ON THE NUMERICAL METHOD OF LINES FOR ONE DIMENSIONAL WATER QUALITY EQUATIONS.

by: R. Vichnevetsky and
Y. S. Shieh *

Department of Computer Science
Livingston College
Rutgers University
The State University of New Jersey
New Brunswick, New Jersey 08903

* Professor R. Vichnevetsky is from the Department of Computer Science
Mr. Shieh is a Graduate Student in the Department of Chemical and Biochemical Engineering.

Dept. of Computer Science Technical Report #20 - Nov. 1972

I. INTRODUCTION

Our interest in this report is in analysing properties of solutions obtained in the application of the continuous-time method of lines to the hyperbolic/parabolic partial differential equations describing one dimensional hydraulic and mass transfer phenomena used in water quality studies of rivers and estuaries.

In this context, "method of lines" (called MOL hereafter) refers to the numerical solution technique in which spatial derivatives are approximated by finite-differences thus replacing a partial differential equation with a coupled system of initial value ordinary differential equations. These are then integrated by classical numerical algorithms for such problems. The Runge Kutta-4 method seems to have been the prevalent algorithm utilised in water quality simulation work, ([2],[4]) but use of other time-integration techniques should be of equal value [3].

It is often the case that the accuracy of the time- integration approximation is higher than that of the spatial-difference approximation (whence the name "method of lines", which would otherwise be somewhat of a misnomer). Without attempting to justify whether this is a desirable choice of parameters, we assume that the time-integration is perfect, and thereby analyse the errors due to the spatial approximation alone.

In a separate report we shall look into the problem of numerical stability and time-integration accuracy, or derivation of maximum permissible values of the time increment Δt in the integration process. (See also ref [11] and [12] in this respect.)

One-dimensional hydrological models

One-dimensional water quality time-dependent mathematical models of rivers and estuaries consist of two types of partial differential equations, describing the hydrodynamic and mass transfer phenomena respectively. The former is expressed as 2 coupled equations of the hyperbolic type, in the simplest case of the form:

$$\left.\begin{aligned} &\frac{\partial h}{\partial t} + \frac{\partial (V \cdot h)}{\partial x} = 0 \\ &\frac{\partial V}{\partial t} + V\frac{\partial V}{\partial x} + k_1\frac{\partial h}{\partial x} + k_2 V \cdot |V| = 0 \end{aligned}\right\} \qquad \text{(i)}$$

(where $h(x,t)$ = water heigt and $V(x,t)$ = water velocity) whilst the latter consits of one transport equation for each species*, with diffusion and eventual coupled reaction terms:

$$\frac{\partial c_i}{\partial t} + \frac{\partial (V \cdot c_i)}{\partial x} = D_i \frac{\partial^2 c_i}{\partial x^2} + \sum_j k_{ij}(c_i, c_j) \qquad \text{(ii)}$$

(Where $C_i(x,t)$= species concentration)

The characteristic form of the hyperbolic system (i) consits of two equations which are (save for the absence of diffusion) similar to the

---

*including the water temperature T(x,t), considered as a "species".

transport equation (ii). In their numerical treatment both (i) and (ii) have therefore strong common properties, which are also those observed in the numerical treatment of the pure transport, hyperbolic equation:

$$\frac{\partial u}{\partial t} + \frac{\partial (V \cdot u)}{\partial x} = 0 \qquad \text{(iii)}$$

The additional terms in either of the aforementioned equations are small. Moreover, they contribute little to the properties and difficulties of numerical integration.

We shall therefore analyze properties of the numerical solutions of (iii), as a model of the same properties found in the numerical treatment of the typical equation (i) and (ii) found in water qualitysimulation.

This analysis is in many aspects qualitative: rather than using the classical form of truncation errors in higher derivative form, we are using both the concept of frequency analysis*, (or solution of the algorithm with periodic, sinusoidal inputs) and the concepts of spurious dispersion and diffusion which are induced by the approximation.

---

*

The concepts of frequency response and transfer functions as tools to analyze water quality in bodies of water are described e.g. in Thomann (1963) and in Davidson, et al.(1971).

We are also restricting our analysis to the case V = constant. The equation (iii) is then

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = 0 \qquad (1)$$

Whilst many problems of interest in water quality simulation involve a variable velocity, the simpler constant velocity model (1) affords a more detailed mathematical analysis, and the qualitative properties of the computation so derived apply equally well to the more complex equations (i) and (ii) on a spatially precewise basis.

Summary of Results

Approximation errors which are inherent to the numerical solution of the hyperbolic/parabolic partial-differential equations modeling one-dimentional water quality place limitations upon the types of prescribed initial and boundary conditions allowed in computer simulation. In the numerical method of lines (which consists in approximating a partial-differential equation by ordinary difference-differential equations of the initial-value type), these limitations are a function of the spatial finite increment Δx, and of its relation to the parameters of the physical problem at hand.

The main results of the analysis contained in this report may be summarized as follows, as they apply to the simulation of non-tidal rivers and estuaries:

- in the numerical simulation of periodic fluctuations of wavelength λ, the ratio $N_\lambda = (\lambda/\Delta x)$, (which is the number of numerical simulation points per wavelength) must always be equal or larger to 2π, and preferably larger than 4π.

- if these fluctuations are created by periodic imposed boundary conditions of frequency Ω (in radians per unit time) this frequency must be constrained upwards by $(\Omega \cdot \Delta x/V) \leq 1$, and preferably $(\Omega \cdot \Delta x/V) \leq .5$, where V is the minimum velocity of the water.

- where central differences in space are used, spurious diffusion is introduced by the approximation when $N_\lambda \leq 2\pi$ or $(\Omega \cdot \Delta x/V) \geq 1$.

- when backward differences in space are used, spurious diffusion is always introduced by the approximation, but is kept to an acceptable value when $N_\lambda \geq 4\pi$

- the velocity of propagation of sinusoidal solutions is a function of λ (or Ω) in the numerical approximations. The resulting velocity error is also kept to an acceptable value when $N_\lambda \geq 4\pi$, in the central difference as well as backward difference cases.

The two latter conclusions are illustrated in Figures Ia, b and c. Central differences are used to obtain numerical solutions with a sinusoidal input to the convection-decay equation for BOD concentration in water:

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = - A \cdot u$$

in fig. (I-a) N_λ is equal to 15 whilst in (I-b) it is equal to 10. The lack of spurious diffusion is observed in both cases by the near correctness of the amplitude, whilst the velocity error is well apparent in the latter case, and negligible in the former.

In fig (I-c), N_λ is equal to 5: both the amplitude and velocity of the numerical solution are seen to be significantly in error.

