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# THE DEVELOPMENT OF A NUMERICAL SOLUTION TO THE TRANSPORT EQUATION

**Report 2** 

## COMPUTATIONAL PROCEDURES

by

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September 1983 Report 2 of a Series

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20. ABSTRACT (Continued).

bydrodynamic interface, and the determination of dispersion coefficients are developed for simulating conditions in Mississippi Sound and adjacent areas.

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#### PREFACE

The computational procedures of the numerical approximation to the transport equation are reported herein. These procedures will be incorporated into a numerical model to be used for evaluating effects of proposed dredged material disposal practices in Mississippi Sound and adjacent areas.

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Computational procedures were developed by the U. S. Army Engineer Waterways Experiment Station (WES) in the Hydraulics Laboratory (HL) under the general supervision of Messrs. H. B. Simmons and F. A. Herrmann, Jr., Chief and Assistant Chief, respectively, HL, and in CERC under the general supervision of Drs. R. W. Whalin and L. E. Link, Chief and Assistant Chief, respectively CERC, and Mr. C. E. Chatham, Chief, Wave Dynamics Division (WDD). This report was prepared by Dr. R. A. Schmalz, Jr., WDD.

Commanders and Directors of WES during this study and the preparation and publication of this report were COL Nelson P. Conover, CE, and COL Tilford C. Creel, CE. Technical Director was Mr. F. R. Brown.

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## DEVELOPMENT OF A NUMERICAL SOLUTION TO THE TRANSPORT EQUATION: Report 2 COMPUTATIONAL PROCEDURES

PART I: INTRODUCTION

This report develops in detail the numerical approximations to the transport equation. In Part II, the linearized form of the equation is the subject of investigation. The stability and truncation error characteristics for the schemes proposed in the first series are developed. In Part III, the nonlinear equation in transformed coordinates is considered. The schemes developed in the first part are extended to the nonlinear equation. In Part IV, the numerical approximations near boundaries, the hydrodynamic interface, and the determination of dispersion coefficients in terms of flow field properties are developed.

This report outlines the development of the salinity algorithm. The next step is the numerical implementation of these procedures.

#### PART II: NUMERICAL APPROXIMATIONS FOR THE TRANSPORT EQUATION IN CARTESIAN COORDINATES

A Cartesian coordinate system is employed in all developments presented in this part. The stability and truncation error of the proposed numerical approximations are investigated for the linearized transport equation. In this manner the most favorable schemes may be determined prior to programming a numerical experimentation. Unfortunately, the transport equation is nonlinear and no formal method of analysis exists to determine the appropriateness of numerical schemes. We follow standard numerical practice and assume schemes which possess favorable computational attributes for the linearized transport equation will also be suitable for the nonlinear equation.

We therefore develop linear forms of the transport equation followed by investigation of several numerical schemes to this form of the equation. The schemes considered are the Leendertse [1] multioperational scheme employing forward time and centered space derivatives (FTCS). The use of upwind space differencing within the Leendertse multioperational scheme is next investigated. The scheme thereby obtained is known as the forward time upwind space (FTUS) scheme. We next investigate several spread time derivative (STCS) schemes and select the most favorable for further development.

#### 1. Linear Forms of the Transport Equation

Let us consider the two-dimensional depth integrated transport equation as follows:

$$\frac{\partial}{\partial t} (hs) + \frac{\partial}{\partial x} (hus) + \frac{\partial}{\partial y} (hvs) = \frac{\partial}{\partial x} \left( hK_x \frac{\partial s}{\partial x} \right) + \frac{\partial}{\partial y} \left( hK_y \frac{\partial s}{\partial y} \right)$$
(1.1)

where

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h = total water depth

- u,v = depth average velocity components in the x and y directions, respectively
  - t = time
- x,y = Cartesian coordinates
  - s = constituent concentration
- K x,K y = Effective dispersion coefficients in the x and y direc tions, respectively (note the \* notation has been dropped)

Equation 1.1 represents the conservative form of the transport equation. To derive the nonconservative form, we expand the left hand side of 1.1 to obtain (noting  $h = \eta - z_h$ ):

$$\mathbf{s} \begin{pmatrix} \frac{\partial \mathbf{n}}{\partial \mathbf{t}} - \frac{\partial \mathbf{z}}{\partial \mathbf{t}} \end{pmatrix} + \mathbf{h} \frac{\partial \mathbf{s}}{\partial \mathbf{t}} + \frac{\partial (\mathbf{h}\mathbf{u})}{\partial \mathbf{x}} \mathbf{s} + \mathbf{h}\mathbf{u} \frac{\partial \mathbf{s}}{\partial \mathbf{x}} + \mathbf{s} \frac{\partial (\mathbf{h}\mathbf{v})}{\partial \mathbf{y}} + \frac{\partial \mathbf{s}}{\partial \mathbf{y}} \mathbf{h}\mathbf{v} \qquad (1.2)$$

Since the bottom is rigid,  $\partial z_b/\partial t = 0$ . Using the continuity relation  $\partial \eta/\partial t + \partial (hu)/\partial x + \partial (hv)/\partial y = 0$  and collecting terms we obtain

$$s\left(\frac{\partial \eta}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y}\right) + h\left(\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y}\right)$$
(1.3)

Then finally the left hand side of Equation 1.1 becomes

$$h\left(\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y}\right)$$
(1.4)

We now rewrite the transport equation for two important special cases. In Case I we assume h is constant and obtain

$$\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y} = \frac{\partial}{\partial x} \left( K_x \frac{\partial s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial s}{\partial y} \right)$$
(1.5)

This result is also obtained if  $|\eta| << |z_b|$ . In Case II we assume h,  $K_x$ , and  $K_y$  are all constant and obtain

$$\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y} = K_x \frac{\partial^2 s}{\partial x^2} + K_y \frac{\partial^2 s}{\partial y^2}$$
(1.6)

We note that in Equations 1.5 and 1.6, although u, v, s are depth integrated quantities and  $K_x$  and  $K_y$  are effective dispersion coefficients, the form of the equations hold for instantaneous velocity or time averaged (over the turbulence) velocity as well. In fact Equation 1.6 or its one-dimensional form is often used since for constant velocity it becomes a linear equation. Therefore, von Neumann stability analysis may be employed to analyze the characteristics of numerical approximations.

#### 2. Leendertse Multioperational Schemes: One-Dimensional Analysis

The following one-dimensional transport equation is employed to determine the dissipative and dispersive properties of the multioperational scheme [1].

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} - D \frac{\partial^2 \rho}{\partial x^2} = 0$$
 (2.1)

A multioperational analog to Equation 2.1 is written as follows:

$$\rho_{j}^{n+1} - \rho_{j}^{n} + \frac{\Delta t}{2\Delta x} u \left[ (1 + \alpha) \rho_{j+1}^{n+1} - 2\alpha \rho_{j}^{n+1} + (\alpha - 1) \rho_{j-1}^{n+1} \right] - \frac{D\Delta t}{\Delta x^{2}} \left( \rho_{j+1}^{n+1} - 2\rho_{j}^{n+1} + \rho_{j-1}^{n+1} \right) = 0 \qquad (2.2a)$$
$$\rho_{j}^{n+2} - \rho_{j}^{n+1} + \frac{\Delta t}{2\Delta x} u \left[ (1 + \alpha) \rho_{j+1}^{n+1} - 2\alpha \rho_{j}^{n+1} + (\alpha - 1) \rho_{j-1}^{n+1} \right]$$

$$-\frac{D\Delta t}{\Delta x^2} \left( \rho_{j+1}^{n+1} - 2\rho_j^{n+1} + \rho_{j-1}^{n+1} \right) = 0 \qquad (2.2b)$$

where

$$\rho_j^n = \rho(j\Delta x, n\Delta t)$$
  
 $\alpha = -1$ , 0, 1 (Note  $\alpha = -1$  for backward difference in space  
 $\alpha = 0$  for centered difference in space  
 $\alpha = 1$  for forward difference in space)

The solutions to the 2.2a and 2.2b are expressed by a Fourier series

$$\rho(\mathbf{x}, \mathbf{t}) = \sum_{m=1}^{\infty} \rho_m^* \exp \left[i(\sigma_m \mathbf{x} + \mathbf{w}_m \mathbf{t})\right]$$
(2.3)  
$$\rho_j^n = \rho(j\Delta \mathbf{x}, n\Delta \mathbf{t}) = \sum_{m=1}^{\infty} \rho_m^* \exp \left[i(\sigma_m j\Delta \mathbf{x} + \mathbf{w}_m n\Delta \mathbf{t})\right]$$

where

w = frequency  

$$\sigma$$
 = wave number  
 $\rho_m^*$  = complex constant for each m  
i =  $\sqrt{-1}$ 

Considering only one general term in Equation 2.3 due to the linearity of Equation 2.2 and substituting in Equation 2.2a we write:

Note

$$\rho * e^{i \left[\sigma(j \pm 1)\Delta x + w(n+1)\Delta t\right]} = \rho_{j \pm 1}^{n+1} = \rho_{j}^{n+1} e^{\pm i\sigma\Delta x}$$

We thus are in a position to determine  $\gamma_j^{n+1}/\rho_j^n$ . Therefore we obtain from Equation 2.2a:

$$\rho_{j}^{n+1} - \rho_{j}^{n} + \frac{u\Delta t}{2\Delta x} \left[ (1+\alpha)\rho_{j}^{n+1}e^{i\sigma\Delta x} - 2\alpha\rho_{j}^{n+1} + (\alpha-1)\rho_{j}^{n+1}e^{-i\sigma\Delta x} \right] - \frac{D\Delta t}{(\Delta x)^{2}} \left( \rho_{j}^{n+1}e^{i\sigma\Delta x} - 2\rho_{j}^{n+1} + \rho_{j}^{n+1}e^{-i\sigma\Delta x} \right) = 0 \quad (2.4)$$

which may be rewritten as follows

$$\lambda_1 \rho_j^{n+1} = \rho_j^n \tag{2.5a}$$

$$\frac{\rho_j^{n+1}}{\rho_j^n} = \frac{1}{\lambda_1}$$
(2.5b)

In order to simplify  $\lambda$ , recall  $\sin \theta = (e^{i\theta} - e^{-i\theta})/2i$ , therefore

$$\sin^2 \theta = \left(\frac{e^{i\theta} - e^{-i\theta}}{2i}\right)^2 = \frac{e^{i2\theta} - 2 + e^{-i2\theta}}{-4}$$
(2.6)

Regrouping  $\lambda_1$  , with the above relations in mind

$$\lambda_{1} = \frac{u\Delta t}{2\Delta x} (e^{i\sigma\Delta x} - e^{-i\sigma\Delta x}) + \frac{u\Delta t}{2\Delta x} \alpha (e^{i\sigma\Delta x} + e^{-i\sigma\Delta x} - 2) - \frac{D\Delta t}{\Delta x^{2}} (e^{i\sigma\Delta x} - 2 + e^{-i\sigma\Delta x}) + 1 \quad (2.7)$$

$$\lambda_{1} = \frac{iu\Delta t}{\Delta x} \sin (\sigma\Delta x) - 2 \frac{u\Delta t}{\Delta x} \alpha \sin^{2} \left(\frac{\sigma\Delta x}{2}\right) + \frac{4D\Delta t}{\Delta x^{2}} \sin^{2} \left(\frac{\sigma\Delta x}{2}\right) + 1$$
$$\lambda_{1} = \left(\frac{4D\Delta t}{\Delta x^{2}} - \frac{2u\Delta t\alpha}{\Delta x}\right) \sin^{2} \left(\frac{\sigma\Delta x}{2}\right) + \frac{iu\Delta t}{\Delta x} \sin (\sigma\Delta x) + 1$$

If we substitute a general term in Equation 2.2 in Equation 2.2b we obtain

$$\rho_{j}^{n+2} - \rho_{j}^{n+1} + \frac{\Delta t u}{2\Delta x} \left[ (1 + \alpha) \rho_{j}^{n+1} e^{i\sigma\Delta x} - 2\alpha \rho_{j}^{n+1} + (\alpha - 1) \rho_{j}^{n+1} e^{-i\sigma\Delta x} \right] - \frac{D\Delta t}{\Delta x^{2}} \left( \rho_{j}^{n+1} e^{i\sigma\Delta x} - 2\rho_{j}^{n+1} + \rho_{j}^{n+1} e^{-i\sigma\Delta x} \right) = 0 \quad (2.8)$$

Which may be written as follows:

$$\lambda_2 \rho_j^{n+1} = \rho_j^{n+2}$$
 (2.9)

Where 
$$\lambda_2 = 1 - \frac{iu\Delta t}{\Delta x} \sin(\sigma\Delta x) + \frac{2u\Delta t\alpha}{\Delta x} \sin^2\left(\frac{\sigma\Delta x}{2}\right) - \frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{\sigma\Delta x}{2}\right)$$

Defining the entire transfer process as

$$\rho_{j}^{n+2} = \lambda_{2} \rho_{j}^{n+1} = \frac{\lambda_{2}}{\lambda_{1}} \rho_{j}^{n}$$
(2.10)

We obtain the amplification factor  $\lambda_2/\lambda_1 = \lambda$  which for stability  $|\lambda| \leq 1$ .

