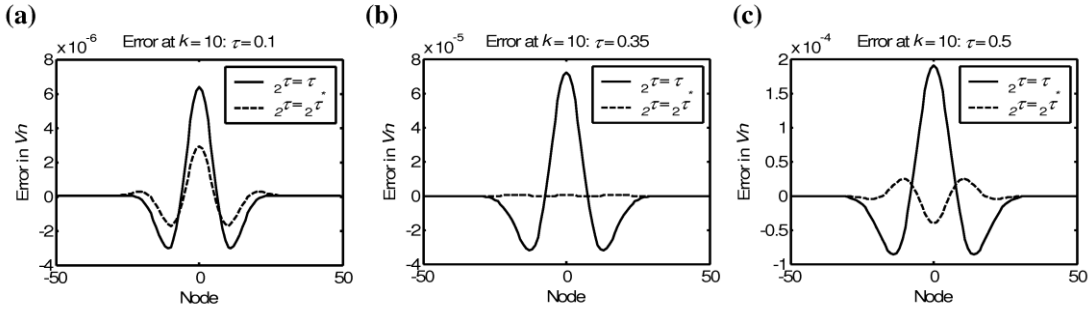


Figure 7: Errors for standard LR models after 10 time steps with initial Gaussian-shaped concentration distribution of cell variance 50 and errors for similar models with the second time step adjusted.

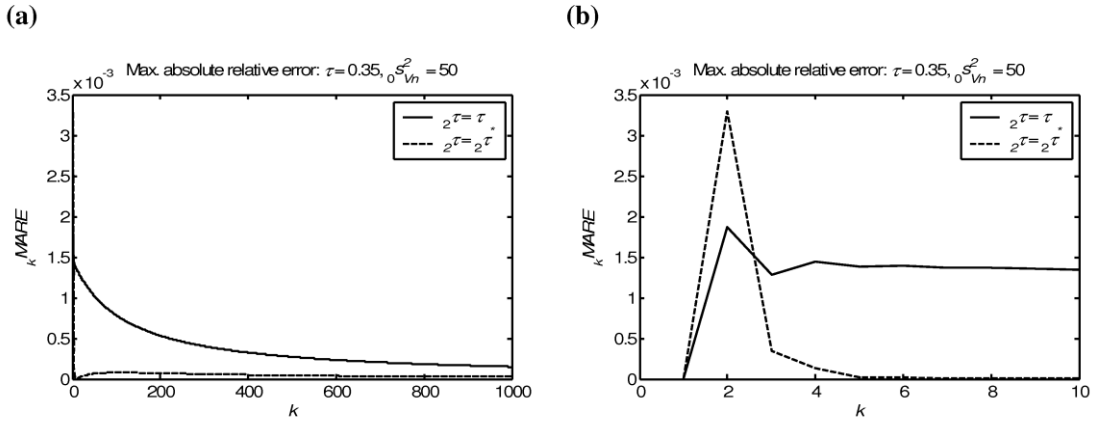


Figure 8: Maximum absolute relative errors plotted against $k$ for standard and adjusted models with initial Gaussian-shaped concentration profiles (a) and the same results for the first 10 time steps (b).

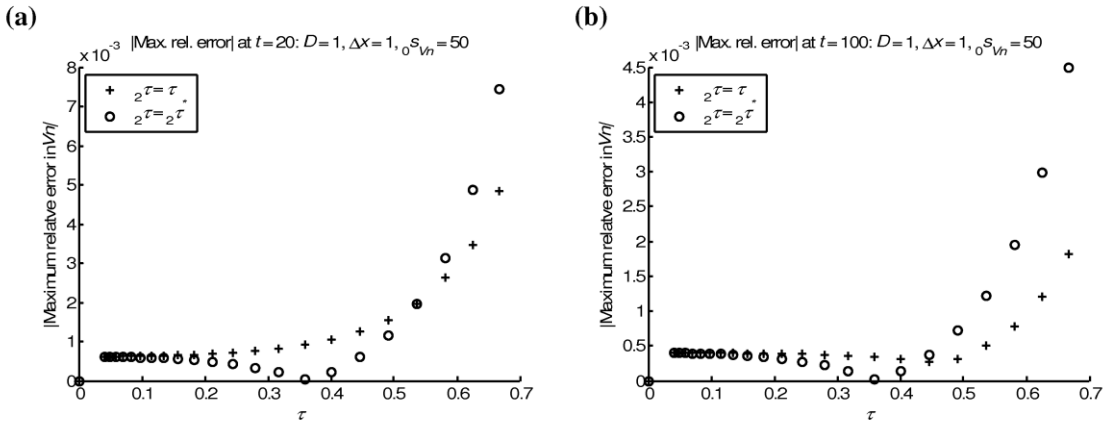


Figure 9: Maximum relative errors measured at $t$ = 20 (a) and $t$ = 100 (b) for standard and adjusted models plotted against $\tau$. Models were initialised with a Gaussian node voltage profile of variance 50.