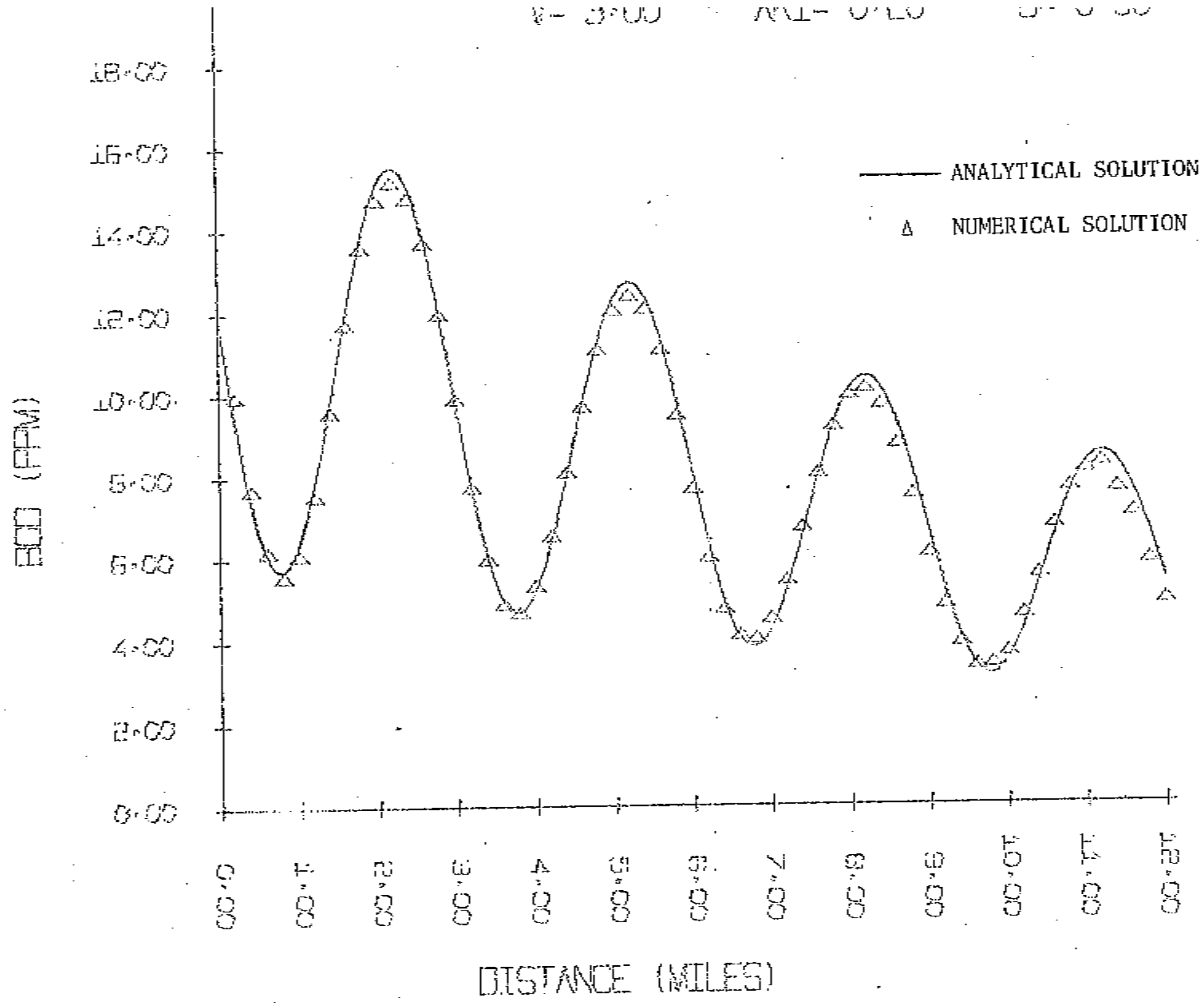


Fig. I-a $N_\lambda \simeq 15$; $(\Omega \cdot \Delta x / V) \simeq 0.4$

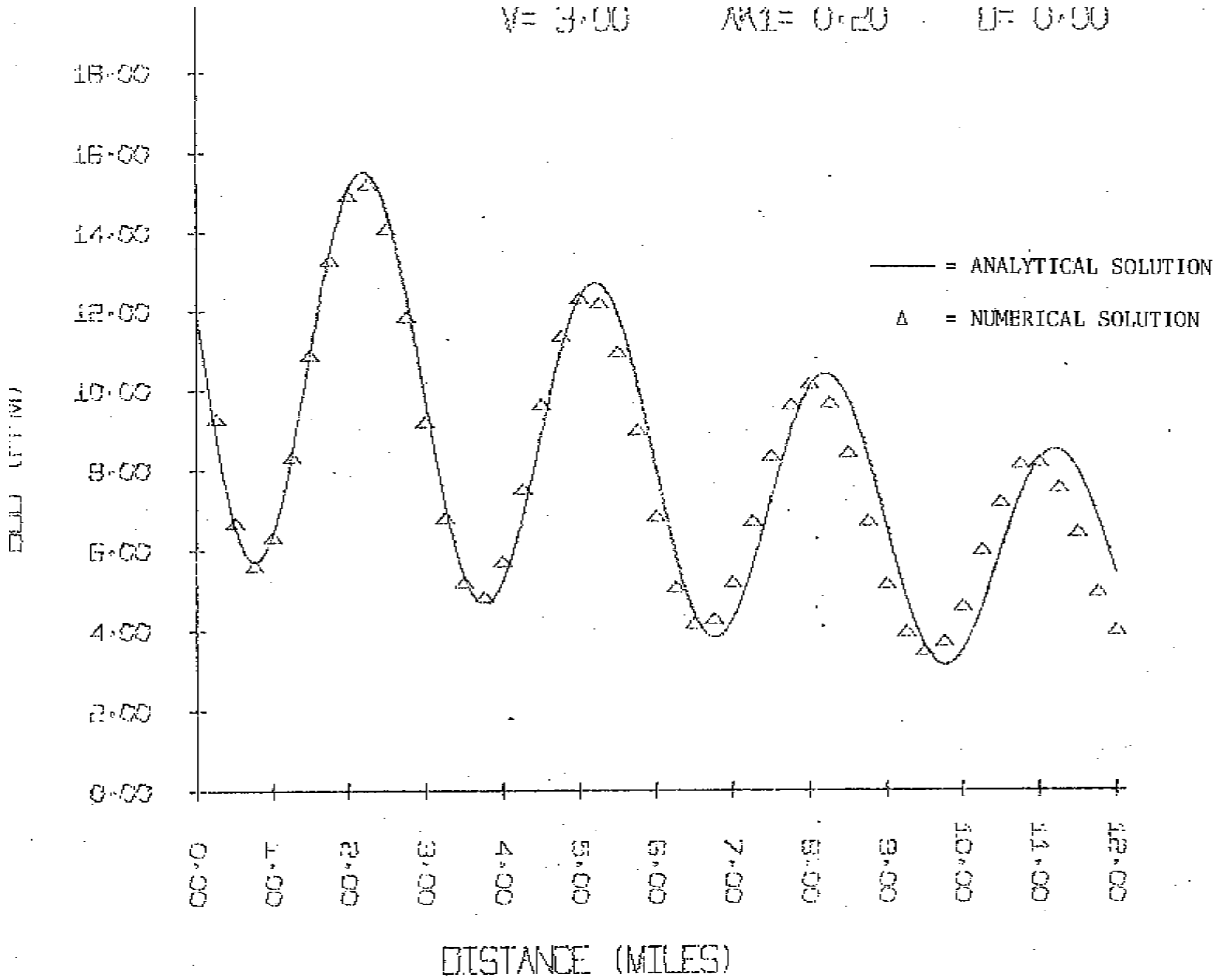


Fig. I-b $N_\lambda \simeq 10$; $(\Omega \cdot \Delta x / V) \simeq .62$

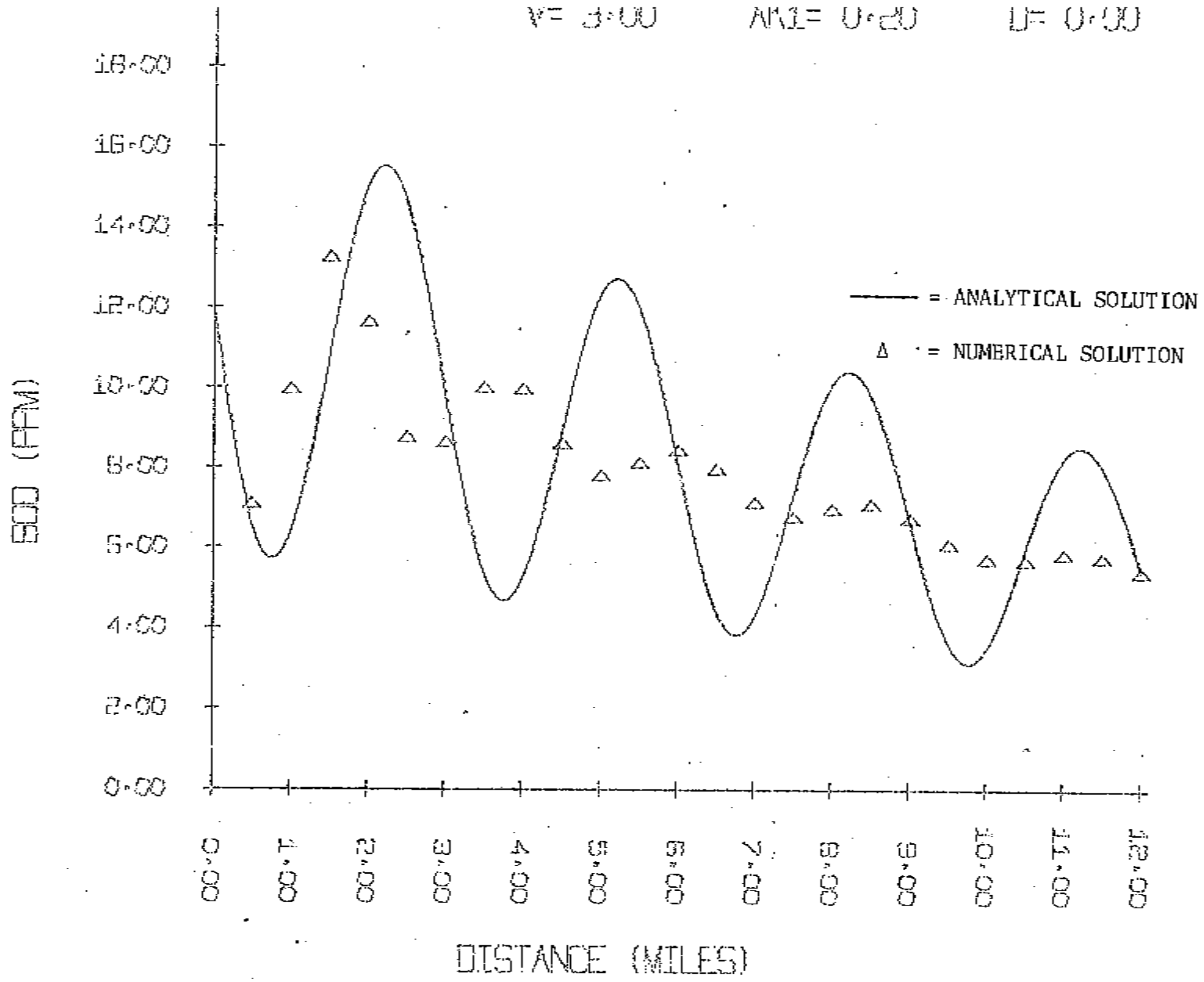


Fig. I-c $N_\lambda \simeq 5$; $(\Omega \cdot \Delta x / V) \simeq 1.2$

II. METHODS OF LINES USING CENTRAL SPATIAL DIFFERENCES

II.1. The method of lines

There are several versions of the MOL as applied to the equation (1), each corresponding to a different approximation of the spatial partial derivative.

The central-differences version of this method consists in replacing thisspatial derivative by the approximation

$$\left(\frac{\partial u}{\partial x}\right)_{x_n} \simeq \frac{u_{n+1} - u_{n-1}}{2 \cdot \Delta x}$$

with

$$\left.\begin{array}{l} u_n(t) \simeq u(x_n, t) \\ x_n \simeq n.\Delta x \;;\; n = 1, 2, \ldots\ldots \end{array}\right\} \qquad (2)$$

Thus, (1) is replaced by the system of ordinary differential equations of the initial value type (see fig 1)

$$\frac{du_n}{dt} = -V\left(\frac{u_{n+1} - u_{n-1}}{2 \cdot \Delta x}\right) ; n = 1, 2, \ldots \qquad (3)$$

which may be integrated in time by the use of classical numerical methods for such problems.

It is assumed that the numerical integration-in-time is perfect. That is, we analyze the consequences of difference approximations such as (2) alone. (We shall consider in section III other difference approximations than (2) to replace $\partial u/\partial x$).

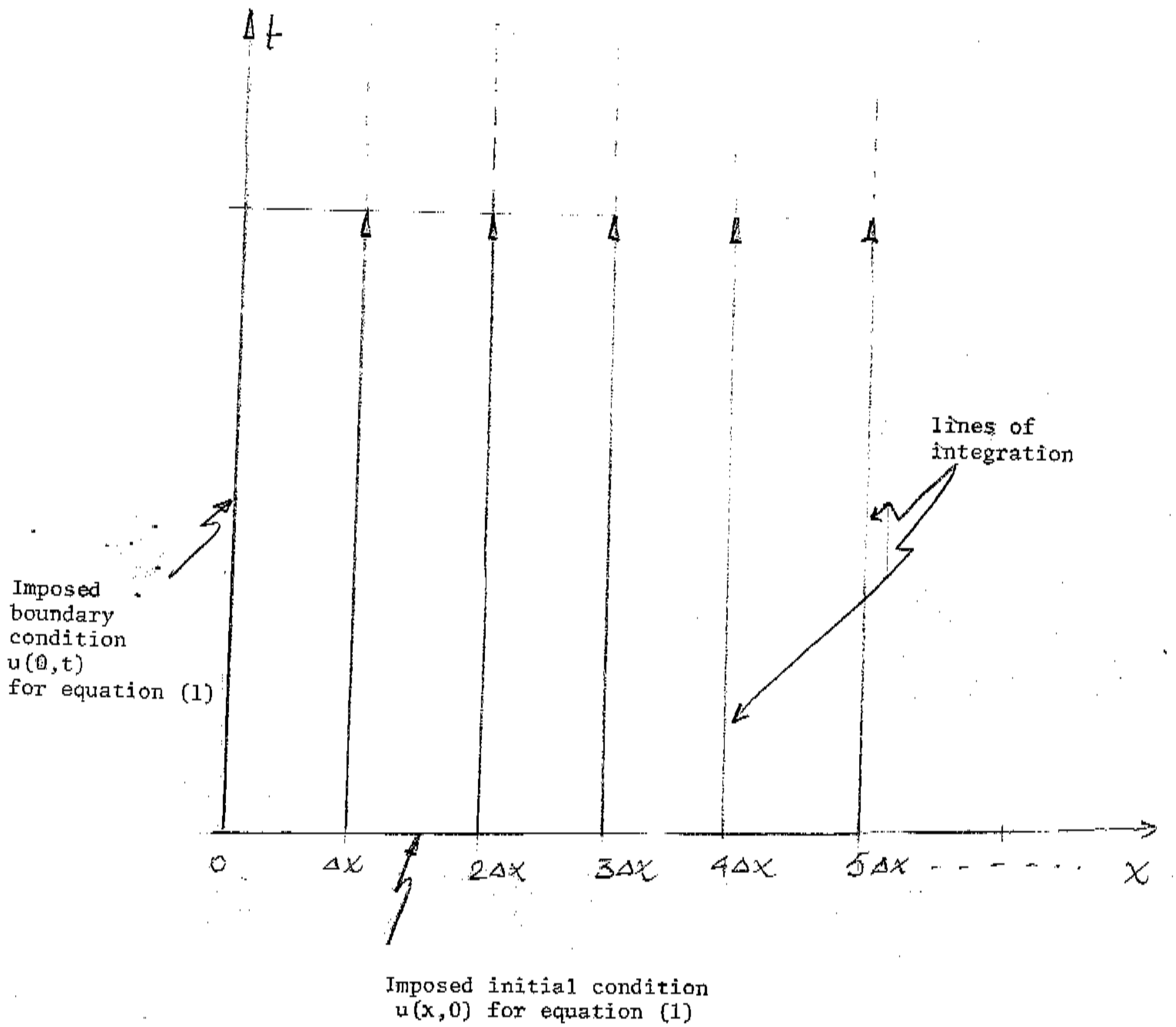


Figure 1. Continuous-Time Method of Lines.