Thus

$$\lambda = \frac{1 + \left(\frac{2u\Delta t\alpha}{\Delta x} - \frac{4D\Delta t}{\Delta x^2}\right) \sin^2\left(\frac{\sigma\Delta x}{2}\right) - \frac{iu\Delta t}{\Delta x}\sin(\sigma\Delta \chi)}{1 + \left(\frac{4D\Delta t}{\Delta x^2} - \frac{2u\Delta t\alpha}{\Delta x}\right)\sin^2\left(\frac{\sigma\Delta x}{2}\right) + \frac{iu\Delta t}{\Delta x}\sin(\sigma\Delta x)}$$
(2.11)

We observe in Equation 2.11 for centered space differences ( $\alpha = 0$ ) and  $|\lambda| \leq 1$ . For backward space differences ( $\alpha = -1$ ) and u > 0  $|\lambda| \leq 1$ , while for u < 0 the cell Peclet number must obey the following relation for  $|\lambda| \leq 1$ .

$$Pe_{c} = \frac{|u|\Delta x}{D} \leq 2 \qquad (2.12)$$

For forward space differences ( $\alpha$  = 1) and  $|u| < 0 ~|\lambda| \leq 1$  , while for

u > 0 relation (Equation 2.12) must again be satisfied for  $\lambda \leq 1$ . Upwind space differences represent a combination of backward and forward differences. For u > 0 backward space differences are employed, while for u < 0 forward space differences are utilized. In this manner unconditional stability is obtained; i.e., the restriction of Equation 2.12 above is removed. Let a =  $(2u\Delta t/\Delta x) \sin^2(\sigma\Delta x/2)$ , b =  $(4D\Delta t/\Delta x^2) \sin^2(\sigma\Delta x/2)$ , and c =  $(u\Delta t/\Delta x) \sin(\sigma\Delta x)$  then

$$|\lambda| = \left| \frac{1 + a\alpha - b - ic}{1 + b - a\alpha + ic} \right| = \frac{\sqrt{\left[ (1 - b) + a\alpha \right]^2 + c^2}}{\sqrt{\left[ (1 + b) - a\alpha \right]^2 + c^2}}$$
(2.13)

Leendertse notes that the general solution to Equation 2.1 may be expressed as

$$\rho(\mathbf{x},t) = \rho^* \exp \left[i(\sigma \mathbf{x} + \mathbf{w}t)\right]$$
(2.14)

Substituting Equation 2.14 into Equation 2.1 we obtain

$$iw\rho(x,t) + iu\sigma\rho(x,t) - Di^{2}\sigma^{2}\rho(x,t) = 0$$
  

$$w + u\sigma - iD\sigma^{2} = 0$$
  

$$w = \sigma(iD\sigma - u)$$
(2.15a)

and

$$\rho(\mathbf{x},t) = \rho^* \exp \left[i\sigma(\mathbf{x} - \mathbf{u}t)\right] \exp \left(-D\sigma^2 t\right) \qquad (2.15b)$$

We observe then that there is a relationship between the temporal frequency and the spatial frequency. As a result, the complete solution may be written in terms of the spatial frequency solely. For a time period  $\Delta t$ , each Fourier component is decreased in amplitude by exp ( $-D\sigma^2\Delta t$ ) and is propagated a distance  $u\Delta t$ .

In the computational procedure a different relationship exists. The eigenvalue or amplification factor may be used to study the dissipative and dispersive effect of the computational procedure by the use of the concept of the complex propagation factor.

The propagation factor is expressed in terms of the dimensionless parameters  $\mathbf{m} = (L/\Delta \mathbf{x})$ ,  $D' = (D\Delta t/\Delta \mathbf{x}^2)$ , and  $U = (u\Delta t/\Delta \mathbf{x})$ . It is defined as the complex ratio of the computed wave to the prototype wave after an interval in which the prototype wave propagates over its wavelength. The modulus of the propagation is a measure of the decay of the amplitude during computation, while the argument is a measure of the computed phase shift.

To determine the factor we use the following previous results for the computed solution. We consider the case  $\alpha = 0$  corresponding to the use of centered space differences. We note from Equation 2.13 for  $\alpha = 0$ 

 $\lambda = \frac{1 - b - ic}{1 + b + ic} \text{ where } b = \frac{4D\Delta t}{\Delta x^2} \sin^2 \frac{\sigma \Delta x}{2} \text{ and } c = \frac{u\Delta t}{\Delta x} \sin (\sigma \Delta x)$  $b = 4D' \sin^2 \frac{\sigma \Delta x}{2} \qquad c = U \sin (\sigma \Delta x) \quad (2.17)$  $\rho_j^{n+2} = \lambda \rho_j^n$ 

From the solution of the PDE in Equation 2.15 itself

$$\rho(j\Delta x, t + 2\Delta t)$$

$$= \rho^{*} \exp \left[i\sigma(j\Delta x - u(t + 2\Delta t))\right] \exp \left[-D\sigma^{2}(t + 2\Delta t)\right]$$

$$\rho(j\Delta x, t + 2\Delta t)$$

$$= \rho^{*} \exp \left[i\sigma(j\Delta x - ut)\right] \exp \left(-D\sigma^{2}t\right) \exp \left(i\sigma u 2\Delta t\right)$$

$$\cdot \exp \left(-D\sigma^{2} 2\Delta t\right) \qquad (2.18)$$

$$\rho(j\Delta x, t + 2\Delta t) = \rho(j\Delta x, t) \exp \left(-D\sigma^{2} 2\Delta t\right) \exp \left(i\sigma u 2\Delta t\right)$$

$$\rho(j\Delta x, t + 2\Delta t) = \rho(j\Delta x, t)\lambda_{s}$$

The complex propagation factor is then given by the following relation

$$f_m = \left(\frac{\lambda}{\lambda_s}\right)^{n/2}$$
 where  $n = \frac{L_m}{u\Delta t}$  (2.19)

Let us expand Equation 2.19 using Equations 2.17 and 2.18

$$T_{m} = \left[ \left( \frac{1 - b - ic}{1 + b + ic} \right) \left( \frac{1}{e^{-D\sigma^{2}2\Delta t}e^{i\sigma u2\Delta t}} \right) \right]^{n/2}$$

$$\sigma = \frac{2\pi}{L_{m}} \qquad L_{m} = m\Delta x \qquad b = 4D' \sin^{2} \left( \frac{\pi}{m\Delta x} \Delta x \right) = 4D' \sin^{2} \left( \frac{\pi}{m} \right)$$

$$c = U \sin \left( \frac{2\pi}{m\Delta x} \Delta x \right) = U \sin \frac{2\pi}{m}$$

$$D\sigma^{2}2\Delta t = D \left( \frac{2\pi}{m\Delta x} \right)^{2}2\Delta t = D \frac{4\pi^{2}}{m^{2}\Delta x^{2}} 2\Delta t = \frac{D\Delta t}{\Delta x^{2}} 2 \left( \frac{2\pi}{m} \right)^{2} = 2D' \left( \frac{2\pi}{m} \right)^{2}$$

$$\sigma u2\Delta t = \frac{2\pi}{m\Delta x} (u2\Delta t) = \frac{4\pi}{m} \frac{u\Delta t}{\Delta x} = \frac{4\pi}{m} U$$

$$T_{m} = \left[ \left( \frac{1 - 4D' \sin^{2} \left( \frac{\pi}{m} \right) - iU \sin \frac{2\pi}{m}}{1 + 4D' \sin^{2} \left( \frac{\pi}{m} \right) + iU \sin \frac{2\pi}{m}} \right) \left( \frac{1}{e^{-2\sigma(2\pi/m)^{2}} e^{i(4\pi/m)U}} \right) \right]^{n/2}$$
(2.20)

Leendertse [1] considers D' = 0.01, 0.04, and U = 0.1, 0.2, 0.5, 1. m is plotted on log scale for the range 2 - 100. (Only two cycles are used.) In working with Equation 2.20 it is instructive to convert the first complex number to polar representation

$$c_{1} = \rho_{1}e^{i\theta_{1}} = \rho_{1} (\cos \theta_{1} + i \sin \theta_{1})$$

$$c_{2} = \rho_{2}e^{i\theta_{2}} = \rho_{2} (\cos \theta_{2} + i \sin \theta_{2})$$

$$\frac{c_{1}}{c_{2}} = \frac{\rho_{1}}{\rho_{2}}e^{i(\theta_{1}-\theta_{2})}$$

Note  

$$c_{1} = \left[ \left( 1 - 4D' \sin^{2} \left( \frac{\pi}{m} \right) \right)^{2} + U^{2} \sin^{2} \frac{2\pi}{m} \right] e^{i \tan^{-1} \left[ U \sin \left( 2\pi/m \right) / \left( 1 - 4D' \sin^{2} \left( \pi/m \right) \right) \right]}$$

$$c_{2} = \left[ \left(1 + 4D' \sin^{2} \left(\frac{\pi}{m}\right)\right)^{2} + U^{2} \sin^{2} \frac{2\pi}{m} \right] e^{i \tan^{-1} \left[U \sin \left(\frac{2\pi}{m}\right) / \left(1 + 4D' \sin^{2} \left(\frac{\pi}{m}\right)\right)\right]}$$

$$\frac{c_1}{c_2} = \frac{\left(1 - 4D'\sin^2\left(\frac{\pi}{m}\right)\right)^2 + U^2\sin^2\frac{2\pi}{m}}{\left(1 + 4D'\sin^2\left(\frac{\pi}{m}\right)\right)^2 + U^2\sin^2\frac{2\pi}{m}} e^{i\left[\tan^{-1}\frac{U\sin(2\pi/m)}{1 - 4D'\sin^2(\pi/m)} - \tan^{-1}\frac{U\sin(2\pi/m)}{1 + 4D'\sin^2(\pi/m)}\right]}$$

We therefore may rewrite Equation 2.20 in final form by defining temporary variables  $a = 1 - 4D' \sin^2 \pi/m$ ,  $b = 1 + 4D' \sin^2 \pi/m$ , and  $c = U \sin (2\pi/m)$ . Note  $n = L_m/u\Delta t = m\Delta x/u\Delta t = m/U$ .

$$T_{m} = \frac{\frac{a^{2} + c^{2}}{b^{2} + c^{2}}}{e^{-2\sigma/(2\pi/m)^{2}}} e^{i \left[ \tan^{-1} (c/a) - \tan^{-1} (c/b) - (4\pi/m)U \right]^{m/2U}}$$
(2.21a)

$$T_{m} = R_{m} e^{i\theta_{m}}$$
(2.21b)

The plot of  $R_m$  versus m is known as the modulus of the propagation factor. The plot of  $\theta_m$  versus m is known as the argument of the propagation factor. An alternate means of considering  $T_m$  is given by Leendertse as  $T(\sigma L)$  where  $T[(2\pi/m\Delta x)L]$  or  $T[(2\pi/m\Delta x)\Delta x] = T(2\pi/m) = T_m$ .  $L = \Delta x$  is a characteristic length equal to the grid size. Although we have not shown the above plots here, Leendertse comments that amplitude and phase characteristics of the multioperational scheme are good for  $m \ge 10$ ,  $L_m \ge 10\Delta x$ .

M

In the simulation of Jamaica Bay  $\Delta x = 500$  ft\* and  $L_m \ge 5000$  ft. \* To convert from feet to meters, multiply by 0.3048. For wavelengths less than 5000 ft the amplitudes will be amplified. The flow conditions considered for initial testing are given in Table I.

u D	$\frac{0.1}{0.01}$ ,	$\frac{0.2}{0.01}$ ,	$\frac{0.5}{0.01}$ ,	$\frac{1.0}{0.01}$	v D	$\frac{0.1}{0.04}$	$\frac{0.2}{0.04}$	$\frac{0.5}{0.04}$	$\frac{1.0}{0.04}$
	¥	¥	¥	¥		t	t	t	¥
P <sub>e</sub>	10	20	50	100	۴e	2.5	5	12.5	25

Table I. Leendertse Flow Conditions

3. Leendertse Multioperational Schemes: Two-Dimensional Analysis (FTCS)

The following two-dimensional transport equation is considered.

$$\frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + v \frac{\partial \eta}{\partial y} = \alpha \left( \frac{\partial^2 \eta}{\partial x^2} + \frac{\partial^2 \eta}{\partial y^2} \right)$$
(3.1)

where

$$\eta \equiv \text{constituent of concern}$$

u,v ≡ constant velocity components in the x and y directions, respectively

 $\alpha \equiv \text{constant dispersion coefficient}$ 

x,y,t are as previously defined

Leendertse [1] employs the scheme originally proposed by Peaceman and Rachford [2] for diffusion problems. Namely, for the X-sweep

$$\left(1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2\right) \eta^{n+1/2} = \left(1 - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2\right) \eta^n \qquad (3.2a)$$

For the Y-sweep

$$\left(1 + \frac{\mathbf{v}\Delta t}{2} \, \delta \mathbf{y} - \frac{\alpha \Delta t}{2} \, \delta \mathbf{y}^2\right) \eta^{n+1} = \left(1 - \frac{\mathbf{u}\Delta t}{2} \, \delta \mathbf{x} + \frac{\alpha \Delta t}{2} \, \delta \mathbf{x}^2\right) \eta^{n+1/2} \quad (3.2b)$$

where

$$\begin{split} \delta \mathbf{x} &= (\eta_{\ell,m+1} - \eta_{\ell,m-1}) \ 2\Delta \mathbf{x} & \delta \mathbf{x}^2 &= (\eta_{\ell,m+1} + \eta_{\ell,m-1} - 2\eta_{\ell,m}) \ \Delta \mathbf{x}^2 \\ \delta \mathbf{y} &= (\eta_{\ell+1,m} - \eta_{\ell-1,m}) \ 2\Delta \mathbf{y} & \delta \mathbf{y}^2 &= (\eta_{\ell+1,m} + \eta_{\ell-1,m} - 2\eta_{\ell,m}) \ \Delta \mathbf{y}^2 \\ \mathbf{x} &= \mathbf{m} \Delta \mathbf{x} \\ \mathbf{y} &= \ell \Delta \mathbf{y} \\ \mathbf{t} &= \mathbf{n} \Delta \mathbf{t} \end{split}$$

If we eliminate the intermediate level  $\eta^{n+1/2}$  , we obtain

$$\frac{\left(1 - \frac{\mathbf{v}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{y} + \frac{\mathbf{\alpha}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{y}^2\right)\boldsymbol{\eta}^{\mathbf{n}}}{\left(1 + \frac{\mathbf{u}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{x} - \frac{\mathbf{\alpha}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{x}^2\right)} = \frac{\left(1 + \frac{\mathbf{v}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{y} - \frac{\mathbf{\alpha}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{y}^2\right)\boldsymbol{\eta}^{\mathbf{n}+1}}{\left(1 - \frac{\mathbf{u}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{x} + \frac{\mathbf{\alpha}\Delta \mathbf{t}}{2}\,\,\delta\mathbf{x}^2\right)}$$
(3.3)

Expanding Equation 3.3 we obtain

$$\begin{pmatrix} 1 + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^2 \end{pmatrix} \begin{pmatrix} 1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2 \end{pmatrix} \eta^{n+1}$$

$$= \left(1 - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2 \right) \left(1 - \frac{u\Delta t}{2} \delta x + \frac{\alpha\Delta t}{2} \delta x^2 \right) \eta^n$$

$$(3.4)$$

Let us substitute  $\eta_{\ell,m}^n = e^{\alpha n \Delta t} e^{i \gamma \ell \Delta y} e^{i \beta m \Delta x}$  into Equation 3.4 and define the following auxillary variables.

$$a_{1} = \frac{u\Delta t}{4\Delta x} \qquad a_{2} = \frac{v\Delta t}{4\Delta y}$$

$$b_{1} = \frac{\alpha\Delta t}{2\Delta x^{2}} \qquad b_{2} = \frac{\alpha\Delta t}{2\Delta y^{2}}$$
(3.5)

If we employ, the results of Equation 2.6, we obtain the following expression for the eigenvalue  $\lambda$  of the numerical approximation.

$$\lambda = \frac{\eta_{\ell,m}^{n+1}}{\eta_{\ell,m}^{n}}$$

$$= \frac{\left(1 - 2ia_{1} \sin \beta \Delta x - 4b_{1} \sin^{2} \frac{\beta \Delta x}{2}\right) \left(1 - 2ia_{2} \sin \gamma \Delta y - 4b_{2} \sin^{2} \frac{\gamma \Delta y}{2}\right)}{\left(1 + 2ia_{1} \sin \beta \Delta x + 4b_{1} \sin^{2} \frac{\beta \Delta x}{2}\right) \left(1 + 2ia_{2} \sin \gamma \Delta y + 4b_{2} \sin^{2} \frac{\gamma \Delta y}{2}\right)}$$
(3.6)

We note then  $|\lambda| \leq 1$  , thus the scheme is unconditionally stable.