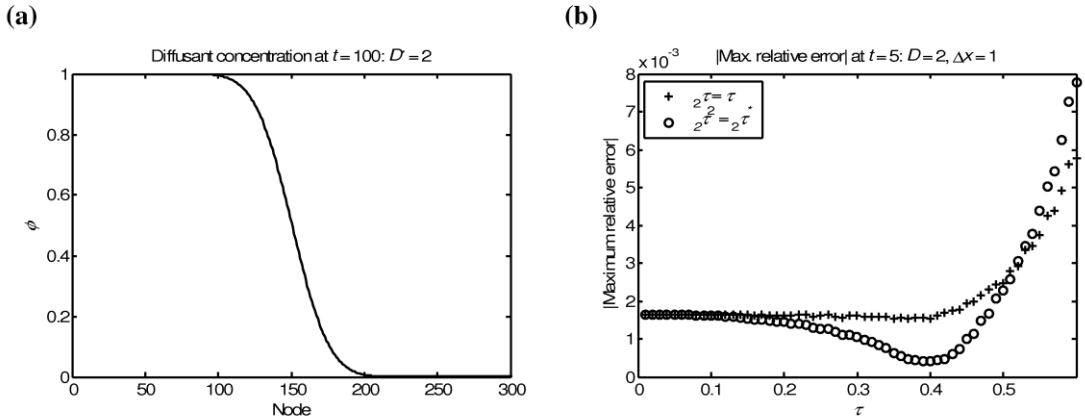


Figure 10: A typical result for an infinite LR model with an initial step input (a) and the maximum relative errors at $t$ = 5 for models with a fixed diffusion coefficient but with different $\Delta t$ (and, therefore, different $\tau$) values.

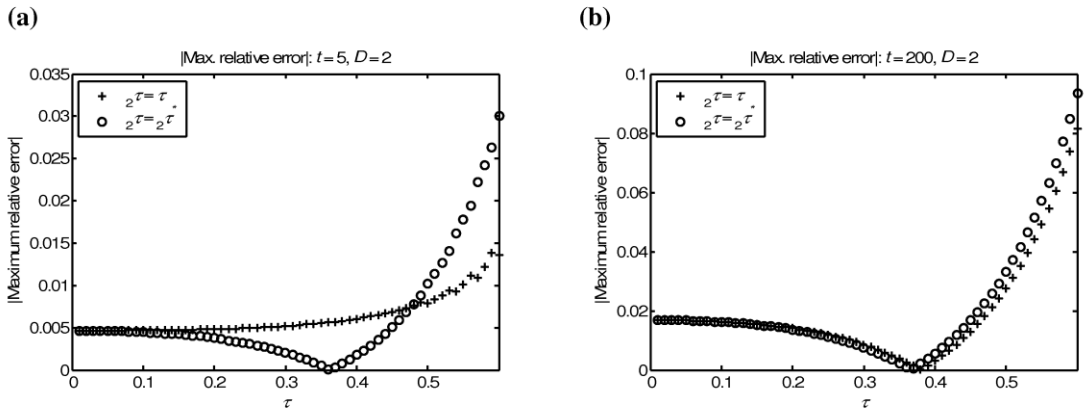


Figure 11: The maximum relative error magnitude at $t$ = 5 (a) and $t$ = 200 (b) for models of a finite space with fixed boundary conditions, a fixed diffusion coefficient, but with different $\Delta t$ (and, therefore, different $\tau$) values.

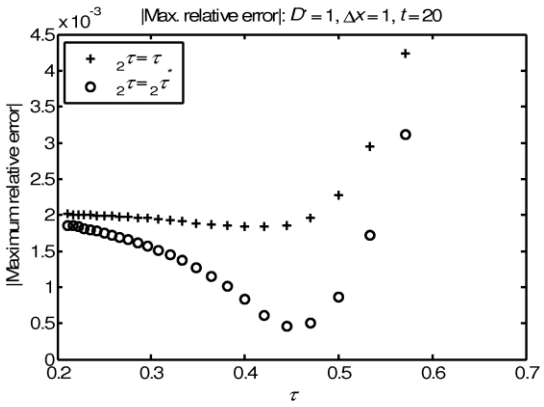


Figure 12: The maximum relative error magnitude after 20 seconds for 2D models with fixed concentration at all boundaries, a fixed diffusion coefficient value, and with different $\Delta t$ (and, therefore, different $\tau$) values.