II.2. PROPERTIES OF SINUSOIDAL SOLUTIONS

Since equation (1) is linear, sinusoidal components of different wavelength in the solution may be analysed separately.

With this in mind, let the boundary condition $u(0,t)$ be:

$$u(0,t) = \sin \Omega t \tag{4}$$

where the time-frequency Ω is expressed in radians per unit time

a) Properties of the exact solution

The steady-state solution of equation (1) in response to this boundary condition is (Fig. 2-a)

$$u(x,t) = \sin \Omega \left(t - \frac{x}{V}\right) \tag{5}$$

(verification by substitution is trivial)

The spatial dependence of this solution is also sinusoidal, with the spatial frequency (in radians per unit length)

$$\omega = \frac{\Omega}{V} \tag{6}$$

and associated wavelength

$$\lambda = \frac{2\pi V}{\Omega} \tag{7}$$

This wave propagates at the phase velocity V, with a constant amplitude.

Note that (5) may also be written as

$$u(x,t) = \sin \omega (Vt - x) \tag{8}$$

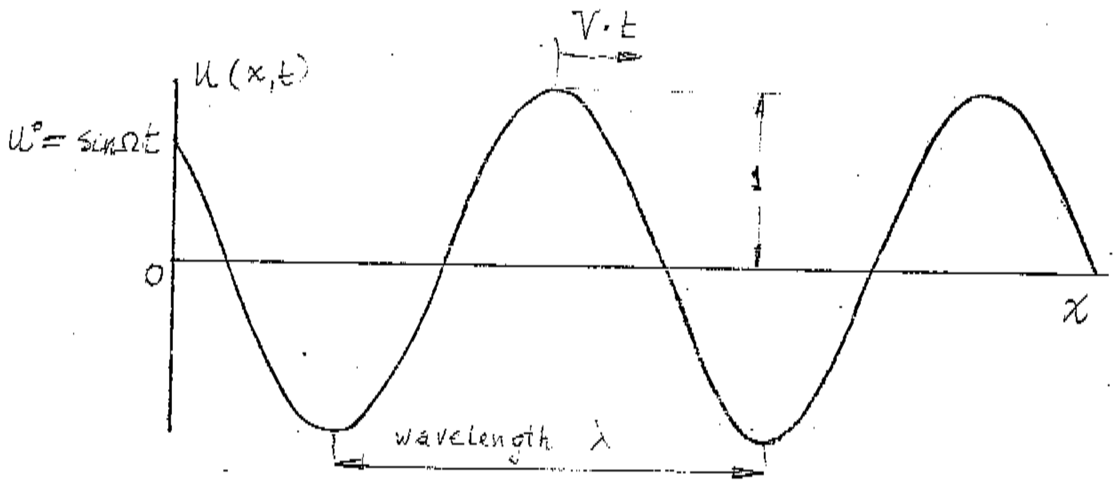


Figure 2-a. Exact response of equation (1) to a sinusoidal imposed boundary value.

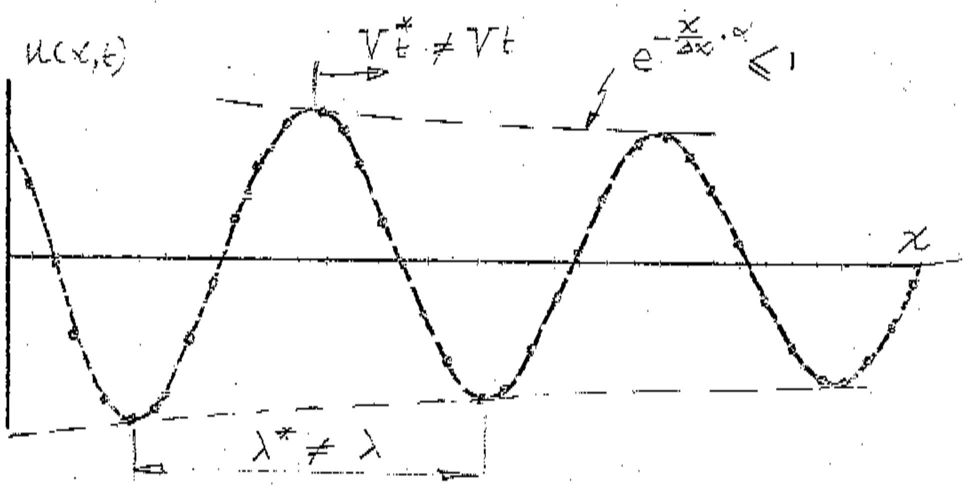


Figure 2-b. Numerical response of equation (1) to a sinusoidal imposed boundary value, obtained numerically by application of the Method of Lines.

b) Properties of the numerical solution (with central differences)

Sinusoidal fluctuations in the solution which are represented numerically with the MOL approximation deviate from the analytic solution. Whilst the sinusoidal nature of the solution is preserved, the amplitude and velocity of propagation become functions of the frequency. We shall analyse this from three different viewpoints

i. By expressing analytically the numerical sinusoidal response, and analysing the distorsion of its characteristics in terms of amplitude, velocity, wavelength, etc.

ii. By expressing the same result as i, in the familiar form of transfer functions.

iii. By an interpretation of the deviation of the numerical solution in terms of the physical concepts of dissipation, diffusion and dispersion.

Analytical form of the numerical sinusoidal response

Let

$$u(n\cdot\Delta x, t) \simeq u_n(t) = e^{-n\alpha} \sin\Omega\left(t - \frac{x}{V^*}\right) \tag{9}$$

be a trial solution of the numerical approximation (3). (Fig. 2-b) with the boundary condition (4), assuming perfect time integration, and where V^* and $e^{-n\alpha}$ are the numerical representations of the corresponding parameters in (5), that is, of V and 1. The particular form of this trial solution is based on the assumption that the sinusoidal response of the numerical approximation is sinusoidal in space, propagates at a velocity V^* (which may be different from V) and has a spatially decaying amplitude expressed by the exponential function $e^{-n\alpha} = e^{-\frac{x}{\Delta x}\cdot\alpha}$ where α is a real number. (when $\alpha = 0$, $e^{-\alpha} = 1$ and there is no decay)

As we shall see, V^* and $e^{-\alpha}$ are functions of the time-frequency ω. Upon substitution of (9) into the MOL equations (3) and elimination of common terms we find

$$\Omega \cdot \cos\Omega\left(t-\frac{x}{V^*}\right) = -\frac{V}{\Delta x}\left[\operatorname{Sh}\alpha \cdot \cos\left(\frac{\Omega \cdot \Delta x}{V^*}\right) \cdot \sin\Omega\left(t-\frac{x}{V^*}\right) - \operatorname{Ch}\alpha \cdot \sin\left(\frac{\Omega \cdot \Delta x}{V^*}\right) \cdot \cos\Omega\left(t-\frac{x}{V^*}\right)\right] \quad (10)$$

which must become an identity with the appropriate values of V^* and α.

<u>Case 1</u>:

For $\frac{\Omega \cdot \Delta x}{V} \leq 1$, expression (10) becomes an identity with $\alpha = 0$ and $(V/\Omega \cdot \Delta x) \cdot \sin(\Omega \cdot \Delta x / V^*) = 1$

That is,

$$\alpha = 0 \text{ or } e^{\alpha} = 1 \quad (11)$$

and

$$V^* = \frac{\Omega \cdot \Delta x}{\operatorname{arc\,sin}(\Omega \cdot \Delta x / V)} = V \cdot \left(\frac{\Omega \cdot \Delta x / V}{\operatorname{arc\,sin}(\Omega \cdot \Delta x / V)}\right) \quad (12)$$

V^* is the <u>phase velocity of the numerical solution</u>.

Likewise, we find by use of the relations (6) and (7):

- <u>spatial frequency of the numerical solution</u> (in radians per unit length):

$$\omega^* = \frac{1}{\Delta x} \cdot \operatorname{arc\,sin}(\Omega \cdot \Delta x / V) = \left(\frac{\operatorname{arc\,sin}(\Omega \cdot \Delta x / V)}{(\Omega \cdot \Delta x / V)}\right) \quad (13)$$

- <u>wave length of the numerical solution</u> (in unit length):

$$\lambda^* = \frac{2\pi \cdot \Delta x}{\operatorname{arc\,sin}(\Omega \cdot \Delta x / V)} = \lambda\left(\frac{(\Omega \cdot \Delta x / V)}{\operatorname{arc\,sin}(\Omega \cdot \Delta x / V)}\right) \quad (14)$$

It may be verified that V^*, ω^* and λ^* converge to V, ω and λ when $(\Omega \cdot \Delta x / V) \to 0$

If we let (see fig. 3)

$$R\left(\frac{\Omega \cdot \Delta x}{V}\right) \triangleq \frac{\operatorname{arc\,sin}(\Omega \cdot \Delta x / V)}{(\Omega \cdot \Delta x / V)} \quad (15)$$

then these relations may be rewritten simply as:

$$V^*/V = 1/R \quad (16)$$

$$\omega^*/\omega = R \quad (17)$$

$$\lambda^*/\lambda = 1/R \quad (18)$$

In summary, sinusoidal fluctuations for which $(\Omega \cdot \Delta x/V) \leq 1$ holds are, with the approximation (3), represented numerically by constant-amplitude sinusoidal solutions, whose velocity, frequency and wavelength distorsion are expressed by (16), (17) and (18), respectively.

A good visualization of this analysis is afforded by expressing the quantity $(\Omega \cdot \Delta x/V)$ by use of the wavelength λ :

$$(\Omega \cdot \Delta x/V) = (2\pi \cdot \Delta x/\lambda)$$

and by noting that $\lambda/\Delta x = N_\lambda$ is the number of spatial increments Δx or number of solution points per exact wavelength λ in the numerical representation. Whence, $(\Omega \cdot \Delta x/V) \equiv (2\pi/N_\lambda)$