If we expand Equation 3.4, we obtain the equivalent two-dimensional difference scheme.

$$\left(1 + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^{2} + \frac{u\Delta t}{2} \delta x + \frac{uv\Delta t^{2}}{4} \delta x \delta y - \frac{\alpha u\Delta t^{2}}{4} \delta y^{2} \delta x - \frac{\alpha \Delta t}{2} \delta x^{2} - \frac{\alpha v\Delta t^{2}}{4} \delta x^{2} \delta y + \left(\frac{\alpha\Delta t}{2}\right)^{2} \delta y^{2} \delta x^{2}\right) \eta^{n+1}$$

$$\left(1 - \frac{u\Delta t}{2} \delta x + \frac{\alpha\Delta t}{2} \delta x^{2} - \frac{v\Delta t}{2} \delta y + \frac{uv\Delta t^{2}}{4} \delta x \delta y - \frac{\alpha v\Delta t^{2}}{4} \delta x^{2} \delta y + \frac{\alpha \Delta t}{4} \delta x^{2} \delta y + \frac{\alpha \Delta t}{2} \delta y^{2} - \frac{\alpha u\Delta t^{2}}{4} \delta y^{2} \delta x + \left(\frac{\alpha\Delta t}{2}\right)^{2} \delta y^{2} \delta x^{2}\right) \eta^{n}$$

$$\left(3.7\right)$$

We observe further that Equation 3.7 may be rewritten as follows

$$\delta_{t}\eta^{n} + v\Delta t \quad \delta y \quad \frac{(\eta^{n+1} + \eta^{n})}{2} + u\Delta t \quad \delta x \quad \frac{(\eta^{n+1} + \eta^{n})}{2}$$

$$- \alpha\Delta t \quad \delta y^{2} \left(\frac{\eta^{n+1} + \eta^{n}}{2}\right) - \alpha\Delta t \quad \delta^{2} x \left(\frac{\eta^{n+1} + \eta^{n}}{2}\right)$$

$$+ \frac{uv\Delta t^{2}}{4} \quad \delta x \delta y \quad (\eta^{n+1} - \eta^{n}) - \frac{\alpha u\Delta t^{2}}{4} \quad \delta y^{2} \delta x \quad (\eta^{n+1} - \eta^{n})$$

$$- \frac{\alpha v\Delta t^{2}}{4} \quad \delta x^{2} \delta y \quad (\eta^{n+1} - \eta^{n}) + \left(\frac{\alpha\Delta t}{2}\right)^{2} \quad \delta y^{2} \delta x^{2} \quad (\eta^{n+1} - \eta^{n}) = 0$$

$$(3.8)$$

where  $\delta_t = \eta^{n+1} - \eta^n$ . We note the underlined terms are additional

terms required by the factorization necessary to obtain the multioperational scheme.

4. Leendertse Multioperational Schemes: Two-Dimensional Analysis (FTUS)

A forward time upwind space scheme may be developed by considering the following general space derivative in operator notation.

$$T_{\mathbf{x}} = \delta_{\mathbf{x}} + g \frac{\Delta \mathbf{x}}{2} \delta \mathbf{x}^{2} \qquad g \in (-1, 0, 1)$$

$$T_{\mathbf{y}} = \delta \mathbf{y} + g \frac{\Delta \mathbf{y}}{2} \delta \mathbf{y}^{2}$$
(4.1)

Where

 $T_x, T_y \equiv$  general first derivative operator

 $\delta x, \delta y \equiv$  centered first derivative operators as previously defined  $\delta x^2, \delta y^2 \equiv$  second derivative operators as previously defined For g = -1, backward space differences are employed. For g = 0, the previous scheme with centered space derivatives is obtained. For g = +1, forward space differences are developed.

If we replace  $\delta_x$  and  $\delta_y$  by  $T_x$  and  $T_y$ , respectively, in Equations 3.2-3.4 and in Equations 3.7 and 3.8 a very general scheme is obtained equivalent to Leendertse's [1] one-dimensional analysis. Correspondingly, in Equation 3.6 it is necessary to make the following assignments to obtain the relation in Equation 4.3 below for the eigenvalue of the general scheme.

$$2ia_{1} \sin \beta \Delta x \rightarrow 2ia_{1} \sin \beta \Delta x - 4a_{1}g \sin^{2} \frac{\beta \Delta x}{2}$$

$$(4.2)$$

$$2ia_{2} \sin \gamma \Delta y \rightarrow 2ia_{2} \sin \gamma \Delta y - 4a_{2}g \sin^{2} \frac{\gamma \Delta y}{2}$$

$$A = \frac{\left[1 + (4a_{1}g - 4b_{1})\sin^{2}\frac{\beta\Delta x}{2} - 2ia_{1}\sin\beta\Delta x\right]\left[1 + (4a_{2}g - 4b_{2})\sin^{2}\frac{\gamma\Delta y}{2} - 2ia_{2}\sin\gamma\Delta y\right]}{\left[1 + (4b_{1} - 4a_{1}g)\sin^{2}\frac{\beta\Delta x}{2} + 2ia_{1}\sin\beta\Delta x\right]\left[1 + (4b_{2} - 4a_{2}g)\sin^{2}\frac{\gamma\Delta y}{2} + 2ia_{2}\sin\gamma\Delta y\right]} (4.3)$$

in which

$$4a_{1}g - 4b_{1} = \left(\frac{u\Delta tg}{\Delta x} - \frac{2\alpha\Delta t}{\Delta x^{2}}\right)$$

$$4a_{2}g - 4b_{2} = \left(\frac{v\Delta tg}{\Delta y} - \frac{2\alpha\Delta t}{\Delta y^{2}}\right)$$
(4.4)

We observe that if we set  $\Delta t \rightarrow \Delta t/2$ ,  $\alpha \rightarrow g$ ,  $D \rightarrow \alpha$  in Equation 2.11, for  $a_2 = b_2 = o$ , we obtain the result given by Equation 4.3. Analogous to the one dimension case, for upwind differencing an unconditionally stable scheme is obtained which we denote as FTUS.

#### 5. Spread Time Derivative Schemes

Let us first define the following average space operators

$$\mu_{x} = \frac{\eta_{\ell, m+1} + \eta_{\ell, m-1}}{2}$$
(5.1a)

$$\mu_{y} = \frac{\eta_{\ell+1,m} + \eta_{\ell-1,m}}{2}$$
 (5.1b)

If one studies the relationship between Equations 3.3 and 3.6 and replaces 1 by  $(2 + \mu_x)/3$  or by  $(2 + \mu_y)/3$ , appropriately, several schemes suggest themselves. In each case, the appropriate time derivative is averaged spatially and a "spread" in space time derivative scheme is obtained. Several such schemes are investigated in turn below. Intermediate level differencing

If we replace 1 by  $(2 + \mu_x)/3$  at the intermediate level we obtain the following relation.

$$\left(1 + \frac{\mathbf{v}\Delta \mathbf{t}}{2} \, \delta \mathbf{y} - \frac{\alpha \Delta \mathbf{t}}{2} \, \delta \mathbf{y}^2\right) \left(\frac{2}{3} + \frac{\mu_{\mathbf{x}}}{3} + \frac{\mathbf{u}\Delta \mathbf{t}}{2} \, \delta \mathbf{x} - \frac{\alpha \Delta \mathbf{t}}{2} \, \delta \mathbf{x}^2\right) \eta_{\ell,m}^{n+1}$$

$$= \left(\frac{2}{3} + \frac{\mu_{\mathbf{x}}}{3} - \frac{\mathbf{u}\Delta \mathbf{t}}{2} \, \delta \mathbf{x} + \frac{\alpha \Delta \mathbf{t}}{2} \, \delta \mathbf{x}^2\right) \left(1 - \frac{\mathbf{v}\Delta \mathbf{t}}{2} \, \delta \mathbf{y} + \frac{\alpha \Delta \mathbf{t}}{2} \, \delta \mathbf{y}^2\right) \eta_{\ell,m}^n$$

$$(5.2)$$

If one substitutes  $\eta_{\ell,m}^n = e^{\alpha n \Delta t} e^{i \gamma \ell \Delta y} e^{i \beta m \Delta x}$  into Equation 5.2 and employs Equation 3.5, the following eigenvalue for the numerical scheme is obtained.

$$\lambda = \frac{\left(\frac{2}{3} + \frac{\cos\beta\Delta x}{3} - 2ia_{1}\sin\beta\Delta x - 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)\left(1 - 2ia_{2}\sin\gamma\Delta y - 4b_{2}\sin^{2}\frac{\gamma\Delta y}{2}\right)}{\left(1 + 2ia_{2}\sin\gamma\Delta y + 4b_{2}\sin^{2}\frac{\gamma\Delta y}{2}\right)\left(\frac{2}{3} + \frac{\cos\beta\Delta x}{3} + 2ia_{1}\sin\beta\Delta x + 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)} (5.3)$$

 $\lambda \leq 1~$  and the scheme is unconditionally stable. The scheme is given by the following relationship.

$$\left(\frac{2}{3} + \frac{\mu_{\mathbf{x}}}{3} + \frac{\mathbf{u}\Delta \mathbf{t}}{2} \, \delta \mathbf{x} - \frac{\alpha\Delta \mathbf{t}}{2} \, \delta \mathbf{x}^2\right) \eta^{n+1/2} = 1 - \frac{\mathbf{v}\Delta \mathbf{t}}{2} \, \delta \mathbf{y} + \frac{\alpha\Delta \mathbf{t}}{2} \, \delta \mathbf{y}^2 \, \eta^n$$

$$\left(1 + \frac{\mathbf{v}\Delta \mathbf{t}}{2} \, \delta \mathbf{y} - \frac{\alpha\Delta \mathbf{t}}{2} \, \delta \mathbf{y}^2\right) \eta^{n+1} = \left(\frac{2}{3} + \frac{\mu_{\mathbf{x}}}{3} - \frac{\mathbf{u}\Delta \mathbf{t}}{2} \, \delta \mathbf{x} + \frac{\alpha\Delta \mathbf{t}}{2} \, \delta \mathbf{x}^2\right) \eta^{n+1/2}$$

$$(5.4)$$

Expanding Equation 5.2 we obtain the equivalent two-dimensional scheme

$$\begin{pmatrix} \frac{2}{3} + \frac{\mu_{x}}{3} + \frac{u\Delta t}{2} & \delta x - \frac{\alpha\Delta t}{2} & \delta x^{2} + \frac{v\Delta t}{3} & \delta y + \frac{v\Delta t}{6} & \delta y \mu_{x} + \frac{uv\Delta t^{2}}{4} & \delta x \delta y \\ & - \frac{\alpha v\Delta t^{2}}{4} & \delta x^{2} \delta y - \frac{\alpha\Delta t}{3} & \delta y^{2} - \frac{\alpha\Delta t}{6} & \delta y^{2} \mu_{x} - \frac{u\alpha\Delta t^{2}}{4} & \delta y^{2} \delta x \\ & + \frac{\alpha^{2}\Delta t^{2}}{4} & \delta y^{2} \delta x^{2} \end{pmatrix} \eta^{n+1}$$

$$= \left( \frac{2}{3} + \frac{\mu_{x}}{3} - \frac{u\Delta t}{2} & \delta x + \frac{\alpha\Delta t}{2} & \delta x^{2} - \frac{v\Delta t}{3} & \delta y - \frac{1}{6} & v\Delta t \delta y \mu_{x} + \frac{uv\Delta t^{2}}{4} & \delta x \delta y \\ & - \frac{\alpha v\Delta t^{2}}{4} & \delta x^{2} \delta y + \frac{\alpha\Delta t}{3} & \delta y^{2} + \frac{\alpha\Delta t}{6} & \delta y^{2} \mu_{x} - \frac{\alpha u\Delta t^{2}}{4} & \delta y^{2} \delta x + \frac{\alpha^{2}\Delta t^{2}}{4} & \delta x^{2} \delta y^{2} \end{pmatrix} \eta^{n}$$

$$(5.5)$$

If we combine like terms in Equation 5.5 we obtain the following relation in which the additional factorization terms (see underlined terms in Equation 3.8) have been omitted.