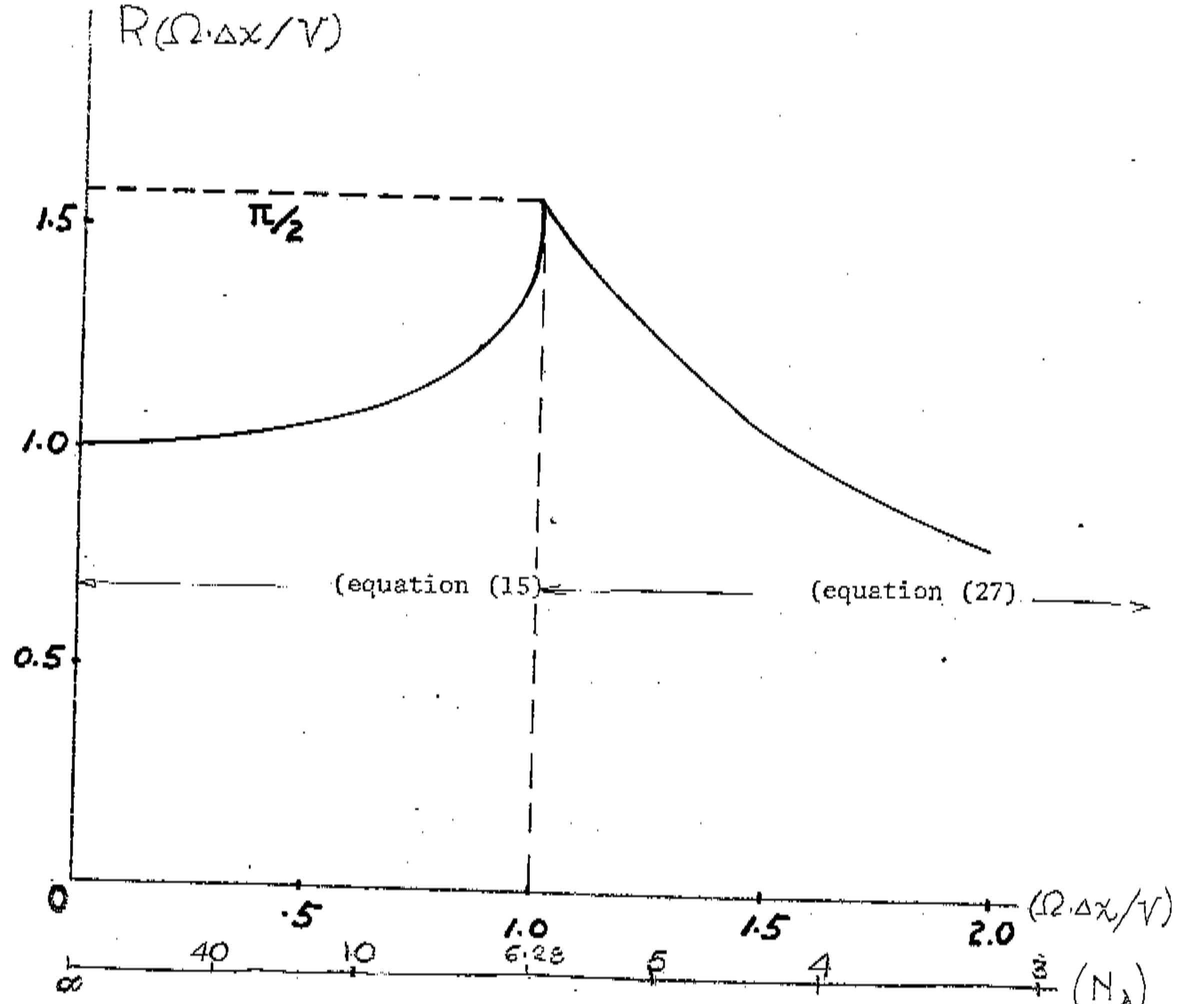
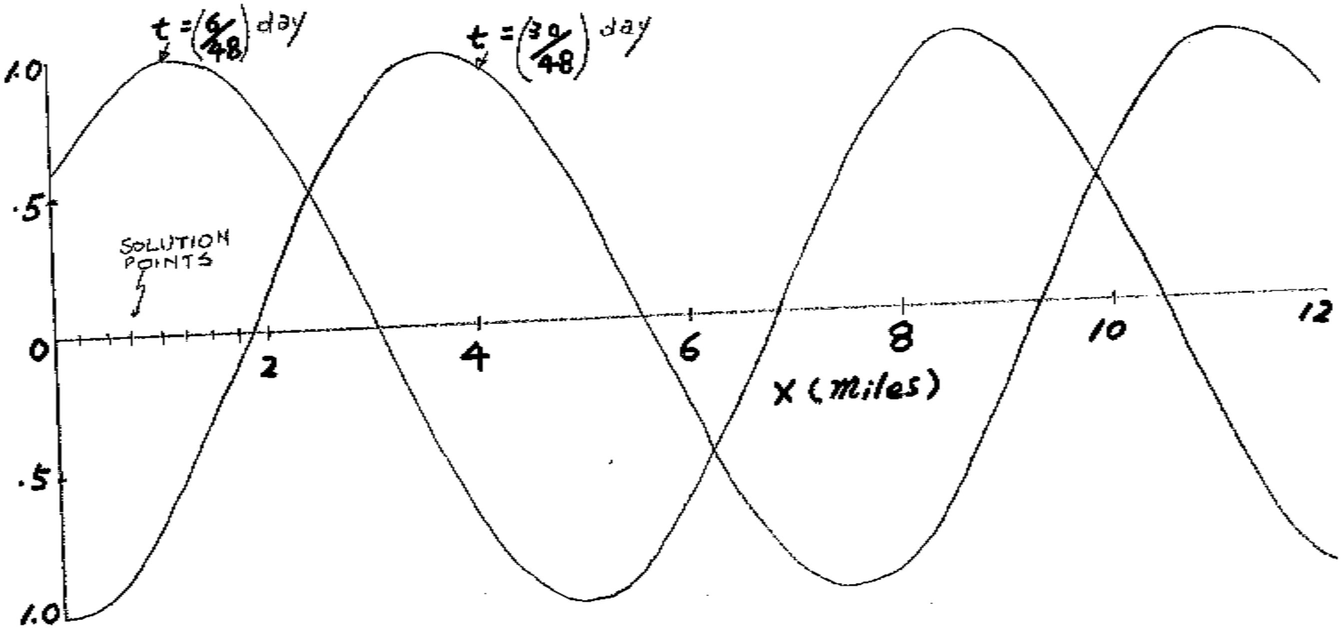


Figure 3. The function R $\left(\frac{\Omega \cdot \Delta x}{V}\right)$ - central differences case.

The N_λ scale gives the number of solution points per exact wavelength λ

$\Omega = 4.188$ $\quad \Delta x = 0.25$ mi $\quad V = 5$ mi/day

$T = 1.5$ $\quad \Delta t = (1/48)$ day $\quad V^* = 4.9$ mi/day



SINUSOIDAL RESPONSE

TYPICAL COMPUTER RESULT - CENTRAL DIFFERENCES - $(\Omega \cdot \Delta x / V) < 1$

(OR $N_\lambda > 2\pi$)

Case 2:

When $\frac{\Omega \cdot \Delta x}{V} > 1$ the identity condition of the left and right hand sides of (10) requires that:

$$(\Omega \cdot \Delta x / V^*) = \pi/2 \tag{19}$$

and

$$(V/\Omega \cdot \Delta x) \cdot Ch\,\alpha = 1 \tag{20}$$

That is:

$$V^* = \frac{2\,\Omega \cdot \Delta x}{\pi} \tag{21}$$

and

$$Ch\,\alpha = \frac{\Omega \cdot \Delta x}{V}$$

or

$$e^{-\alpha} = e^{-\arg \cdot Ch(\;\cdot \Delta x / V)} \tag{22}$$

We will show later [equation (38)] that this function may also be expressed as

$$e^{-\alpha} = \frac{\Omega \cdot \Delta x}{V} - \sqrt{\left(\frac{\Delta x}{V}\right)^2 - 1} \tag{22-a}$$

We may observe that we have the interesting properties :

• phase velocity of the numerical solution=

$$V^* = 2\Omega \cdot \Delta x / \pi \tag{23}$$

which is independent of V

• spatial frequency of the numerical solution=

$$\omega^* = \pi/2 \cdot \Delta x = \text{constant} \tag{24}$$

• wavelength of the numerical solution=

$$\lambda^* = 4 \cdot \Delta x = \text{constant} \tag{25}$$

Also in this case, the amplitude of the solution is not constant but decays with n as

$$e^{-n \cdot \arg\, Ch(\Omega \cdot \Delta x / V)} = \left(\left(\frac{\Omega \cdot \Delta x}{V}\right) - \sqrt{\left(\frac{\Omega \cdot \Delta x}{V}\right)^2 - 1}\right)^n \tag{26}$$

The relations (23), (24) and (25) may be rewritten as before in the form

$$\frac{V}{V^*} = \frac{\omega^*}{\omega} = \frac{\lambda}{\lambda^*} = R$$

where R is now the function = (for $\frac{\omega \cdot \Delta x}{V} \geqslant 1$):

$$R = \frac{\pi}{2} \cdot \frac{1}{(\Omega \cdot \Delta x / V)} \tag{27}$$

(Note that $R = 1$ for $\left(\frac{\Omega \cdot \Delta x}{V}\right) = \pi/2$).

II. 3. SELECTION OF A SPATIAL INCREMENT

If we choose a deviation of 10% in the ratio $\frac{V^*}{V}$), or ($|R-1| \leq .1$) as an upper bound of the acceptable approximation error, this leads (in the central differences case) to a maximum permissible value of $(\omega \cdot \Delta x / V)$ of about .7.

This also leads to the condition = $(N_\lambda)_{min} = \frac{\lambda_{min}}{\Delta x} \geqslant 2\pi/.7 \simeq 9$

Which is equivalent to stating that one should choose a minimum of 9 spatial increments Δx per shortest wavelength of interest. (Choosing $N_\lambda = 10$, which corresponds to $(\Omega_{max} \cdot \Delta x / V = \pi/5)$ is an easily remembered criterion).

II. 4. LAPLACE TRANSFORM ANALYSIS

A Laplace transform analysis confirms the results of the preceding section, and affords in addition an explanation of the observed response of the approximation to a step-variation at the boundary.

Consider equation (1) with the boundary conditions=

$$\left.\begin{array}{l} u(x,0) = 0 \\ u(0,t) = u_0(t) \quad \text{given} \end{array}\right\} \tag{28}$$

For fixed values of x, let

$$U(s,x) \triangleq \int_0^\infty u(x,t)\cdot e^{-st}\,dt = \mathcal{L}[u(x,t)]$$

be the Laplace transform of the solution. By substitution into (1) it is easily found that $U(s,x)$ satisfies the relation

$$U(s,x) = U(s,0)\cdot e^{-sx/V} \tag{29}$$

The factor $e^{-sx/V}$ is the transfer function (or ratio of Laplace transforms) for the solution between the points x (the output) and o (the input).

As one may expect, the exact relation (29)is not satisfied by the solution of the numerical approximation (3).

To obtain an equivalent transfer-function expression for this approximation let $U_n(s)$ be the Laplace-transform of $u_n(t)$

Call $E(s)$ the (yet unknown) transfer function between x_n and x_{n+1} for all n, that is:

---

*The assumption that $E(s)$ is independent of n implies that x_{max} or $n_{max} = \infty$. Whilst this is never verified in practice, proper numerical handling of the boundary condition in $x = x_{max}$ (as e.g. in ref. [13]) has the effect of making this assumption verified to a degree of accuracy more than compatible with the other assumptions in the present problem.

$$E(s) \triangleq \frac{U_{n+1}(s)}{U_n(s)} = \frac{U_n(s)}{U_{n-1}(s)} = \cdots \tag{30}$$

The equation (3) may then be rewritten as:

$$s \cdot U_n(s) = -\frac{V}{\Delta x}\left[\frac{E(s) - E^{-1}(s)}{2}\right] \cdot U_n(s)$$

or

$$s = -\frac{V}{\Delta x}\left[\frac{E(s) - E^{-1}(s)}{2}\right] \tag{31}$$

By letting $E(s) = e^{-\beta(s)}$, we may ·ite

$$s = +\frac{V}{\Delta x} \cdot \mathrm{Sh}\,\beta \qquad (\text{from}(31))$$

whence $\beta = \arg \mathrm{Sh}\,(s \cdot \Delta x / V)$

and

$$E(s) = e^{-\arg \mathrm{Sh}\,(s \cdot \Delta x / V)} \tag{32}$$

Thus,

$$\frac{U_{n+1}(s)}{U_n(s)} = E(s) = e^{-\arg \mathrm{Sh}(s \cdot \Delta x / V)} \tag{33}$$

and

$$\frac{U_n(s)}{U_0(s)} = \left[E(s)\right]^n = e^{-n \arg \mathrm{Sh}(s \cdot \Delta x / V)} \tag{34}$$

which are transfer-function representations of the difference approximation process (3).

The transfer function $e^{-\arg Sh \frac{s\cdot\Delta x}{V}}$

Consider the transfer function $E(s) = e^{-\arg Sh \frac{s\cdot\Delta x}{V}}$ along the imaginary axis $s = i\omega$.

a) $\dfrac{\Omega\cdot\Delta x}{V} < 1$

One has then $\arg Sh\, i\left(\frac{\Omega\cdot\Delta x}{V}\right) = i \,\mathrm{arc}\sin\left(\frac{\Omega\cdot\Delta x}{V}\right)$

whence

$$E = e^{-i\,\mathrm{arc}\sin\left(\frac{\Omega\cdot\Delta x}{V}\right)} \tag{35}$$

which has the amplitude

$$|E| = 1 \tag{36}$$

and the phase

$$\angle E = -\,\mathrm{arc}\sin\left(\frac{\cdot\Delta x}{V}\right) \tag{37}$$

b) $\dfrac{\Omega\cdot\Delta x}{V} \geqslant 1$

Then we may return to equation(31) which yields, successively:

$$E^2 + 2i\frac{\Omega\cdot\Delta x}{V}E - 1 = 0$$

which has the two roots

$$E = -i\left(\frac{\Omega\cdot\Delta x}{V} \pm \sqrt{\left(\frac{\Omega\cdot\Delta x}{V}\right)^2 - 1}\right)$$

It may be easily shown that only the minus sign is to be used. Thus

$$E = -i\left(\frac{\Omega\cdot\Delta x}{V} - \sqrt{\left(\frac{\Omega\cdot\Delta x}{V}\right)^2 - 1}\right) \tag{38}$$

which has the phase $\angle E = -\frac{\pi}{2}$ and the decaying amplitude shown in the following figure. This function may also be expressed as

$$E = e^{-i\frac{\pi}{2} - \arg Ch\left(\frac{\Omega\cdot\Delta x}{2}\right)} = -i\cdot e^{-\arg Ch\left(\frac{\Omega\cdot\Delta x}{2}\right)} \tag{38-2}$$

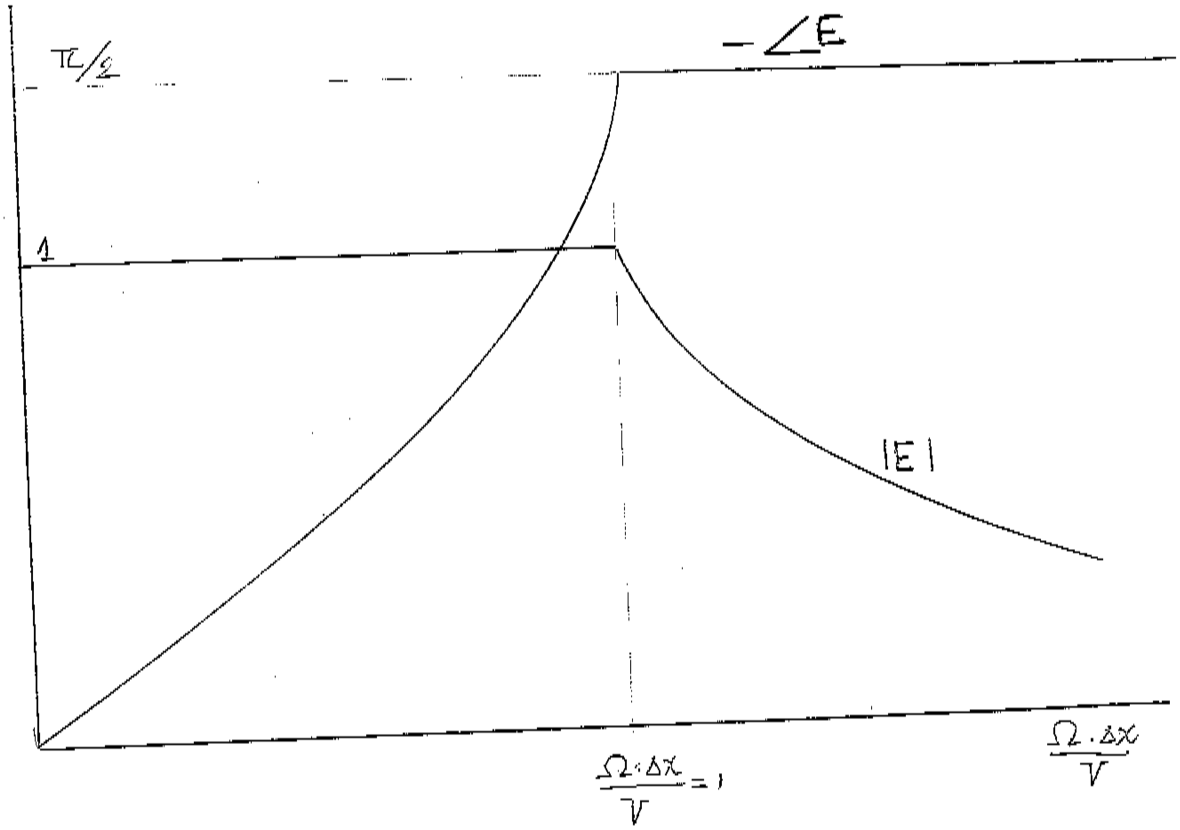

$-\angle E$
$\pi/2$
1
$|E|$
$\frac{\Omega \cdot \Delta x}{V} = 1$
$\frac{\Omega \cdot \Delta x}{V}$

Figure 4.

The relation between this analysis in terms of transfer functions and the sinusoidal response analysis of the preceding section is expressed by the identities =

$$|E| \equiv e^{-\alpha} \tag{39}$$

and

$$\frac{\angle E}{(\Omega \cdot \Delta x / V)} \equiv -R \tag{40}$$

II.5. STEP RESPONSE OF THE APPROXIMATION

Consider now the case where the initial state is $u(x,0) = 0$ and the imposed boundary condition is the step function

$$u(0,t) = H(t) = \begin{cases} 0 & \text{for } t \leq 0 \\ 1 & \text{for } t > 0 \end{cases}$$

It has the Laplace transform

$$V_0(s) = \frac{1}{s} \tag{41}$$

The exact solution of equation (1) with these initial/boundary conditions is simply (Fig. 5) :

$$u(x,t) = \mathcal{L}^{-1}\left[\frac{1}{s}\cdot e^{-\frac{s\cdot x}{V}}\right] = H\left(t - \frac{x}{V}\right)$$

An analytical expression of the corresponding numerical response is, from (34) and (41):

$$u_n(t) = \mathcal{L}^{-1}\left[\frac{1}{s}\, e^{-n\,\arcsin(s\cdot\Delta x/V)}\right]$$

$$= \mathcal{L}^{-1}\left[\frac{1}{s}\sqrt{\left(\frac{s\cdot\Delta x}{V}\right)^2 + 1} - s\right]^n \tag{42}$$

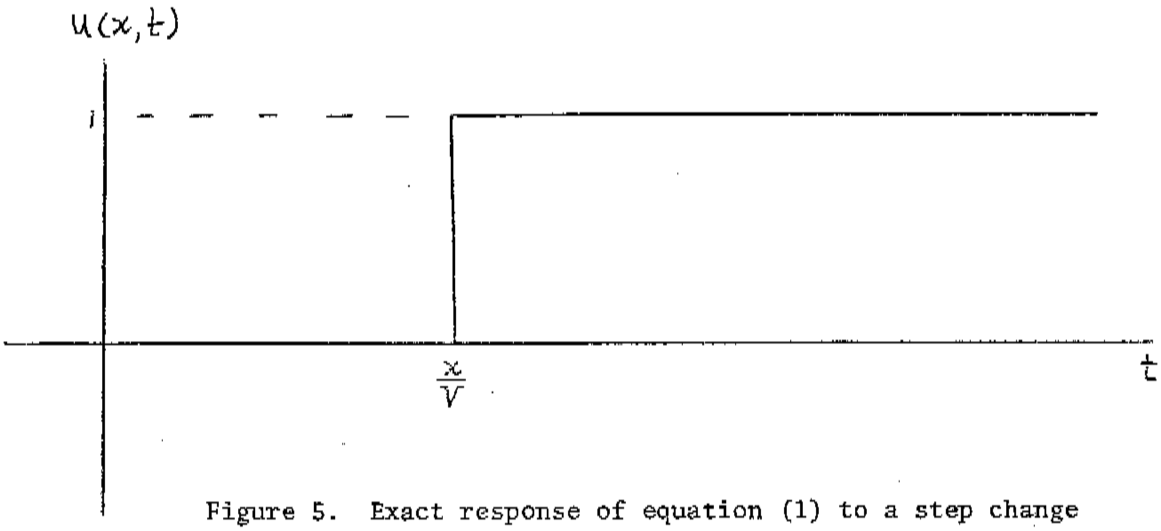
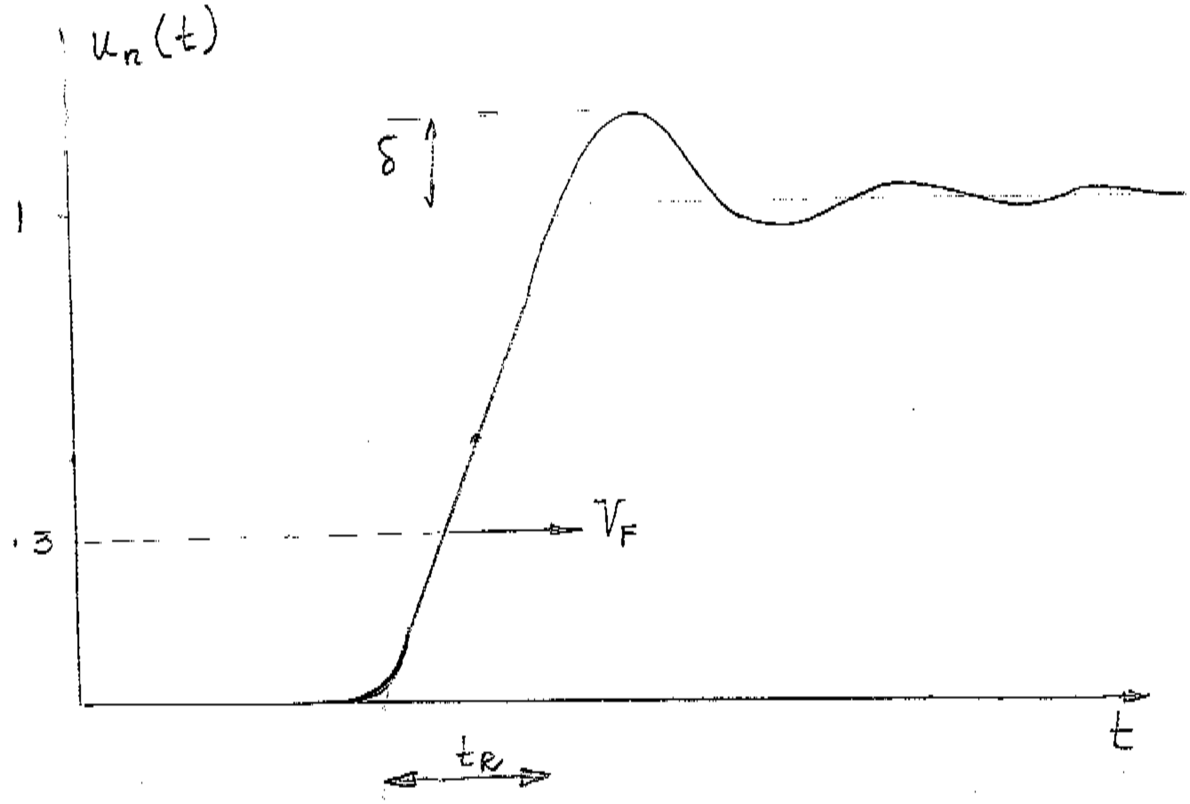


Figure 5. Exact response of equation (1) to a step change in the boundary condition u(0,t).



Definitions of rise time t_R , overshoot δ and front velocity V_F of the numerical solutions.