$$\begin{pmatrix} \frac{2}{3} + \mu_{\mathbf{x}} \\ \frac{1}{3} \end{pmatrix} \delta_{\mathbf{t}} \eta^{\mathbf{n}} + \mathbf{u} \Delta t \delta \mathbf{x} \begin{pmatrix} \underline{\eta^{n+1} + \eta^{\mathbf{n}}} \\ \frac{1}{2} \end{pmatrix} - \alpha \Delta t \delta \mathbf{x}^{2} \begin{pmatrix} \underline{\eta^{n+1} + \eta^{\mathbf{n}}} \\ \frac{1}{2} \end{pmatrix}$$

$$+ \frac{2}{3} \mathbf{v} \Delta t \delta \mathbf{y} \begin{pmatrix} \underline{\eta^{n+1} + \eta^{\mathbf{n}}} \\ \frac{1}{2} \end{pmatrix} - \frac{2}{3} \alpha \Delta t \delta \mathbf{y}^{2} \begin{pmatrix} \underline{\eta^{n+1} + \eta^{\mathbf{n}}} \\ \frac{1}{2} \end{pmatrix}$$

$$+ \frac{1}{3} \mathbf{v} \Delta t \delta \mathbf{y} \mu_{\mathbf{x}} \begin{pmatrix} \underline{\eta^{n+1} + \eta^{\mathbf{n}}} \\ \frac{1}{2} \end{pmatrix} - \frac{1}{3} \alpha \Delta t \delta \mathbf{y}^{2} \mu_{\mathbf{x}} \begin{pmatrix} \underline{\eta^{n+1} + \eta^{\mathbf{n}}} \\ \frac{1}{2} \end{pmatrix} \approx 0$$

$$(5.6)$$

#### Opposite intermediate level differencing

If we replace 1 by  $(2+\mu_y)/3$  at time levels n and n+1 and employ standard time differencing at  $\eta^{n+1/2}$  the following relation is obtained

$$\begin{pmatrix} \frac{2}{3} + \frac{\mu_y}{3} + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^2 \end{pmatrix} \begin{pmatrix} 1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2 \end{pmatrix} \eta^{n+1}$$

$$= \left(1 - \frac{u\Delta t}{2} \delta x + \frac{\alpha\Delta t}{2} \delta x^2\right) \left(\frac{2}{3} + \frac{\mu_y}{3} - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2\right) \eta^n$$
(5.7)

If one substitutes  $\eta_{\ell,m}^n = e^{\alpha n \Delta t} e^{i \gamma \ell \Delta y} e^{i \beta m \Delta x}$  into Equation 5.7, the following eigenvalue is obtained.

$$\lambda = \frac{\left(1 - 2ia_{1}\sin\beta\Delta x - 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)\left(\frac{2}{3} + \frac{\cos\gamma\Delta y}{3} - 2ia_{2}\sin\gamma\Delta y - 4b_{2}\sin^{2}\frac{\gamma\Delta y}{2}\right)}{\left(\frac{2}{3} + \frac{\cos\gamma\Delta y}{3} + 2ia_{2}\sin\gamma\Delta y + 4b_{2}\sin^{2}\frac{\gamma\Delta y}{2}\right)\left(1 + 2ia_{1}\sin\beta\Delta x + 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)}$$
(5.8)

Since  $\lambda \leq 1$ , this scheme is also unconditionally stable. The scheme is given by the following relationship.

$$\left(1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2\right) \eta^{n+1/2} = \left(\frac{2}{3} + \frac{\mu y}{3} - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2\right) \eta^n$$

$$\left(\frac{2}{3} + \frac{\mu y}{3} + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^2\right) \eta^{n+1} = \left(1 - \frac{u\Delta t}{2} \delta x + \frac{\alpha\Delta t}{2} \delta x^2\right) \eta^{n+1/2}$$

$$(5.9)$$

Expanding Equation 5.7 the following equivalent two dimensional scheme is obtained.

$$\begin{pmatrix} \frac{2}{3} + \frac{\mu_y}{3} + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^2 + \frac{u\Delta t}{3} \delta x + \frac{u\Delta t}{6} \delta x \mu_y + \frac{uv\Delta t^2}{4} \delta y \delta x \\ - \frac{\alpha u\Delta t^2}{4} \delta y^2 \delta x - \frac{\alpha\Delta t}{3} \delta x^2 - \frac{\alpha\Delta t}{6} \delta x^2 \mu_y - \frac{\alpha v\Delta t^2}{4} \delta x^2 \delta y \\ + \frac{\alpha^2 \Delta t^2}{4} \delta x^2 \delta y^2 \right) \eta^{n+1}$$

$$= \left( \frac{2}{3} + \frac{\mu_y}{3} - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2 - \frac{u\Delta t}{3} \delta x - \frac{u\Delta t}{6} \delta x \mu_y + \frac{uv\Delta t^2}{4} \delta y \delta x \\ - \frac{\alpha u\Delta t^2}{4} \delta y^2 \delta x + \frac{\alpha\Delta t}{3} \delta x^2 + \frac{\alpha\Delta t}{6} \delta x^2 \mu_y - \frac{\alpha v\Delta t^2}{4} \delta x^2 \delta y + \frac{\alpha^2 \Delta t^2}{4} \delta x^2 \delta y \right) \eta^n$$

$$(5.10)$$

Equation 5.10 may be written neglecting the factorization terms as follows.

$$\begin{pmatrix} \frac{2 + \mu_y}{3} \end{pmatrix} \delta_t \eta^n + v \Delta t \delta y \left( \frac{\eta^{n+1} + \eta^n}{2} \right) - \alpha \Delta t \delta y^2 \left( \frac{\eta^{n+1} + \eta^n}{2} \right)$$

$$+ \frac{2}{3} u \Delta t \delta x \left( \frac{\eta^{n+1} + \eta^n}{2} \right) - \frac{2}{3} \alpha \Delta t \delta x^2 \left( \frac{\eta^{n+1} + \eta^n}{2} \right)$$

$$+ \frac{1}{3} u \Delta t \delta x \mu_y \left( \frac{\eta^{n+1} + \eta^n}{2} \right) - \frac{1}{3} \alpha \Delta t \delta x^2 \mu_y \left( \frac{\eta^{n+1} + \eta^n}{2} \right) \approx 0$$

$$(5.11)$$

#### Advanced level differencing

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ė

If one employs spread time derivatives at the most advanced levels in each sweep  $(\eta^{n+1/2*} \text{ and } \eta^{n+1})$  and utilizes previous procedures, the following eigenvalue is obtained for this scheme.

$$\lambda = \frac{\left(1 - 2ia_1 \sin \beta \Delta x - 4b_1 \sin^2 \frac{\beta \Delta x}{2}\right) \left(1 - 2ia_2 \sin \gamma \Delta y - 4b_2 \sin^2 \frac{\gamma \Delta y}{2}\right)}{\left(\frac{2}{3} + \frac{\cos \beta \Delta x}{3} + 2ia_1 \sin \beta \Delta x + 4b_1 \sin^2 \frac{\beta \Delta x}{2}\right) \left(\frac{2}{3} + \frac{\cos \gamma \Delta y}{3} + 2ia_2 \sin \gamma \Delta y + 4b_2 \sin^2 \frac{\gamma \Delta y}{2}\right)}$$
(5.12)

Consider a stability investigation in the following manner. First, note by trigonometric identity

$$\sin^2 \frac{\beta \Delta x}{2} = \frac{1 - \cos \beta \Delta x}{2}$$
 and  $\sin^2 \frac{\gamma \Delta y}{2} = \frac{1 - \cos \gamma \Delta y}{2}$ 

Consider  $\gamma \Delta y = (0) = \beta \Delta x$ , then since sin (0) = 0 and cos (0) = 1, Equation 5.12 becomes

$$\lambda = \frac{9}{4} \rightarrow |\lambda| > 1$$

and the method is unstable. Therefore, this scheme will not be further considered.

#### Retarded level differencing

If one employs spread time differencing at the most retarded time level in both sweeps, the eigenvalue is given by the following relation.

$$\lambda = \frac{\left(\frac{2}{3} + \frac{\cos\beta\Delta x}{3} - 2ia_{1}\sin\beta\Delta x - 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)\left(\frac{2}{3} + \frac{\cos\gamma\Delta y}{3} - 2ia_{2}\sin\gamma\Delta y - 4b_{2}\sin^{2}\frac{\gamma\Delta y}{2}\right)}{\left(1 + 2ia_{2}\sin\gamma\Delta y + 4b_{2}\sin^{2}\frac{\gamma\Delta y}{2}\right)\left(1 + 2ia_{1}\sin\beta\Delta x + 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)}$$
(5.13)

This scheme is unconditionally stable and is given by the following relation.

$$\left(1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2\right) \left(1 + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^2\right) \eta^{n+1}$$

$$= \left(\frac{2}{3} + \frac{\mu_y}{3} - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2\right) \left(\frac{2}{3} + \frac{\mu_x}{3} - \frac{u\Delta t}{2} \delta x + \frac{\alpha\Delta t}{2} \delta x^2\right) \eta^n$$

$$(5.14)$$

The sweep equations then become

$$\left(1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha \Delta t}{2} \delta x^2\right) \eta^{n+1/2} = \left(\frac{2}{3} + \frac{\mu_y}{3} - \frac{v\Delta t}{2} \delta y + \frac{\alpha \Delta t}{2} \delta y^2\right) \eta^n$$

$$\left(1 + \frac{v\Delta t}{2} \delta y - \frac{\alpha \Delta t}{2} \delta y^2\right) \eta^{n+1} = \left(\frac{2}{3} + \frac{\mu_x}{3} - \frac{u\Delta t}{2} \delta x + \frac{\alpha \Delta t}{2} \delta x^2\right) \eta^{n+1/2}$$

$$(5.15)$$

If Equation 5.14 is expanded the following relation is obtained.

$$\begin{pmatrix} 1 + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2 + \frac{v\Delta t}{2} \delta y + \frac{uv\Delta t^2}{4} \delta x \delta y - \frac{\alpha v\Delta t^2}{4} \delta x^2 \delta y \\ - \frac{\alpha\Delta t}{2} \delta y^2 - \frac{\alpha u\Delta t^2}{4} \delta y^2 \delta x + \frac{\alpha^2 \Delta t^2}{4} \delta x^2 \delta y^2 \right) \eta^{n+1} \\ = \left( \frac{4}{9} + \frac{2}{9} \mu_y - \frac{v\Delta t}{3} \delta y + \frac{\alpha\Delta t}{3} \delta y^2 + \frac{2}{9} \mu_x + \frac{\mu_y \mu_x}{9} - \frac{v\Delta t}{6} \delta y \mu_x \right)$$
(5.16)  
$$+ \frac{\alpha\Delta t}{6} \delta y^2 \mu_x - \frac{u\Delta t}{3} \delta x - \frac{u\Delta t}{6} \delta x \mu_y + \frac{uv\Delta t^2}{4} \delta y \delta x - \frac{\alpha u\Delta t^2}{4} \delta y^2 \delta x \\ + \frac{\alpha\Delta t}{3} \delta x^2 + \frac{\alpha\Delta t}{6} \delta x^2 \mu_y - \frac{\alpha v\Delta t^2}{4} \delta x^2 \delta y + \frac{\alpha^2 \Delta t^2}{4} \delta x^2 \delta y^2 \right) \eta^n$$

Equation 5.16 may be recast into the following form (ignoring  $\Delta t^2$  factorization terms).

$$\eta^{n+1} - \frac{4 + 2(\mu_x + \mu_y) + \mu_x \mu_y}{9} \eta^n + v\Delta t \delta y \frac{\eta^{n+1}}{2} + \frac{(2 + \mu_x)}{6} \eta^n + u\Delta t \delta x \frac{\eta^{n+1}}{2} + \frac{(2 + \mu_y)}{6} \eta^n - \alpha \Delta t \delta y^2 \frac{\eta^{n+1}}{2} + \frac{(2 + \mu_x)}{6} \eta^n \quad (5.17)$$
$$- \alpha \Delta t \delta x^2 \frac{\eta^{n+1}}{2} + \frac{(2 + \mu_y)}{6} \eta^n = 0$$

#### Complete time level differencing

If one employs spread time differencing at all time levels in both sweeps, the scheme eigenvalue is given by the following relation

$$\lambda = \frac{\left(\frac{2}{3} + \frac{\cos\beta\Delta x}{3} - 2ia_{1}\sin\beta\Delta x - 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)\left(\frac{2}{3} + \frac{\cos\gamma\Delta y}{2} - 2ia_{2}\sin\gamma\Delta y - 4b_{2}\sin^{2}\frac{Y\Delta y}{2}\right)}{\left(\frac{2}{3} + \frac{\cos\gamma\Delta y}{3} + 2ia_{2}\sin\gamma\Delta y + 4b_{2}\sin^{2}\frac{Y\Delta y}{2}\right)\left(\frac{2}{3} + \frac{\cos\beta\Delta x}{3} + 2ia_{1}\sin\beta\Delta x + 4b_{1}\sin^{2}\frac{\beta\Delta x}{2}\right)}$$
(5.18)

This scheme is unconditionally stable. Corresponding to Equation 5.18, the scheme becomes

$$\left(\frac{2}{3} + \frac{\mu_x}{3} - \frac{u\Delta t}{2} \delta x + \frac{\alpha\Delta t}{2} \delta x^2\right) \left(\frac{2}{3} + \frac{\mu_y}{3} - \frac{v\Delta t}{2} \delta y + \frac{\alpha\Delta t}{2} \delta y^2\right) \eta^n$$

$$= \left(\frac{2}{3} + \frac{\mu_y}{3} + \frac{v\Delta t}{2} \delta y - \frac{\alpha\Delta t}{2} \delta y^2\right) \left(\frac{2}{3} + \frac{\mu_x}{3} + \frac{u\Delta t}{2} \delta x - \frac{\alpha\Delta t}{2} \delta x^2\right) \eta^{n+1}$$

$$(5.19)$$

In multioperational form, the scheme is given by

$$\left(\frac{2}{3} + \frac{\mu_{y}}{3} + \frac{v\omega t}{2} \, \delta y - \frac{\alpha \Delta t}{2} \, \delta y^{2}\right) \eta^{n+1/2} = \left(\frac{2}{3} + \frac{\mu_{x}}{3} - \frac{u\Delta t}{2} \, \delta x + \frac{\alpha \Delta t}{2} \, \delta x^{2}\right) \eta^{n}$$

$$\left(\frac{2}{3} + \frac{\mu_{x}}{3} + \frac{u\Delta t}{2} \, \delta x - \frac{\alpha \Delta t}{2} \, \delta x^{2}\right) \eta^{n+1} = \left(\frac{2}{3} + \frac{\mu_{y}}{3} - \frac{v\Delta t}{2} \, \delta y + \frac{\alpha \Delta t}{2} \, \delta y^{2}\right) \eta^{n+1/2}$$

$$(5.20)$$

If we expand Equation 5.19

$$\begin{pmatrix} \frac{4}{9} + \frac{2}{9} \mu_{y} + \frac{v\Delta t}{3} \delta y - \frac{\alpha\Delta t}{3} \delta y^{2} + \frac{2}{9} \mu_{x} + \frac{\mu_{x}\mu_{y}}{9} + \frac{v\Delta t}{6} \delta y\mu_{x} - \frac{\alpha\Delta t}{6} \delta y^{2}\mu_{x} \\ + \frac{u\Delta t}{3} \delta x + \frac{u\Delta t}{6} \delta x\mu_{y} + \frac{uv\Delta t^{2}}{4} \delta y\delta x - \frac{\alpha u\Delta t^{2}}{4} \delta y^{2}\delta x - \frac{\alpha\Delta t}{3} \delta x^{2} \\ - \frac{\alpha\Delta t}{6} \delta x^{2}\mu_{y} - \frac{\alpha v\Delta t^{2}}{4} \delta x^{2}\delta y + \frac{\alpha^{2}\Delta t^{2}}{4} \delta x^{2}\delta y^{2} \right) \eta^{n+1}$$

$$= \left( \frac{4}{9} + \frac{2}{9} \mu_{x} - \frac{u\Delta t}{3} \delta x + \frac{\alpha\Delta t}{3} \delta x^{2} + \frac{2}{9} \mu_{y} + \frac{\mu_{x}\mu_{y}}{9} - \frac{u\Delta t}{6} \delta x\mu_{y} + \frac{\alpha\Delta t}{6} \delta x^{2}\mu_{y} \right)$$

$$- \frac{v\Delta t}{3} \delta y - \frac{v\Delta t}{6} \delta y\mu_{x} + \frac{uv\Delta t^{2}}{4} \delta y\delta x - \frac{\alpha v\Delta t^{2}}{4} \delta x^{2}\delta y + \frac{\alpha\Delta t}{3} \delta^{2}y \\ + \frac{\alpha\Delta t}{6} \delta y^{2}\mu_{x} - \frac{\alpha u\Delta t^{2}}{4} \delta y^{2}\delta x + \frac{\alpha^{2}\Delta t^{2}}{4} \delta x^{2}\delta y^{2} \right) \eta^{n}$$

Collecting similar terms (ignoring factorization terms) we obtain

$$\left( \frac{4 + 2(\mu_{y} + \mu_{x}) + \mu_{y}\mu_{x}}{9} \right) \delta_{t} \eta^{n} + v \Delta t \delta y \left( \frac{\eta^{n+1} + \eta^{n}}{3} + \frac{\mu_{x}}{6} (\eta^{n+1} + \eta^{n}) \right)$$

$$- \alpha \Delta t \delta y^{2} \left( \frac{\eta^{n+1} + \eta^{n}}{3} + \frac{\mu_{x}}{6} (\eta^{n+1} + \eta^{n}) \right) + u \Delta t \delta x \left( \frac{\eta^{n+1} + \eta^{n}}{3} + \frac{\mu_{y}}{6} (\eta^{n+1} + \eta^{n}) \right) \quad (5.22)$$

$$- \alpha \Delta t \delta x^{2} \left( \frac{\eta^{n+1} + \eta^{n}}{3} + \frac{\mu_{y}}{6} (\eta^{n+1} + \eta^{n}) \right) \approx 0$$

Summary of spread time derivative schemes

The following four unconditionally stable schemes have been introduced: (a) intermediate level differencing, (b) opposite intermediate level differencing, (c) retarded level differencing, and (d) complete time level differencing. The first two of these schemes employ spread time derivatives in only one coordinate direction, while the second two schemes employ spread time derivatives in both directions. For a two-dimensional computation, the first two schemes appear less desirable than the last two schemes. These last two schemes are therefore further investigated within a formal truncation error analysis.

#### 6. Formal Truncation Error, Eigenvalue, and Complex Propagation Factor Analysis

In order to compare the schemes developed with respect to truncation error, Taylor series expansions were developed for the constituent terms common to all schemes. In Tables II and III the expansions are carried through third order, while in Tables IV and V the expansions are carried through fourth order terms. Substituting the appropriate expansions for the terms in each scheme, it is shown that all schemes are consistent with the linearized transport equation. The order of the principal truncation error is given in Table VI for each scheme.

We note that the complete time level differencing spread time derivative scheme is truly second order. Therefore, it is the more accurate of the two spread time derivative schemes and will be the subject of further numerical development.

The Leendertse multioperational schemes in tandem form a lower order (FTUS) and higher order (FTCS) pair, which may be developed within flux corrected transport.

## Table II. Time Level n Taylor Series Expansions (Third Order)

 $\eta_{\ell,m}^n = \eta_{\ell,m}^n$  $\mu_{\mathbf{y}} \eta_{\boldsymbol{\ell},\mathbf{m}}^{n} = \eta_{\boldsymbol{\ell},\mathbf{m}}^{n} + \frac{\Delta \mathbf{y}^{2}}{2!} \frac{\partial^{2} \eta}{\partial \mathbf{y}^{2}}$  $\delta y \eta_{\ell,m}^{n} = \frac{1}{2\Delta y} \left( 2\Delta y \frac{\partial \eta}{\partial y} + \frac{\Delta y^{3}}{3} \frac{\partial^{3} \eta}{\partial y^{3}} \right)$  $\mu_{\mathbf{x}} \eta_{\ell,m}^{n} = \eta_{\ell,m}^{n} + \frac{\Delta \mathbf{x}^{2}}{2!} \frac{\partial^{2} \eta}{\partial \mathbf{x}^{2}}$  $\delta x \eta_{\ell,m}^{n} = \frac{1}{2\Delta x} \left( 2\Delta x \frac{\partial \eta}{\partial x} + \frac{\Delta x^{3}}{3} \frac{\partial^{3} \eta}{\partial x^{3}} \right)$  $\mu_{\mathbf{x}}\mu_{\mathbf{y}}\eta_{\boldsymbol{\ell},\mathbf{m}}^{n} = \eta_{\boldsymbol{\ell},\mathbf{m}}^{n} + \frac{\Delta \mathbf{x}^{2}}{2!} \frac{\partial^{2} \eta}{\partial \mathbf{x}^{2}} + \frac{\Delta \mathbf{y}^{2}}{2!} \frac{\partial^{2} \eta}{\partial \mathbf{x}^{2}}$  $\delta y \mu_{x} \eta_{\ell,m}^{n} = \frac{1}{2\Delta y} \left( 2\Delta y \frac{\partial \eta}{\partial y} + \Delta x^{2} \Delta y \frac{\partial^{3} \eta}{\partial x^{2} \partial y} + \frac{\Delta x^{3}}{3} \frac{\partial^{3} \eta}{\partial x^{3}} \right)$  $\delta x \mu_y \eta_{\ell,m}^n = \frac{1}{2\Delta x} \left( 2\Delta x \frac{\partial \eta}{\partial x} + \Delta x \Delta y^2 \frac{\partial^3 \eta}{\partial x \partial y^2} + \frac{\Delta x^3}{3} \frac{\partial^3 \eta}{\partial x^3} \right)$  $\delta x \delta y \eta_{\ell,m}^{n} = \frac{1}{4\Delta x \Delta y} \left( 4\Delta x \Delta y \frac{\partial^{2} \eta}{\partial x \partial y} \right)$ 

## Table III. Time Level n+1 Taylor Series Expansions (Third Order)
# Table IV. Time Level n Taylor Series Expansions (Fourth Order)

$$\begin{split} \delta y^2 \eta_{\ell,m}^n &= \frac{1}{\Delta y^2} \left( \Delta y^2 \frac{\partial^2 \eta}{\partial y^2} + \frac{\Delta y^4}{12} \frac{\partial^4 \eta}{\partial y^4} \right) \\ \delta y^2 \mu_x \eta_{\ell,m}^n &= \frac{1}{\Delta y^2} \left( \Delta y^2 \frac{\partial^2 \eta}{\partial y^2} + \frac{\Delta x^2 \Delta y^2}{2} \frac{\partial^4 \eta}{\partial x^2 \partial y^2} + \frac{\Delta y^4}{12} \frac{\partial^4 \eta}{\partial y^4} \right) \\ \delta y^2 \delta x \eta_{\ell,m}^n &= \frac{1}{2\Delta x \Delta y^2} \left( 2\Delta x \Delta y^2 \frac{\partial^3 \eta}{\partial x \partial y^2} \right) \\ \delta x^2 \eta_{\ell,m}^n &= \frac{1}{\Delta x^2} \left( \Delta x^2 \frac{\partial^2 \eta}{\partial x^2} + \frac{\Delta x^4}{12} \frac{\partial^4 \eta}{\partial x^4} \right) \\ \delta x^2 \mu_y \eta_{\ell,m}^n &= \frac{1}{\Delta x^2} \left( \Delta x^2 \frac{\partial^2 \eta}{\partial x^2} + \frac{\Delta x^2 \Delta y^2}{2} \frac{\partial^4 \eta}{\partial x^2 \partial y^2} + \frac{\Delta x^4}{12} \frac{\partial^4 \eta}{\partial x^4} \right) \\ \delta x^2 \delta y^2 \eta_{\ell,m}^n &= \frac{1}{\Delta x^2 \Delta y^2} \left( \Delta x^2 \Delta y^2 \frac{\partial^4 \eta}{\partial x \partial y^2} \right) \\ \delta x^2 \delta y \eta_{\ell,m}^n &= \frac{1}{\Delta x^2 \Delta y^2} \left( 2\Delta y \Delta x^2 \frac{\partial^4 \eta}{\partial x \partial y^2} \right) \end{split}$$

 $\delta y^2 \eta_{\ell,m}^{n+1} = \frac{1}{\Delta y^2} \left( \Delta y^2 \frac{\partial^2 \eta}{\partial y^2} + \Delta y^2 \Delta t \frac{\partial^3 \eta}{\partial y^2 \partial t} + \frac{\Delta y^4}{12} \frac{\partial^4 \eta}{\partial y^4} + \frac{\Delta y^2 \Delta t^2}{2} \frac{\partial^4 \eta}{\partial y^2 \partial t^2} \right)$  $\delta y^{2} \mu_{x} \eta_{\ell,m}^{n+1} = \frac{1}{\Lambda y^{2}} \left( \Delta y^{2} \frac{\partial^{2} \eta}{\partial y^{2}} + \Delta y^{2} \Delta t \frac{\partial^{3} \eta}{\partial y^{2} \partial t} + \frac{\Delta t^{2} \Delta y^{2}}{2} \frac{\partial^{4} \eta}{\partial t^{2} \partial y^{2}} \right)$ +  $\frac{\Delta x^2 \Delta y^2}{2} \frac{\partial^4 \eta}{\partial y^2 \partial y^2} + \frac{\Delta y^4}{12} \frac{\partial^4 \eta}{\partial y^4}$  $\delta y^2 \delta x n_{\ell,m}^{n+1} = \frac{1}{2 \Delta x \Delta y^2} \left( 2 \Delta x \Delta y^2 \frac{\partial^3 n}{\partial x \partial y^2} + 2 \Delta t \Delta x \Delta y^2 \frac{\partial^4 n}{\partial t \partial x \partial y^2} \right)$  $\delta x^{2} n_{\ell,m}^{n+1} = \frac{1}{\Delta x^{2}} \left( \Delta x^{2} \frac{\partial^{2} n}{\partial x^{2}} + \Delta x^{2} \Delta t \frac{\partial^{3} n}{\partial x^{2} \partial t} + \frac{\Delta x^{4}}{12} \frac{\partial^{4} n}{\partial x^{4}} + \frac{\Delta x^{2} \Delta t^{2}}{2} \frac{\partial^{4} n}{\partial x^{2} \partial t^{2}} \right)$  $\delta \mathbf{x}^{2} \boldsymbol{\mu}_{\mathbf{y}} \quad \boldsymbol{\eta}_{\ell,\mathbf{m}}^{\mathbf{n+1}} = \frac{1}{\Delta \mathbf{x}^{2}} \left( \Delta \mathbf{x}^{2} \frac{\partial^{2} \boldsymbol{\eta}}{\partial \mathbf{x}^{2}} + \Delta \mathbf{x}^{2} \Delta \mathbf{t} \frac{\partial^{3} \boldsymbol{\eta}}{\partial \mathbf{x}^{2} \partial \mathbf{t}} + \frac{\Delta \mathbf{t}^{2} \Delta \mathbf{x}^{2}}{2} \frac{\partial^{4} \boldsymbol{\eta}}{\partial \mathbf{t}^{2} \partial \mathbf{x}^{2}} \right)$ +  $\frac{\Delta \mathbf{x}^2 \Delta \mathbf{y}^2}{2} \frac{\partial^4 \mathbf{n}}{\partial \mathbf{x}^2 \partial \mathbf{y}^2} + \frac{\Delta \mathbf{x}^4}{12} \frac{\partial^4 \mathbf{n}}{\partial \mathbf{x}^4}$  $\delta \mathbf{x}^2 \delta \mathbf{y}^2 \quad \mathbf{n}_{\ell,m}^{n+1} = \frac{1}{\Delta \mathbf{x}^2 \Delta \mathbf{y}^2} \left( \Delta \mathbf{x}^2 \Delta \mathbf{y}^2 \quad \frac{\partial^4 \mathbf{n}}{\partial \mathbf{x}^2 \partial \mathbf{y}^2} + \Delta t \Delta \mathbf{x}^2 \Delta \mathbf{y}^2 \quad \frac{\partial^5 \mathbf{n}}{\partial t \partial \mathbf{x}^2 \partial \mathbf{y}^2} \right)$  $\delta \mathbf{x}^{2} \delta \mathbf{y} \, \mathbf{n}_{\ell,\mathbf{m}}^{\mathbf{n+1}} = \frac{1}{2 \Delta \mathbf{y} \Delta \mathbf{x}^{2}} \left( 2 \Delta \mathbf{y} \Delta \mathbf{x}^{2} \, \frac{\partial^{3} \mathbf{n}}{\partial \mathbf{y} \partial \mathbf{x}^{2}} + 2 \Delta t \Delta \mathbf{y} \Delta \mathbf{x}^{2} \, \frac{\partial^{4} \mathbf{n}}{\partial t \partial \mathbf{y} \partial \mathbf{x}^{2}} \right)$ 

Table V. Time Level n+1 Taylor Series Expansions (Fourth Order)

Scheme	Equation	Order of Truncation Error*
Multioperational Leendertse		
FTCS	3.7	0 ( $\Delta t^2$ , $\Delta x^2$ , $\Delta y^2$ )
FTUS	3.7 and 4.1	0 (Δt <sup>2</sup> , Δx, Δy)
Spread Time Derivative		
Complete Level	5.21	0 ( $\Delta t^2$ , $\Delta x^2$ , $\Delta y^2$ )
Retarded Level	5.16	$0 \left( \Delta t^2, \frac{\Delta x^2}{\Delta t}, \frac{\Delta y^2}{\Delta t} \right) * *$

# Table VI. Truncation Error Analysis Results



#### Eigenvalue analysis

To facilitate this analysis, the following dimensionless quantities are defined. In the general two-dimensional case, the dispersion coefficients are different in each coordinate direction and are represented by  $D_{_{\rm X}}$  and  $D_{_{\rm V}}$ , respectively.