There are many interesting properties which can be derived from an analytical investigation of this expression, but it is somewhat beyond the scope of this report. A summary of these properties (largely supported by numerical experimental verifications) will suffice:

The characteristic shape of the step-response solution is shown in Figure (6). Except for the initial distortion of the initial step $u_o(t) = H(t)$ into the oscillating function $u_1(t)$ in Figure (6), there is little further distortion in the propagation of the numerical solution for n = 3,...,etc., (i.e. for increasing x). The characteristics of these solutions may be described in terms of rise time t_R, overshoot δ and front velocity V_F as defined in Figure (7).

(a) Rise time of the numerical solution

The rise-time of the numerical solutions is for all practical purposes constant (i.e., independent of n and equal to

$$t_R \simeq \frac{2\pi \cdot \Delta x}{V}$$

The period of the oscillatory response is slightly longer than $(2 \cdot t_R)$ for the first oscillation, and approaches this number assymptotically for the succeeding oscillations as their amplitude tends to zero.

(b) Overshoot of the numerical solution

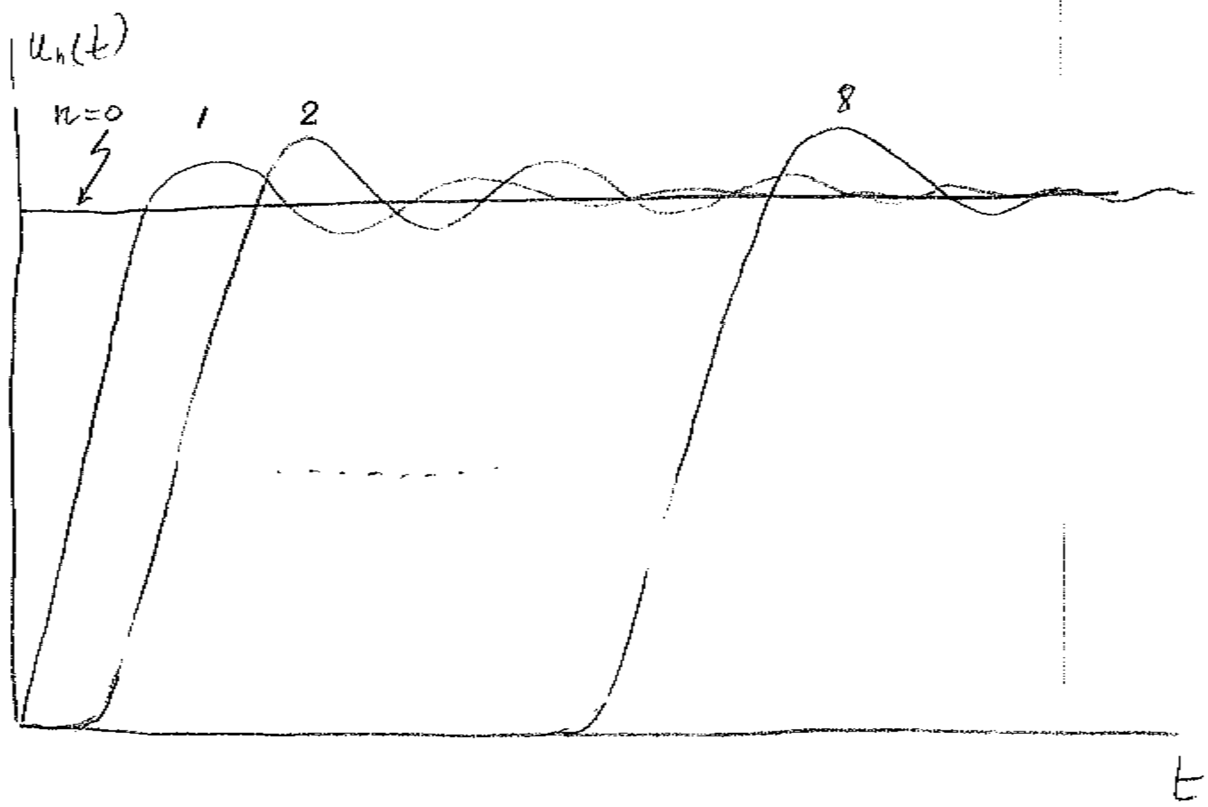
The overshoot of the numerical solutions $u_n(t)$ is more or less constant with n, equal to

$$\delta \simeq \text{constant} \simeq .2$$

(c) Front velocity of the numerical solution

The numerical front velocity V_F is practically equal to the exact velocity

$$V_F \simeq V$$



The family of numerical solutions to the MOL equations (3) -

$u_o(t)$ = H(t) = step function - (experimental results).

III. METHODS OF LINES USING NON CENTRAL SPATIAL DIFFERENCES

III.1.

A more general form than (2)for the approximation of the spatial derivative $\frac{\partial u}{\partial x}$ in (1) is the non-central differences expression*

$$\left(\frac{\partial u}{\partial x}\right)_n \simeq \frac{(1+\beta)\,u_{n+1} - 2\beta\, u_n - (1-\beta)\, u_{n-1}}{2 \cdot \Delta x} \tag{45}$$

For $\beta = 0$, this expression is the central differences approximation (2) used before ; for $\beta = 1$, we obtain forward differences:

$$\left(\frac{\partial u}{\partial x}\right)_n \simeq \frac{u_{n+1} - u_n}{\Delta x} \tag{46}$$

and for $\beta = -1$ we have backward differences:

$$\left(\frac{\partial u}{\partial x}\right)_n \simeq \frac{u_n - u_{n-1}}{\Delta x} \tag{47}$$

We may rewrite (45) as

$$\left(\frac{\partial u}{\partial x}\right)_n \simeq \left(\frac{u_{n+1} - u_{n-1}}{2 \cdot \Delta x}\right) + \frac{\beta \cdot \Delta x}{2}\left(\frac{u_{n+1} - 2u_n + u_{n-1}}{\Delta x^2}\right) \tag{48}$$

It thus becomes apparent that (45) is a consistent approximation of

$$\frac{\partial u}{\partial x} + \frac{\beta \cdot \Delta x}{2} \cdot \frac{\partial^2 u}{\partial x^2} \tag{49}$$

and that, if it is used to approximate (1) by

$$\frac{du_n}{dx} = -V\left(\frac{(1+\beta)\,u_{n+1} - 2\beta u_n - (1-\beta)\,u_{n-1}}{2 \cdot \Delta x}\right) \tag{50}$$

then this approximation is consistent with the differential equation

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = -\frac{V \cdot \beta \cdot \Delta x}{2} \cdot \frac{\partial^2 u}{\partial x^2} \tag{51}$$

We shall restrict the ensuing analysis to the case $\beta = -1$, that is the backward differences case. The system of ordinary differential equations to be integrated numerically is now

$$\frac{du_n}{dt} = -V\left(\frac{u_n - u_{n-1}}{\Delta x}\right) \;;\quad n = 1, 2, \cdots\cdots \tag{52}$$

---

* See e.g. Leendertse - (1971)

III.2. PROPERTIES OF SINUSOIDAL SOLUTIONS WITH BACKWARD SPATIAL DIFFERENCES

In a manner similar to that of section II-2 , we seek analytically the solution of the MOL approximation (52) in response to the sinusoidal boundary condition $u(0,t) = \sin t$. As before, let a trial solution be $u_n(t) = e^{-n\alpha_B} \cdot \sin\omega\left(t - \frac{x_n}{V_B^*}\right)$ where α_B and V_B^* have the same interpretation as in the central difference case (i.e. they describe the space-decay and phase-velocity characteristics of the numerical solution.)

By substitution of this trial solution in (52) we obtain, after elimination of common terms:

$$\Omega \cdot \cos\Omega\left(t - \frac{x_n}{V_B^*}\right) = -\frac{V}{\Delta x}\left[\sin\Omega\cdot\left(t - \frac{x_n}{V_B^*}\right) - e^{\alpha}\left(\sin\Omega\left(t - \frac{x_n}{V_B^*}\right)\cdot\cos\left(\frac{\Omega\cdot\Delta x}{V_B^*}\right)\right.\right.$$
$$\left.\left. + \cos\Omega\left(t - \frac{x_n}{V_B^*}\right)\cdot\sin\left(\frac{\Omega\cdot\Delta x}{V_B^*}\right)\right)\right] \tag{53}$$

whence, by identification;

$$1 - e^{\alpha}\cdot\cos\left(\Omega\cdot\Delta x / V_B^*\right) = 0 \tag{54}$$

and

$$\Omega = (V/\Delta x)\cdot e^{\alpha}\cdot\sin\left(\Omega\cdot\Delta x / V_B^*\right) \tag{55}$$

which yield the expressions:

$$V_B^* = V\left(\frac{(\Omega\cdot\Delta x / V)}{\arctan(\Omega\cdot\Delta x / V)}\right) \tag{56}$$

$$e^{-\alpha} = 1 / \sqrt{1 + (\Omega\Delta x / V)^2} \tag{57}$$

Likewise, we obtain as before:

• spatial frequency of the numerical solution:

$$\omega_B^* = \frac{1}{\Delta x}\arctan\left(\Omega\cdot\Delta x / V\right) = \omega\cdot\left(\frac{\arctan(\Omega\cdot\Delta x / V)}{(\Omega\cdot\Delta x / V)}\right) \tag{58}$$

• wavelength of the numerical solution;

$$\lambda_B^* = \frac{2\pi\cdot\Delta x}{\arctan(\Omega\cdot\Delta x / V)} = \lambda\cdot\left(\frac{(\Omega\cdot\Delta x / V)}{\arctan(\Omega\cdot\Delta x / V)}\right) \tag{59}$$

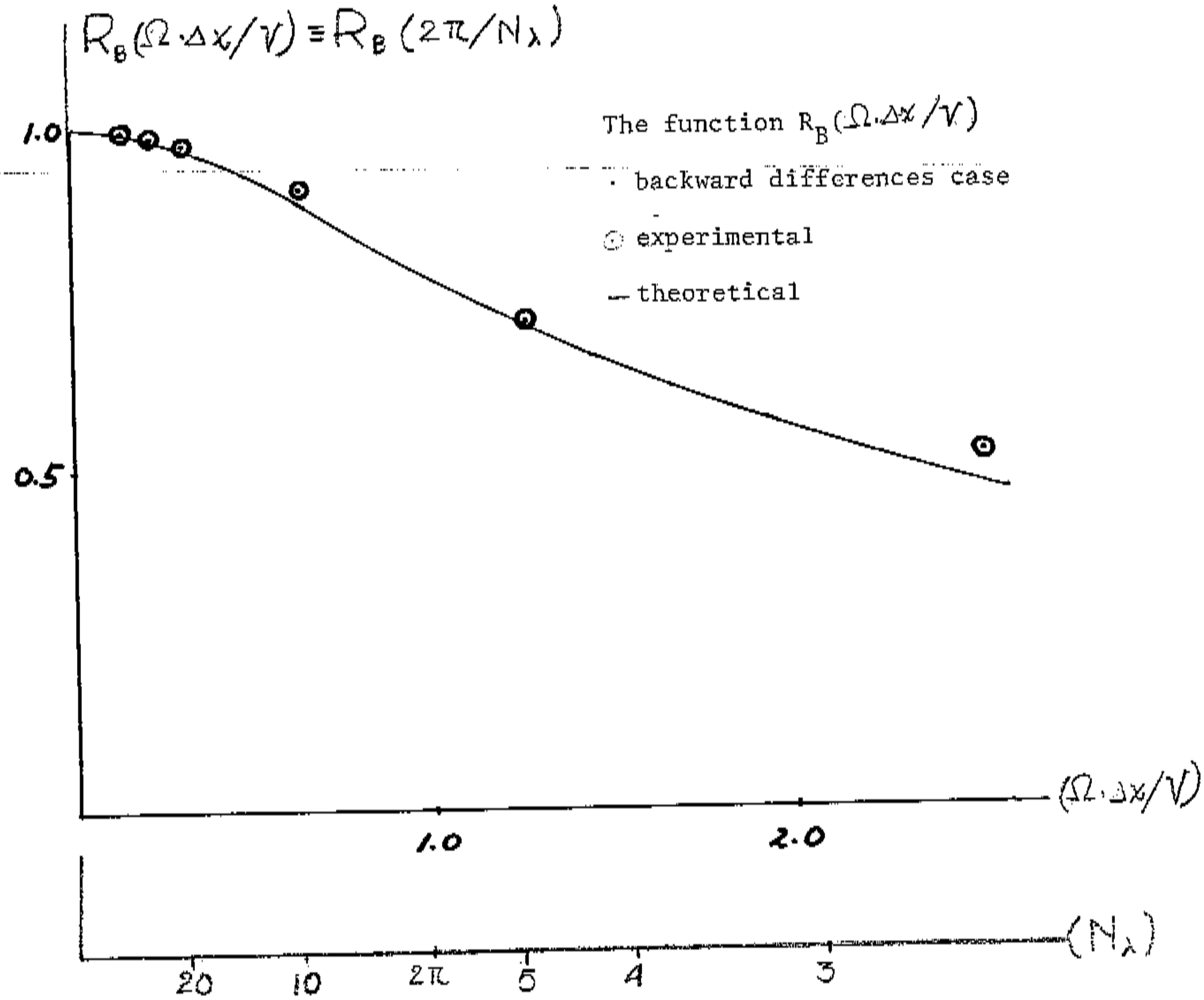
By contrast with the central differences case, these expressions apply for all values of $\left(\frac{\Omega . \Delta x}{V}\right)$.