In previous paragraphs, D and  $\alpha$  have been used to represent, a constant dispersion coefficient in the one- and two-dimensional cases.

$$\sigma_{n} = \frac{2\pi}{n\Delta x} = \frac{2\pi}{L_{n}} \qquad \sigma_{m} = \frac{2\pi}{m\Delta y} \qquad U = \frac{u\Delta t}{\Delta x} \qquad V = \frac{v\Delta t}{\Delta y} \qquad (6.1)$$

$$\sigma_{n}^{2} = \frac{4\pi^{2}}{n^{2}\Delta x^{2}} = \left(\frac{2\pi}{L_{n}}\right)^{2} \qquad \sigma_{m}^{2} = \frac{4\pi^{2}}{m^{2}\Delta y^{2}} \qquad D_{x}^{*} = \frac{D_{x}\Delta t}{\Delta x^{2}} \qquad D_{y}^{*} = \frac{D_{y}\Delta t}{\Delta y^{2}} \qquad (6.1)$$

#### General two-dimensional scheme

Consider equation (4.3) which determines the eigenvalue for the following three schemes if u, v > 0:

(i) g = -1 : Upwind differencing (FTUS)
(ii) g = 0 : Centered differencing (FTCS)
(iii) g = +1 : Forward differencing (FTFS)

Noting  $a_1 = U/4$ ,  $a_2 = V/4$ ,  $b_1 = D'_x/2$ , and  $b_2 = D'_y/2$  the following expression is obtained. ( $\beta \approx \sigma_n$ ,  $\gamma = \sigma_m$ )

$$\lambda_{s} = \frac{\left[1 + (gU - 2D'_{x}) \sin^{2}\left(\frac{\pi}{m}\right) - i \frac{U}{2} \sin\left(\frac{2\pi}{m}\right)\right]}{\left[1 + (2D'_{x} - gU) \sin^{2}\left(\frac{\pi}{m}\right) + i \frac{U}{2} \sin\left(\frac{2\pi}{m}\right)\right]} \\ \times \frac{\left[1 + (gV - 2D'_{y}) \sin^{2}\left(\frac{\pi}{n}\right) - i \frac{V}{2} \sin\left(\frac{2\pi}{n}\right)\right]}{\left[1 + (2D'_{y} - gV) \sin^{2}\left(\frac{\pi}{n}\right) + i \frac{V}{2} \sin\left(\frac{2\pi}{n}\right)\right]} = \lambda_{sx} \cdot \lambda_{sy}$$
(6.2)

#### Spread time derivative scheme

The complete spread time derivative scheme eigenvalue given in (5.18) may be written as follows in terms of dimensionless quantities.

$$\lambda_{s} = \frac{\left[\frac{2}{3} + \frac{\cos\left(\frac{2\pi}{m}\right)}{3} - i\frac{U}{2}\sin\left(\frac{2\pi}{m}\right) - 2D'_{x}\sin^{2}\left(\frac{\pi}{m}\right)\right]}{\left[\frac{2}{3} + \frac{\cos\left(\frac{2\pi}{m}\right)}{3} + i\frac{U}{2}\sin\left(\frac{2\pi}{m}\right) + 2D'_{x}\sin^{2}\left(\frac{\pi}{m}\right)\right]}$$
(6.3)

$$\times \frac{\left[\frac{2}{3} + \frac{\cos\left(\frac{2\pi}{n}\right)}{3} - i\frac{V}{2}\sin\left(\frac{2\pi}{n}\right) - 2D_{y}\sin^{2}\left(\frac{\pi}{n}\right)\right]}{\left[\frac{2}{3} + \frac{\cos\left(\frac{2\pi}{n}\right)}{3} + i\frac{V}{2}\sin\left(\frac{2\pi}{n}\right) + 2D_{y}\sin^{2}\left(\frac{\pi}{n}\right)\right]} = \lambda_{sx} \cdot \lambda_{sy}$$

#### Computation

The eigenvalue of each scheme,  $\lambda_s$ , has been expressed in terms of the x and y wave numbers, n and m respectively. The eigenvalues are compute for n and m values from 2-9 over three log cycles. Note  $L_n = n\Delta x$  and  $L_m = m\Delta y$ , such that the wavelengths are expressed in terms of the grid spacing interval.

#### Complex propagation factor analysis

In order to compute this quantity, it is first necessary to determine the eigenvalue of the analytical solution,  $\lambda_a$ . Consider

$$\frac{\partial n}{\partial t} + u \frac{\partial n}{\partial x} + v \frac{\partial n}{\partial y} = D_x \frac{\partial^2 n}{\partial x^2} + D_y \frac{\partial^2 n}{\partial y^2}$$
(6.4)

Then  $\eta \sim C_n \exp \{i\beta_n t + i(\sigma_n x + \sigma_m y)\}$  is attempted as a solution. Calculating the derivatives:

 $\frac{\partial \eta}{\partial t} = i\beta_{\eta}\eta$ 

 $\frac{\partial n}{\partial x} = i\sigma_n \eta \qquad \qquad \frac{\partial^2 n}{\partial x^2} = -\sigma_n^2 \eta \qquad (6.5)$  $\frac{\partial n}{\partial y} = i\sigma_n \eta \qquad \qquad \frac{\partial^2 n}{\partial y^2} = -\sigma_n^2 \eta$ 

Then

 $(\beta_n + u\sigma_n + v\sigma_m)\mathbf{i} = -\sigma_n^2 \mathbf{D}_{\mathbf{x}} - \sigma_m^2 \mathbf{D}_{\mathbf{y}}$ (6.6)

or

$$\beta_{n} = i \left( \sigma_{n}^{2} D_{x} + \sigma_{m}^{2} D_{y} \right) - u \sigma_{n} - v \sigma_{m}$$
(6.7)

$$\beta_n = \sigma_n (iD_x \sigma_n - u) + \sigma_m (iD_y \sigma_m - v)$$

Thus the solution may be expressed as follows.

$$C \sim C_{n} \exp \left\{ \left[ -\left(\sigma_{n}^{2}D_{x} + \sigma_{m}^{2}D_{y}\right) - i(u\sigma_{n} + v\sigma_{m})\right] t + i(\sigma_{n}x + \sigma_{m}y) \right\}$$

$$C \sim C_{n} \exp \left[ -\left(\sigma_{n}^{2}D_{x} + \sigma_{m}^{2}D_{y}\right) t \right] \exp \left[ i\sigma_{n}(x - ut) + i\sigma_{m}(y - vt) \right]$$

$$C \sim C_{n} \exp \left( -\sigma_{n}^{2}D_{x}t \right) \exp \left[ i\sigma_{n}(x - ut) \right]$$

$$(6.8)$$

× exp 
$$\left(-\sigma_{m}^{2}D_{y}t\right)$$
 exp  $\left[i\sigma_{m}(y - vt)\right]$ 

Therefore the analytical eigenvalue is given

$$\lambda_{a} = \frac{C_{t+\Delta t}}{C_{t}}$$

$$= \exp\left(-\sigma_{n}^{2}D_{x}\Delta t\right) \exp\left(-i\sigma_{n}^{u}\Delta t\right) \exp\left(-\sigma_{m}^{2}D_{y}\Delta t\right) \exp\left(-i\sigma_{m}^{v}v\Delta t\right)$$
(6.9)

In terms of dimensionless quantities, we finally obtain:

$$\lambda_{a} = \left\{ \exp\left[ -\left(\frac{2\pi}{n}\right)^{2} D_{x}^{\dagger} \right] \exp\left(-i \frac{2\pi}{n} U\right) \right\}$$

$$\left\{ \exp\left[ -\left(\frac{2\pi}{m}\right)^{2} D_{y}^{\dagger} \right] \exp\left[ -i\left(\frac{2\pi}{m}\right) V \right] \right\} = \lambda_{ax} \cdot \lambda_{ay}$$
(6.10)

The complex propagation factor, C , is computed as follows.

$$C = \left(\frac{\lambda_{sx}}{\lambda_{ax}}\right)^{M} \left(\frac{\lambda_{sy}}{\lambda_{ay}}\right)^{N}$$
(6.11)

where  $M = \frac{m}{U}$  and  $N = \frac{n}{V}$ We note:  $uM\Delta t = L_m = m\Delta x$ 

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$$vN\Delta t = L_n = n\Delta y$$

A computer program has been written to determine both the eigenvalue and complex propagation factor for the previous schemes at different values of x and y wave numbers, m and n, respectively.

Initially the one-dimensional case with U = 0.2, V = 0.0,  $D'_x = 0.01$ , and  $D'_y = 0$  was computed and results compared with Leendertse's analysis. The results matched exactly. Next, a two dimensional case with U = 1.0 = V and  $D'_x = D'_y = 0.1$  was considered. Finally, the following prototype condition case was considered.

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$$U = \frac{u\Delta t}{\Delta x} = \frac{(3 \text{ fps})(360 \text{ sec})}{(4000 \text{ ft})} = 0.27 = \frac{v\Delta t}{\Delta y} = V$$

$$D'_{x} = \frac{D_{x}\Delta t}{\Delta x^{2}} = \frac{(100 \text{ ft}^{2}/\text{sec})(360 \text{ sec})}{(4000 \text{ ft})^{2}} = 0.00225 = \frac{D_{y}\Delta t}{\Delta y^{2}} = D'_{y}$$
(6.12)

Results for the three cases above and the program listing are presented in Appendices A-D.

## 7. Flux-Corrected Transport

In the implementation of this method, both higher and lower order in space schemes are considered. The schemes are written in the following flux formats.

$$\eta_{\ell,m}^{I} = \eta_{\ell,m}^{n} - (\Delta x \Delta y)^{-1} \left( F_{\ell+1/2,m}^{I} - F_{\ell-1/2,m}^{I} + F_{\ell,m+1/2}^{I} - F_{\ell,m-1/2}^{I} \right)$$
(7.1)

where  $t = n\Delta t$ ,  $x = m\Delta x$ ,  $y = \ell \Delta y$ 

 $n_{\ell,m}^n \equiv \text{concentration at location (l,m) at time level n}$   $\Delta x \equiv x \text{ space step}$  $\Delta y \equiv y \text{ space step}$ 

I ≅ general index at time level n+1 which we set equal to H and L for the higher and lower order schemes, respectively.

$$F_{\ell+1/2,m+1/2}^{1} \equiv$$
 fluxes through the appropriate cell faces of cell ( $\ell,m$ ). Form dependent upon the finite difference formulation.

We observe from (7.1) that the difference between the higher and lower order scheme at (l,m) may be written as follows:

$$\eta_{\ell,m}^{H} - \eta_{\ell,m}^{L} = -(\Delta x \Delta y)^{-1} \left[ \left( F_{\ell+1/2,m}^{H} - F_{\ell+1/2,m}^{L} \right) - \left( F_{\ell-1/2,m}^{H} - F_{\ell-1/2,m}^{L} \right) + \left( F_{\ell,m+1/2}^{H} - F_{\ell,m+1/2}^{L} \right) \right]$$

$$- \left( F_{\ell,m-1/2}^{H} - F_{\ell,m-1/2}^{L} \right) \left[ \left( 7.2 \right) - \left( F_{\ell,m-1/2}^{H} - F_{\ell,m-1/2}^{L} \right) \right]$$

Note this difference is expressed as an array of fluxes between adjacent grid points and is the condition required to implement flux-corrected transport. We next develop the expressions for the above fluxes for the higher  $(F^{H})$  and lower  $(F^{L})$  order schemes.

For the higher order scheme we employ the FICS scheme written below in which the factorization terms necessary for the multioperational method are underlined.

$$\eta_{\rm H}^{n+1} = \eta^n - \frac{v\Delta t}{2} \, \delta y \left( \eta_{\rm H}^{n+1} + \eta^n \right) - \frac{u\Delta t}{2} \, \delta x \left( \eta_{\rm H}^{n+1} + \eta^n \right) \\ + \frac{\alpha \Delta t}{2} \, \delta y^2 \left( \eta_{\rm H}^{n+1} + \eta^n \right) + \frac{\alpha \Delta t}{2} \, \delta x^2 \left( \eta_{\rm H}^{n+1} + \eta^n \right) \\ - \frac{uv\Delta t^2}{4} \, \delta y \delta x \left( \eta_{\rm H}^{n+1} - \eta^n \right) + \frac{\alpha u\Delta t^2}{4} \, \delta y^2 \delta x \left( \eta_{\rm H}^{n+1} - \eta^n \right) \\ + \frac{\alpha v\Delta t^2}{4} \, \delta x^2 \delta y \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) \\ - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{n+1} - \eta^n \right) - \frac{\alpha^2 \Delta t^2}{4} \, \delta y^2 \delta x^2 \left( \eta_{\rm H}^{$$

Ignoring the factorization terms (7.3) may be written in the form of (7.1). The total fluxes are presented as the sum of the advective and diffusive fluxes by defining:

$$F_{\ell+1/2,m}^{H} = F_{\ell+1/2,m}^{HA} + F_{\ell+1/2,m}^{HO}$$

$$F_{\ell,m+1/2}^{H} = F_{\ell,m+1/2}^{HA} + F_{\ell,m+1/2}^{HO}$$
(7.4)

where,

 $F_{\ell+1/2,m+1/2}^{H} \equiv$  higher order scheme fluxes  $F_{\ell+1/2,m+1/2}^{HA} \equiv$  higher order scheme advective fluxes  $F_{\ell+1/2,m+1/2}^{HO} \equiv$  higher order scheme diffusive fluxes Expanding Equation (7.3) using the definitions listed at the top of

page 16 one then obtains:

$$F_{\ell+1/2,m}^{HA} = v \Delta t \Delta x \left[ \frac{\left( \eta_{H}^{n+1} + \eta_{H}^{n} \right)_{\ell+1,m}}{2} + \frac{\left( \eta_{H}^{n+1} + \eta_{H}^{n} \right)_{\ell,m}}{2} \right] / 2.$$
(7.5)

$$F_{\ell,\underline{m+1/2}}^{\text{HA}} = u\Delta t\Delta y \left[ \frac{\left( \eta_{\text{H}}^{n+1} + \eta^{n} \right)_{\ell,\underline{m+1}}}{2} + \frac{\left( \eta_{\text{H}}^{n+1} + \eta^{n} \right)_{\ell,\underline{m}}}{2} \right] / 2. \quad (7.6)$$

$$F_{\ell+1/2,m}^{HO} = -\alpha \Delta t \Delta x \left( n_{\ell+1,m}^{H} + n_{\ell+1,m}^{n} - n_{\ell,m}^{H} - n_{\ell,m}^{n} \right) / 2\Delta y \qquad (7.7)$$

$$F_{\ell-1/2,m}^{HO} = -\alpha \Delta t \Delta x \left( \eta_{\ell,m}^{H} + \eta_{\ell,m}^{n} - \eta_{\ell-1,m}^{H} - \eta_{\ell-1,m}^{n} \right) / 2\Delta y$$
(7.8)

$$F_{\ell,m+1/2}^{HO} = -\alpha \Delta t \Delta y \left( \eta_{\ell,m+1}^{H} + \eta_{\ell,m+1}^{n} - \eta_{\ell,m}^{H} - \eta_{\ell,m}^{n} \right) / 2\Delta x \qquad (7.9)$$

$$F_{\ell,m-1/2}^{HO} = -\alpha \Delta t \Delta y \left( \eta_{\ell,m}^{H} + \eta_{\ell,m}^{n} - \eta_{\ell,m-1}^{H} - \eta_{\ell,m-1}^{n} \right) / 2\Delta x \quad (7.10)$$

Next consider the FTUS lower order scheme given below. For  $g = \overline{+1}$ ,  $u, v \gtrless 0$ , respectively. Factorization terms are again underlined.

$$n_{L}^{n+1} = n^{n} - \frac{v\Delta t}{2} \left[ \delta y + g \frac{(u_{y} - 1)}{\Delta y} \right] \left( n_{L}^{n+1} + n^{n} \right) \\ - \frac{u\Delta t}{2} \left[ \delta x + \frac{g(u_{x} - 1)}{\Delta x} \right] \left( n_{L}^{n+1} + n^{n} \right) + \frac{\alpha\Delta t}{2} \delta y^{2} \left( n_{L}^{n+1} + n^{n} \right) \\ + \frac{\alpha\Delta t}{2} \delta x^{2} \left( n_{L}^{n+1} + n^{n} \right) - \frac{uv\Delta t^{2}}{4} \left[ \delta y \delta x + \frac{\delta xg(u_{y} - 1)}{\Delta y} + \frac{\delta yg(u_{x} - 1)}{\Delta x} \right]$$
(7.11)  
$$+ \frac{g^{2}(u_{x} - 1)(u_{y} - 1)}{\Delta x\Delta y} \left[ \left( n_{L}^{n+1} - n^{n} \right) + \frac{\alpha u\Delta t^{2}}{4} \delta y^{2} \left[ \delta x + \frac{g(u_{x} - 1)}{\Delta x} \right] \left( n_{L}^{n+1} - n^{n} \right) \right] \\ + \frac{uv\Delta t^{2}}{4} \delta x^{2} \left[ \delta y + \frac{g(u_{y} - 1)}{\Delta y} \right] \left( n_{L}^{n+1} - n^{n} \right) - \frac{\alpha^{2} \Delta t^{2}}{4} \delta y^{2} \delta x^{2} \left( n_{L}^{n+1} - n^{n} \right)$$

If, as in the previous case, the factorization terms are ignored, (7.11) may be written in the form of (7.1). Total fluxes are, as before, presented as the sum of advective and diffusive fluxes. Thus

$$F_{\ell,\pm1/2,m}^{L} = F_{\ell,\pm1/2,m}^{LA} + F_{\ell,\pm1/2,m}^{LO}$$

$$F_{\ell,m\pm1/2}^{L} = F_{\ell,m\pm1/2}^{LA} + F_{\ell,m\pm1/2}^{LO}$$
(7.12)

where,

Expanding Equation (7.11) one then obtains:

$$F_{\ell,m+1/2}^{LA} = \begin{cases} u \Delta t \Delta y \left( \frac{n+1}{L} + n^{n} \right)_{\ell,m} & u > 0 \\ u \Delta t \Delta y \left( \frac{n+1}{L} + n^{n} \right)_{\ell,m} & u > 0 \\ u \Delta t \Delta y \left( \frac{n+1}{L} + n^{n} \right)_{\ell,m+1} & u < 0 \end{cases}$$
(7.13)

$$F_{\ell,m-1/2}^{LA} = \begin{cases} u\Delta t\Delta y \left( \frac{\eta_{L}^{n+1} + \eta^{n}}{2} \right)_{\ell,m-1} & u > 0 \\ u\Delta t\Delta y \left( \frac{\eta_{L}^{n+1} + \eta^{n}}{2} \right)_{\ell,m} & u < 0 \end{cases}$$
(7.14)

$$F_{l+1/2,m}^{LA} = \begin{cases} v \Delta t \Delta x \left( \frac{n_{L}^{n+1} + n^{n}}{2} \right)_{l,m} & v > 0 \\ v \Delta t \Delta x \left( \frac{n_{L}^{n+1} + n^{n}}{2} \right)_{l+1,m} & v < 0 \end{cases}$$
(7.15)

$$F_{\ell-1/2,m}^{LA} = \begin{cases} v \Delta t \Delta x \left( \frac{n_{L}^{n+1} + n^{n}}{2} \right)_{\ell-1,m} & v > 0 \\ v \Delta t \Delta x \left( \frac{n_{L}^{n+1} + n^{n}}{2} \right)_{\ell,m} & v < 0 \end{cases}$$
(7.16)

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 $F^{LO}_{\ \ \underline{l+1/2},\underline{m+1/2}}$  are as given in (7.7)-(7.10) if one replaces H with L .

The flux-corrected transport method is completed as follows: 1. Compute the anti-diffusive fluxes,  $A_{\ell+1/2,m+1/2}$ :

$$A_{\ell+1/2, m+1/2} = F_{\ell+1/2, m+1/2}^{H} - F_{\ell+1/2, m+1/2}^{L}$$

2. Determine the limited anti-diffusive fluxes,  $A_{\ell+1/2,m+1/2}^{c}$ :

$$A_{\ell+1/2,m+1/2}^{c} = C_{\ell+1/2,m+1/2} \cdot A_{\ell+1/2,m+1/2} = 0 < C_{\ell+1/2,m+1/2} < 1$$

The determination of  $C_{l+1/2,m+1/2}$  is given by Zalesak as outlined in [3].

3. Apply the limited anti-diffusive fluxes:

$$\eta_{\ell,m}^{n+1} = \eta_{\ell,m}^{L} - (\Delta x \Delta y)^{-1} \left( A_{\ell+1/2,m}^{c} - A_{\ell-1/2,m}^{c} + A_{\ell,m+1/2}^{c} - \dot{A}_{\ell,m-1/2}^{c} \right)$$

## PART 111: NUMERICAL APPROXIMATIONS FOR THE TRANSPORT EQUATION IN TRANSFORMED COORDINATES

The transport equation is transformed from x-y space to  $\alpha_1 - \alpha_2$ space by means of an exponential stretch. Subsequently, the extensions of the numerical approximations to the nonlinear transformed transport equation are presented. It is instructive to note, that even the linearized transport equation becomes nonlinear in transformed coordinates.

## 1. Development of the Tranformed Equation

The following coordinate transformation is considered by Butler

$$x = a_{1} + b_{1} \alpha_{1}^{c_{1}} \iff \alpha_{1} = \left(\frac{x - a_{1}}{b_{1}}\right)^{1/c_{1}}$$
(1.1)

$$y = a_2 + b_2 \alpha_2^{c_2} \longrightarrow \alpha_2 = \left(\frac{y - a_2}{b_2}\right)^{1/c_2}$$
 (1.2)

Then for an arbitrary hydrodynamic variable  $\rho(x,y,t)$ 

$$\frac{\partial \rho}{\partial x} = \frac{\partial \rho}{\partial \alpha_1} \frac{d\alpha_1}{dx} \qquad \frac{\partial \rho}{\partial y} = \frac{\partial \rho}{\partial \alpha_2} \frac{d\alpha_2}{dy}$$
(1.3)

$$\frac{\partial^{2} \rho}{\partial x^{2}} = \frac{\partial}{\partial \alpha_{1}} \left( \frac{\partial \rho}{\partial x} \right) \frac{d\alpha_{1}}{dx} = \frac{\partial}{\partial \alpha_{1}} \left( \frac{\partial \rho}{\partial \alpha_{1}} \frac{d\alpha_{1}}{dx} \right) \frac{d\alpha_{1}}{dx} = \frac{d\alpha_{1}}{dx} \left[ \frac{\partial^{2} \rho}{\partial \alpha_{1}^{2}} \frac{d\alpha_{1}}{dx} + \frac{\partial \rho}{\partial \alpha_{1}} \frac{\partial}{\partial \alpha_{1}} \left( \frac{d\alpha_{1}}{dx} \right) \right] (a)$$

$$\frac{\partial^{2} \rho}{\partial y^{2}} = \frac{\partial}{\partial \alpha_{2}} \left( \frac{\partial \rho}{\partial y} \right) \frac{d\alpha_{2}}{dy} = \frac{\partial}{\partial \alpha_{2}} \left( \frac{\partial \rho}{\partial \alpha_{2}} \frac{d\alpha_{2}}{dy} \right) \frac{d\alpha_{2}}{dy} = \frac{d\alpha_{2}}{dy} \left[ \frac{\partial^{2} \rho}{\partial \alpha_{2}^{2}} \frac{d\alpha_{1}}{dy} + \frac{\partial \rho}{\partial \alpha_{1}} \frac{\partial}{\partial \alpha_{1}} \left( \frac{d\alpha_{1}}{dx} \right) \right] (b)$$

If we introduce  $\mu_1 = dx/d\alpha_1$  and  $\mu_2 = dy/d\alpha_2$  then

$$\frac{\partial \rho}{\partial x} = \frac{1}{\mu_1} \frac{\partial \rho}{\partial \alpha_1} \qquad \frac{\partial \rho}{\partial y} = \frac{1}{\mu_2} \frac{\partial \rho}{\partial \alpha_2} \qquad (1.5)$$

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{1}{\mu_1} \left[ \frac{1}{\mu_1} \frac{\partial^2 \rho}{\partial \alpha_1^2} + \frac{\partial \rho}{\partial \alpha_1} \frac{\partial}{\partial \alpha_1} \left( \frac{1}{\mu_1} \right) \right]$$
(1.6)

$$\frac{\partial^2 \rho}{\partial y^2} = \frac{1}{\mu_2} \left[ \frac{1}{\mu_2} \frac{\partial^2 \rho}{\partial \alpha_2^2} + \frac{\partial \rho}{\partial \alpha_2} \frac{\partial}{\partial \alpha_2} \left( \frac{1}{\mu_2} \right) \right]$$
(1.7)

Considering Equation 1.4a in an alternate manner

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial \rho}{\partial \alpha_1} \frac{d \alpha_1}{d x} \right) = \frac{\partial}{\partial x} \left( \frac{\partial \rho}{\partial \alpha_1} \right) \frac{d \alpha_1}{d x} + \frac{\partial \rho}{\partial \alpha_1} \frac{d^2 \alpha_1}{d x^2}$$
(1.8)

Noting  $\partial/\partial x = (\partial/\partial \alpha_1)(d\alpha_1/dx) = (\partial/\partial \alpha_1)(1/\mu_1)$ 

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial^2 \rho}{\partial \alpha_1^2} \left( \frac{d\alpha_1}{dx} \right)^2 + \frac{\partial \rho}{\partial \alpha_1} \frac{d^2 \alpha_1}{dx^2}$$
(1.9)

Employing previous notation, Equation 1.9 is rewritten as follows:

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial^2 \rho}{\partial \alpha_1^2} \left( \frac{1}{\mu_1} \right)^2 + \frac{\partial \rho}{\partial \alpha_1} \frac{d}{dx} \left( \frac{1}{\mu_1} \right)$$
(1.10)

Note, however, from the relation between  $\partial/\partial x$  and  $\partial/\partial \alpha_1$  we obtain

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial^2 \rho}{\partial \alpha_1^2} \left( \frac{1}{\mu_1} \right)^2 + \frac{\partial \rho}{\partial \alpha_1} \frac{d}{d\alpha_1} \left( \frac{1}{\mu_1} \right) \frac{1}{\mu_1}$$
(1.11)

This relation is equivalent to Equation 1.4.