If we let $R_B(\Omega . \Delta x/V)$ be the function :(figure 7)

$$R_B(\Omega . \Delta x/V) = \frac{\arctan (\Omega . \Delta x / V)}{(\Omega . \Delta x / V)} \tag{60}$$

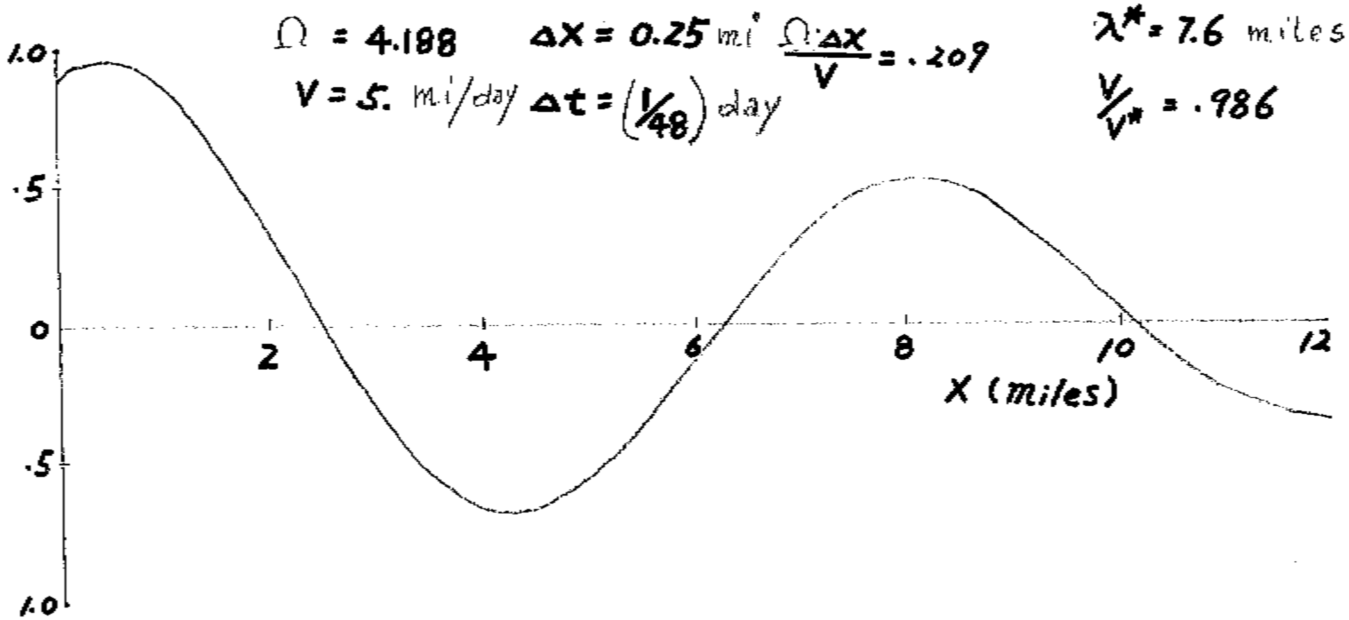
then the preceding relations may be rewritten as:

$$\frac{V}{V_B^*} = \frac{\omega_B^*}{\omega} = \frac{\lambda}{\lambda_B^*} = R_B \tag{61}$$



$R_B(\Omega\cdot\Delta x/V) \equiv R_B(2\pi/N_\lambda)$
1.0
0.5
The function $R_B(\Omega\cdot\Delta x/V)$
backward differences case
experimental
theoretical
$(\Omega\cdot\Delta x/V)$
1.0
2.0
(N_λ)
20
10
2π
5
4
3

Figure 7.



SINUSOIDAL RESPONSE

TYPICAL COMPUTER RESULT - BACKWARD DIFFERENCES -

→ THE OBSERVED REDUCTION OF AMPLITUDE WITH X IS DUE TO THE SPURIOUS DIFFUSION INTRODUCED BY THE THE BACKWARD DIFFERENCE APPROXIMATION -

Fig. 8

III.3. SELECTION OF A SPATIAL INCREMENT Δx

The condition $|(R-1)| \leqslant .1$ which we have chosen is section II-3 as a reasonable criterion for choosing Δx leads in this case to

$$(\Omega_{max} \cdot \Delta x / V) = (2\pi / N_{\lambda_{min}}) \simeq .6$$

Likewise, this leads to the condition

$$N_{\lambda_{min}} \geqslant \frac{2\pi}{.6} \simeq 10.5$$

Here again, a choice of about 10 spatial increments Δx per shortest wavelength λ_{min} emerges as a good practical rule.

This result agrees well with similar guidelines derived by Leendertse in reference [7].

III.4. LAPLACE TRANSFORM ANALYSIS (backward differences)

By Laplace transformation of equation (52), we find

$$E(s) = \frac{1}{1 + s \cdot \Delta x / V} \tag{62}$$

where $E(s)$ is, as before defined by the ratio

$$E(s) \triangleq \frac{U_n(s)}{U_{n-1}(s)} = \frac{U_{n+1}(s)}{U_n(s)} \tag{63}$$

for the backward difference equations (52). The amplitude and phase characteristics of $E(s)$ are (fig. 9).

$$|E(i\Omega)| = \frac{1}{\sqrt{1 + \left(\frac{\Omega \cdot \Delta x}{V}\right)^2}} = e^{-\alpha_B} \tag{64}$$

and

$$\angle E(i\Omega) = -\arctan(\Omega \cdot \Delta x / V) \tag{65}$$

Here again, we find that the relations (39) and (40) hold.

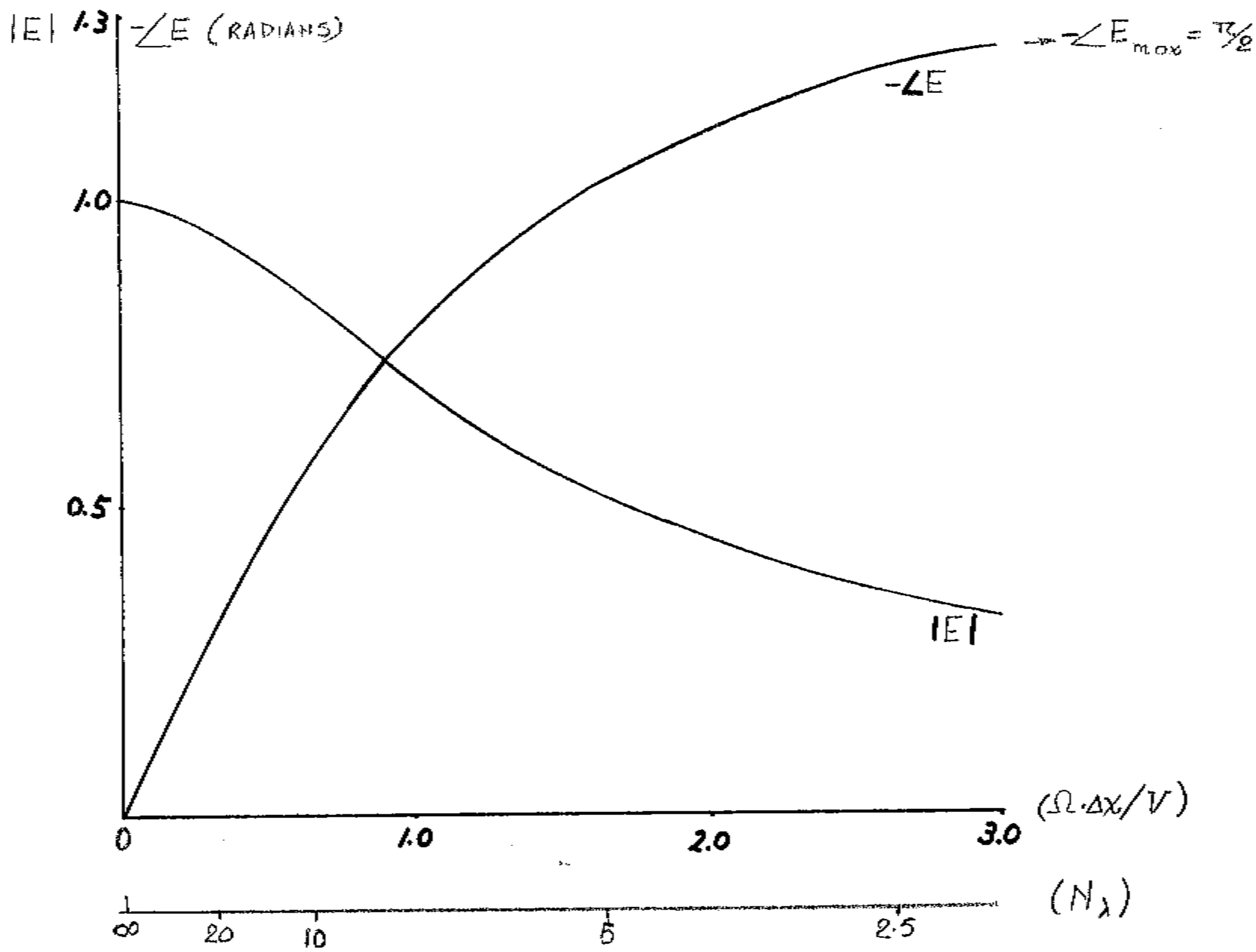


Figure 9. Transfer function ($\not{s}$) of the MOL approximation - Backward differences case

III.5. RESPONSE TO A STEP CHANGE IN THE BOUNDARY VALUE (backward differences)

An exact analytic expression of the response to the unit-step change in the boundary condition $u(o,t)$ can be derived in this case=

$$u_n(t) = \mathcal{L}^{-1}\left[\frac{1}{s}\left(\frac{1}{1+(s\cdot\Delta x/V)}\right)^n\right]$$

$$= \int_0^t \frac{1}{(n-1)!}\cdot\left(\frac{V\cdot t}{\Delta x}\right)^{n-1}\cdot e^{-\frac{V\cdot t}{\Delta x}}\cdot d\left(\frac{V\cdot t}{\Delta x}\right) \qquad (66)$$

This family of responses is shown in fig(9). By contrast with the central difference case where the rise-time of the responses was constant, we may observe now that the rise time is increasing with n; this is directly due to the spurious diffusion term introduced by the backward-differences utilised, as described by equation (51 -a).

It may also be observed that there is no overshoot in this family of solutions. Because of the increasing rise time with n, a definition of the wave front V_F becomes somewhat subjective, and deserves no more exact analysis than to say that it is closely related to V.

* The integrant of (66) is a Poisson distribution of order (n-1):

$$\frac{1}{(n-1)!}\cdot\left(\frac{V\cdot t}{\Delta x}\right)^{n-1}\cdot e^{-\frac{Vt}{\Delta x}} = P_{n-1}\left(\frac{V\cdot t}{\Delta x}\right)$$

Applying integration by parts to (66), one finds that $u_n(t)$ may also be expressed as a sum of Poisson distributions =

$$u_n(t) = 1 - \sum_k P_{n-k}\left(\frac{V\cdot t}{\Delta x}\right) \qquad (66\text{-a})$$

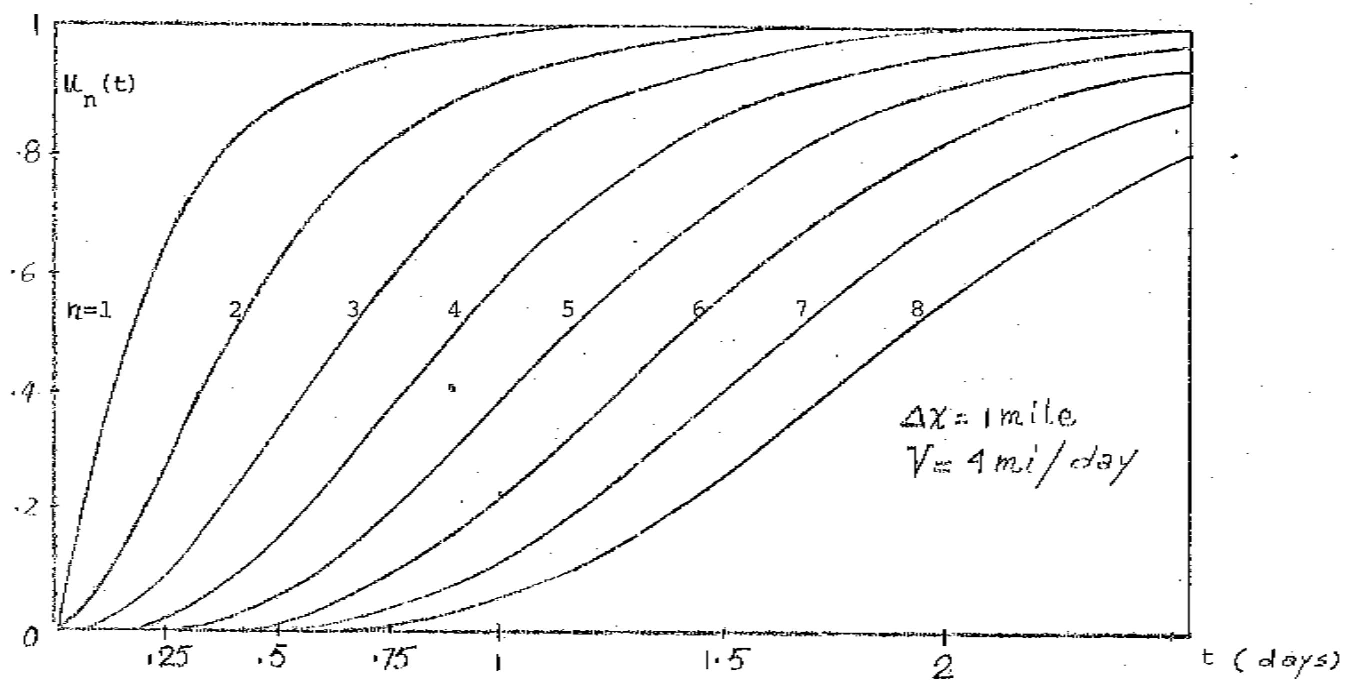


Figure 10. Step response of the MOL approximation - Backward differences case. (Note that the increase in rise-time t_R with n is indicative of the spurious diffusion induced by the approximation).

IV. QUALITATIVE PROPERTIES OF METHODS OF LINES

IV.1. CONSERVATIVE PROPERTY

The exact solution of the transport equation (1) has the property of conservation:

We may derive:

$$\frac{d}{dt}\int_A^B u\,dx = -V\left(u(B,t)-u(A,t)\right) \qquad (68)$$

When the solution is equal at the 2 boundaries of the domain of integration (or more precisely when $V_A u_A = V_B u_B$) then (67) is equal to zero and we have the conservation equation: $\int_A^B u\,dt$ = constant.

In the MOL approximation, the counterpart of (67) is (from (3)):

$$\frac{d}{dt}\sum_{n_A}^{n_B} u_n\cdot\Delta x = -\frac{V}{2}\sum_{n_A+1}^{n_B-1}(u_{n+1}-u_{n-1}) = -\frac{V}{2}(u_{n_B}-u_{n_A}) \qquad (69)$$

When the numerical solution is equal at the 2 boundaries of the domain of integration $u_{n_B} = u_{n_A}$, the conservation property holds, namely:

$$\int u(x)\,dx \simeq \sum_{n=n_{A+1}}^{n_B-1} u_n\cdot\Delta x = \text{constant} \qquad (70)$$

This property also holds in the backward difference case. Indeed, we have then =

$$\frac{d}{dt}\left[\sum_{n_A+1}^{n_B} u_n\cdot\Delta x\right] = -V\left(u_{n_B}-u_{n_A}\right) \qquad (71)$$

which is zero when $u_{n_A-1} = u_{n_B}$

IV.2. QUALITATIVE PROPERTIES OF SINUSOIDAL SOLUTION OF THE MOL APPROXIMATION

Periodic fluctuations which are represented numerically with the MOL approximation deviate from the analytic solution. A qualitative way to analyse these deviations is to characterise them by dissipative diffusive and dispersive effects. While the equation which we attempt to integrate is (1), its numerical approximation is, for sinusoidal solutions of frequency ω, consistent with a differential equation of the form

$$\frac{\partial u}{\partial t} + V^* \frac{\partial u}{\partial x} = D^* \frac{\partial^2 u}{\partial x^2} - K^* u \tag{72}$$

The dissipative, diffusive and dispersive effects of the approximation are described by the functions V^*, D^* and K^* respectively, in the following manner:

a). If sinusoidal solutions of different frequency ω do not travel at the same velocity, non sinusoidal solutions will loose their shape as they propagate: this is the <u>dispersive</u> effect of the approximation, and is measured by the difference $V^*(\omega) - V$

b). If sinusoidal solutions decay in amplitude with ω as described by the spurious diffusion term $D^* \frac{\partial^2 u}{\partial x^2}$ in equation (72), then this effect of the approximation is called <u>diffusive</u> and is measured by D^*.

c). If sinusoidal solutions decay in amplitude with ω as described by the spurious term $-K^* u$ then this effect of the approximation is called <u>dissipative</u> and is measured by K^*.

In this respect, we may summarize the preceding analysis as follows:

a) Spurious dispersion

The central-differences approximation (3) as well as the backward differences (52) introduce a spurious dispersive effect, which is described by equations (12) and (56), respectively.

b) Spurious diffusion

According to (51), the backward-differences scheme (52) is consistent with the equation

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = V \cdot \frac{\Delta x}{2} \cdot \frac{\partial^2 u}{\partial x^2} \qquad \text{(51-a)}$$

whose right hand side is a spurious diffusion term introduced by the approximation.

By contrast with this scheme the central differences case (2), corresponding to $\beta = 0$ does not introduce spurious diffusion. This conclusion has, of course, a finite range of applicability. Non-diffusivity of the solution can be equated to constant-amplitude property of steady-state sinusoidal solutions, and our analysis of section ( ) has shown that this, indeed, is the case for $(\Omega \cdot \Delta x / V) \leqslant 1$ only. Outside of this range, the consistency of (48) with (51) does not hold for sinusoidal solutions of time-frequency Ω, and spurious diffusion does in fact occur.

In the forward differences case ($\beta > 0$), equation (51) contains a "negative diffusion" spurious term. It so happens that in this case, the equations (50) are computationally unstable. I.e., the system of ordinary differential equations (50) is then unstable in the classical or Liapunov sense (ref [10]) and is therefore a non-acceptable model to approximate the partial differential equation (1).

c) Spurious dissipation

There is no spurious dissipative effect in the MOL approximation, neither in the central-differences case (3) nor in the backward differences case (52). Indeed, this may be proved by observing that dissipation implies non-conservation in the sense of non-applicability of equation (68)*. But we have seen, via equations (70) and (71) that the conservative property of (7) is preserved in the MOL approximations (3) and (56); q.e.d.

---

* for the dissipative equation $\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = -K u$ we find:

$$\frac{d}{dt}\int_A^B u\, dx = -V(u_B - u_A) - K\int_A^B u\, dx$$

REFERENCES

[1] Davidson, B., and Y. Shie h. 1971. "Direct Field Determination of the Natural Reaeration Coefficient by Frequency Response Analysis", Water Resources Research, Vol. 7, No. 6, December.

[2] Collins, J., and S. H. Fersht. 1968. "Mixed Technique for Computing Surges in Channels", Proc. ASCE 94, No. HY2, March.

[3] Hicks, J. S. and J. Wei. 1967. "Numerical Solution of Parabolic Partial Differential Equations by Use of the Method of Lines", JACM, Vol. 14, No. 3, July 1967, pp. 549-562.

[4] Jeglic, J. M. 1966. "DECS III - Mathematical Simulation of the Estuarine Behavior", Report No. 1032, General Electric Re-entry Systems Dept., December 1966, revised, July, 1967.

[5] Lapidus, L., and J. H. Seinfeld. 1971. Numerical Solution of Ordinary Differential Equations. Academic Press, New York.

[6] Leendertse, J. J. 1971. "Digital Techniques: Finite Differences", in Estuarine Analysis: An Assessment, pp. 277-302. Water Quality Office, Environmental Protection Agency, Washington, D. C. U. S. Govt. Printing Office, Stock Number 5501-0129.

[7] Papoulis, A. 1962. "The Fourier Integral and its Applications", McGraw-Hill Book Co., Inc.

[8] Richtmyer, R. D. and E. R. W. Morton. 1967. "Difference Methods for Initial Value Problems", Interscience Publishers Inc., New York., pp. 405.

[9] Thomann, Robert V. 1963. "Mathematical Model for Dissolved Oxygen", Proc. ASCE 89, No. SA 5 (October).

[10] Vichnevetsky, R. 1967. "Error Analysis in the Computer Simulation of Dynamic Systems: Variational Aspects of the Problem", IEEE Transactions on Electronic Computers, Vol. EC-16, No. 4, August, pp. 403-411.

[11] Vichnevetsky, R. 1971. "Numerical Stability of Methods of Lines for Partial Differential Equations", DCS Report No. 13, Department of Computer Science, Rutgers University.

[12] Vichnevetsky, R. 1972. "Stability Charts of Methods of Lines for Partial Differential Equations", Proceedings, Sixth Annual Princeton Conference on Information Science and Systems, Princeton University, March.

[13] Vichnevetsky, R. and Tomalesky, A. W. "Spurious Wave Phenomena in Numerical Approximations of Hyperbolic Equations", Proceedings, Fifth Annual Princeton Conference on Information and Systems Science, March, 1971.