If we consider a hydrodynamic variable  $\rho(\alpha_1, \alpha_2, t)$  and let  $i^*, j^*, n$  be defined such that

$$\rho_{i^{*},j^{*}}^{n} = \rho(i^{*}\Delta\alpha_{2}, j^{*}\Delta\alpha_{1}, n\Delta t) \qquad (1.12)$$

Then let i , j , n be such that

$$\rho_{i,j}^{n} = \rho \left[ a_{2} + b_{2} (i \star \Delta \alpha_{2})^{c_{2}}, a_{1} + b_{1} (j \star \Delta \alpha_{1})^{c_{1}}, n \Delta t \right]$$
(1.13)

We employ uniform spacing in  $\alpha_1 - \alpha_2$  space and irregular spacing in x-y space. We may evaluate the derivatives with respect to x and y as follows.

$$\frac{\partial \rho}{\partial \mathbf{x}} \begin{vmatrix} \mathbf{n} \\ \mathbf{i}, \mathbf{j} \end{vmatrix} = \frac{\partial \rho}{\partial \alpha_1} \begin{vmatrix} \mathbf{n} & \frac{d\alpha_1}{d\mathbf{x}} \\ \mathbf{i}^*, \mathbf{j}^* \end{vmatrix} \mathbf{j}^*$$
(1.14)

where

$$\frac{d\alpha_{1}}{dx} = \frac{1}{c_{1}b_{1}} \left(\frac{x - a_{1}}{b_{1}}\right)^{(1-c_{1})/c_{1}} = f(x)$$

$$f\left(a_{1} + b_{1}\alpha_{1}^{c_{1}}\right) = \frac{1}{c_{1}b_{1}} \alpha_{1}^{(1-c_{1})} = f(\alpha_{1}) - \frac{d\alpha_{1}}{dx} \bigg|_{j^{*}} = f(j^{*}\Delta\alpha_{1})$$

and

$$\frac{\partial \rho}{\partial y} \begin{vmatrix} n \\ i, j \end{vmatrix} = \frac{\partial \rho}{\partial \alpha_2} \begin{vmatrix} n & \frac{d \alpha_2}{d y} \\ i^{*}, j^{*} \end{vmatrix}$$
(1.15)

where

$$\frac{d\alpha_2}{dy} = \frac{1}{c_2 b_2} \left( \frac{y - a_2}{b_2} \right)^{(1 - c_2)/c_2} = g(y)$$

$$g\left(a_2 + b_2 \alpha_2^c\right) = \frac{1}{c_2 b_2} \alpha_2^{(1 - c_2)} \equiv g(\alpha_2) \quad \frac{d\alpha_2}{dy} \bigg|_{i^*} = g(i^* \Delta \alpha_2)$$

For the second derivative term we obtain

$$\frac{\partial^2 \rho}{\partial x^2} \bigg|_{i,j}^{n} = \frac{d\alpha_1}{dx} \bigg|_{j} \left\{ \frac{\partial^2 \rho}{\partial \alpha_1} \bigg|_{i^*,j^*}^{n} \frac{d\alpha_1}{dx} \bigg|_{j} + \frac{\partial \rho}{\partial \alpha_1} \bigg|_{i^*,j^*}^{n} \frac{d}{d\alpha_1} \left( \frac{d\alpha_1}{dx} \right) \bigg|_{j^*} \right\} \quad (1.16)$$
where

$$\frac{d}{d\alpha_1} \left( \frac{d\alpha_1}{dx} \right) = \frac{d}{d\alpha_1} \left[ f\left( a_1 + b_1 \alpha_1^c \right) \right] = \frac{(1 - c_1)}{c_1 b_1} \alpha_1^{-c_1} = h(\alpha_1)$$

$$\frac{d}{d\alpha_1} \left( \frac{d\alpha_1}{d\alpha_1} \right) = h(\alpha_1)$$

$$\frac{d}{d\alpha_1} \left( \frac{1}{dx} \right) \Big|_{j^*} = h(j^* \Delta \alpha_1)$$

Similarly, for  $\frac{\partial^2 \rho}{\partial y^2}$ . The underlined terms in Equations 1.6 and i,j

1.7, although they may be computed exactly, are approximated using finite differencing on  $\mu_1$  and  $\mu_2$  .

Transforming Equation 1.1 in Part I in x-y space to  $\alpha_1 - \alpha_2$ space we obtain the following result.

$$(ds)_{t} + \frac{(dus)_{\alpha_{1}}}{\mu_{1}} + \frac{(dvs)_{\alpha_{2}}}{\mu_{2}} = \frac{1}{\mu_{1}} \left[ dK_{\alpha_{1}} \frac{(s)_{\alpha_{1}}}{\mu_{1}} \right]_{\alpha_{1}} + \frac{1}{\mu_{2}} \left[ dK_{\alpha_{2}} \frac{(s)_{\alpha_{2}}}{\mu_{2}} \right]_{\alpha_{2}} (1.17)$$

where d is introduced as the depth in place of h

$$()_{t} = \partial/\partial t$$
$$()_{\alpha_{1}} = \partial/\partial \alpha_{1}$$
$$()_{\alpha_{2}} = \partial/\partial \alpha_{2}$$

Equation 1.17 is the relation that is the subject of numerical approximation. Let us consider the space staggered grid shown in Figure 1. The datum convention is illustrated in Figure 2.



Figure 1. Space staggered finite difference grid in transformed coordinates





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Let us introduce the following notation as a prelude to the approximations. Define for an arbitrary variable  $F_{n,m}^k$ , where  $t = k\Delta t$ ,  $y = n\Delta y$ ,  $x = m\Delta x$ :

$$\delta_{t}^{k} \left( F_{n,m}^{k} \right) = F_{n,m}^{k+1/2} - F_{n,m}^{k}$$
(1.18a)

$$\delta' t^{k}(F^{k}_{n,m}) = F^{k+1}_{n,m} - F^{k}_{n,m}$$
 (1.18b)

$$\delta_{\alpha_{1}}(\mathbf{F}_{n,m}^{k}) = \mathbf{F}_{n,m+1/2}^{k} - \mathbf{F}_{n,m-1/2}^{k}$$
(1.18c)

$$\delta_{\alpha_2}(\mathbf{F}_{n,m}^k) = \mathbf{F}_{n+1/2,m}^k - \mathbf{F}_{n-1/2,m}^k$$
(1.18d)

$$\frac{\alpha_1}{F_{n,m}} = \frac{\left(F_{n,m+1/2}^k + F_{n,m-1/2}^k\right)}{2}$$
(1.18e)

$$\frac{\alpha_2}{F_{n,m}} = \frac{\left(F_{n+1/2,m}^k + F_{n-1/2,m}^k\right)}{2}$$
(1.18f)

# 2. Leendertse FTCS Multioperational Scheme

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The following finite difference equation is considered as an approximation to the nonlinear transport equation (1.17)

$$\sum_{k=1}^{k} (ds) + \frac{\Delta t}{2\Delta \alpha_{1}(\mu_{1})_{m}} \delta_{\alpha_{1}} \left( \frac{\alpha_{1}}{d} k + 1 \frac{\alpha_{1}}{s} k + 1_{u} k + 1 + \frac{\alpha_{1}}{d} k \frac{\alpha_{1}}{s} k_{u} k \right)$$

$$+ \frac{\Delta t}{2\Delta \alpha_{2}(\mu_{2})_{n}} \delta_{\alpha_{2}} \left( \frac{\alpha_{2}}{d} k + 1 \frac{\alpha_{2}}{s} k + 1_{v} k + 1 + \frac{\alpha_{2}}{d} k \frac{\alpha_{2}}{s} k_{v} k \right)$$

$$- \frac{\Delta t}{2(\Delta \alpha_{1})^{2}(\mu_{1})_{m}} \delta_{\alpha_{1}} \left[ \frac{\alpha_{1}}{d} k + 1_{\alpha_{1}} \frac{\kappa_{1}^{k+1}}{\alpha_{1}} \frac{\delta_{\alpha_{1}}(s^{k+1})}{(\mu_{1})_{m}} + \frac{\alpha_{1}}{d} k \kappa_{\alpha_{1}}^{k} \frac{\delta_{\alpha_{1}}(s^{k})}{(\mu_{1})_{m}} \right]$$

$$- \frac{\Delta t}{2(\Delta \alpha_{2})^{2}(\mu_{2})_{n}} \delta_{\alpha_{2}} \left[ \frac{\alpha_{2}}{d} k + 1_{\alpha_{2}} \frac{\kappa_{1}^{k+1}}{\alpha_{2}^{k}} \frac{\delta_{\alpha_{2}}(s^{k+1})}{(\mu_{2})_{n}} + \frac{\alpha_{2}}{d} k \kappa_{\alpha_{2}}^{k} \frac{\delta_{\alpha_{2}}(s^{k})}{(\mu_{2})_{n}} \right] = 0 \quad \text{at } (n,m)$$

The above equation is assumed to be contained within the following multioperational difference equations. For the linear case obtained for  $(\mu_2)_n = (\mu_1)_m = 1$ ,  $K_{\alpha_2}$ ,  $K_{\alpha_1}$  constants in space and time, and u, v, d constant in space and time, the constituent intermediate time level may be eliminated in the multioperational approach and the total difference equation obtained equals the above difference equation plus some higher order in time factorization terms. The total difference equation is consistent with the linear transport equation. For the nonlinear case considered, it is not possible to eliminate the constituent intermediate time level. Thus the exact form of the factorization terms may not be determined. However, their numerical effect may be tested.

The approximations for the X-Sweep may now be written as follows

$$\delta_{t}^{k}(ds) + \frac{\Delta t \quad \delta_{\alpha_{1}}}{2\Delta \alpha_{1}(\mu_{1})_{m}} \left( \frac{\alpha_{1}}{d^{k+1/2^{\star}}} \frac{\alpha_{1}}{s^{k+1/2^{\star}}} \frac{\alpha_{1}}{u^{k+1/2^{\star}}} \right)$$

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$$-\frac{\Delta t \, \delta_{\alpha_{1}}}{2\Delta \alpha_{1}^{2}(\mu_{1})_{m}} \left[ \frac{\alpha_{1}}{d^{k+1/2*}} \kappa_{\alpha_{1}}^{k+1/2*} \frac{\delta_{\alpha_{1}}(s^{k+1/2*})}{(\mu_{1})_{m}} \right]$$
(2.2)

+ 
$$\frac{\Delta t}{2(\mu_2)_n \Delta \alpha_2} \delta_{\alpha_2} \left( \frac{\alpha_2}{d^k} \frac{\alpha_2}{s^k v^k} \right)$$

$$-\frac{\Delta t \delta_{\alpha_2}}{2\Delta \alpha_2^2(\mu_2)_n} \left[ \frac{\alpha_1}{d} \kappa_{\alpha_2}^k \frac{\delta_{\alpha_2}(s^k)}{(\mu_2)_n} \right] = 0 \quad \text{at } (n,m)$$

Expand (2.2) using (1.18) and collect all terms at time level  $k+1/2^{*}$ to obtain:  $(K_{x} \equiv K_{\alpha_{1}})$   $(d_{s})_{n,n}^{k+1/2^{*}} + \frac{\Delta t}{2\Delta \alpha_{1}(u_{1})_{m}} \left[ \frac{\left( \frac{n_{n,m+1}^{k+1/2^{*}} - h_{n,m+1} + \frac{n_{n,m}^{k+1/2^{*}}}{2} - h_{n,m} \right)}{2} u_{n,m+1/2}^{k+1/2^{*}} \frac{\left( \frac{s_{n,m+1}^{k+1/2^{*}} + s_{n,m}^{k+1/2^{*}}}{2} \right)}{2} \right]$   $- \frac{\left( \frac{n_{n,m-1}^{k+1/2^{*}} - h_{n,m-1} + n_{n,m}^{k+1/2^{*}} - h_{n,m} \right)}{2} u_{n,m-1/2}^{k+1/2^{*}} \frac{\left( \frac{s_{n,m+1}^{k+1/2^{*}} - s_{n,m}^{k+1/2^{*}}}{2} \right)}{2} \right]$  $- \frac{\Delta t}{2\Delta \alpha_{1}^{2}(u_{1})_{m}} \left[ \frac{\left( \frac{n_{n,m+1}^{k+1/2^{*}} - h_{n,m} + \frac{n_{n,m-1}^{k+1/2^{*}} - h_{n,m} \right)}{2} \left( \frac{s_{n,m-1}^{k+1/2^{*}} - s_{n,m}^{k+1/2^{*}}}{(u_{1})_{m+1/2}} \right) \frac{s_{n,m-1}^{k+1/2^{*}} - s_{n,m-1}^{k+1/2^{*}}}{(u_{1})_{m+1/2}} x_{n,m+1/2}^{k+1/2^{*}} \right]}{\left( \frac{n_{n,m-1}^{k+1/2^{*}} - h_{n,m-1} + \frac{n_{n,m-1}^{k+1/2^{*}} - h_{n,m}}{2} \right)}{2} \left( \frac{s_{n,m-1}^{k+1/2^{*}} - \frac{s_{n,m-1}^{k+1/2^{*}} - s_{n,m-1}^{k+1/2^{*}}}}{2} \right)}{2}$ Collecting all terms in (2.2) at time level k denoting the result as

$$B_{m}, \text{ we obtain: } (K_{y} \equiv K_{\alpha_{2}})$$

$$u_{m} := (d_{s})_{n,m}^{k} - \frac{\Delta t}{2\Delta \alpha_{2}(u_{2})_{n}} \left[ \frac{\left( n_{n+1,m}^{k} - n_{n+1,m} + n_{n,m}^{k} - n_{n,m} \right)}{2} v_{n+1/2,m}^{k} \frac{v_{n+1/2,m}^{k}}{2} \frac{\left( s_{n+1,m}^{k} + s_{n,m}^{k} \right)}{2} \right]$$

$$- \frac{\left( n_{n-1,m}^{k} - n_{n-1,m} + n_{n,m}^{k} - n_{n,m} \right)}{2} v_{n-1/2,m}^{k} \frac{\left( s_{n-1,m}^{k} + s_{n,m}^{k} \right)}{2} \right]$$

$$+ \frac{\Delta t}{2(u_{2})_{n}(\Delta \alpha_{2})^{2}} \left[ \frac{\left( n_{n+1,m}^{k} - n_{n+1,m} + n_{n,m}^{k} - n_{n,m} \right) \left( s_{n+1,m}^{k} - s_{n,m}^{k} \right)}{2} \frac{s_{n+1/2,m}^{k}}{2} v_{n+1/2,m}^{k} - \frac{\left( n_{n-1,m}^{k} - n_{n,m} + n_{n,m}^{k} - n_{n,m} \right) \left( s_{n+1,m}^{k} - s_{n-1,m}^{k} \right)}{2} v_{n+1/2,m}^{k} \left[ 1 n (2.3) \text{ we define } -a_{n,m-1}, a_{n,m+1}, \text{ and } a_{n,m} \text{ as follows} \right]$$

$$(2.4)$$

$$-a_{n,m-1} = \frac{\Delta t \left(\frac{\alpha_1}{d}\right)_{k+1/2*}}{2\Delta \alpha_1 (\mu_1)_m} \left[\frac{u_{n,m-1/2}^{k+1/2*}}{2 + \frac{(\kappa_x)_{n,m-1/2}^{k+1/2*}}{\Delta \alpha_1 (\mu_1)_{m-1/2}}\right]$$
(2.5)

$$a_{n,m+1} = \frac{\Delta t \left(\frac{\alpha_1}{d}\right)_{\substack{k+1/2 \\ n,m+1/2}}}{2\Delta \alpha_1 (\mu_1)_m} \left[\frac{u_{n,m+1/2}^{k+1/2 *}}{2} - \frac{(K_x)_{n,m+1/2}^{k+1/2 *}}{\Delta \alpha_1 (\mu_1)_{m+1/2}}\right]$$
(2.6)

$$a_{n,m} = d_{n,m}^{k+1/2*} + \frac{\Delta t}{2\Delta \alpha_{1}(\mu_{1})_{m}} \left[ \frac{\left(\frac{\alpha_{1}}{du}\right)_{k+1/2*}_{n,m+1/2}}{2} - \frac{\left(\frac{\alpha_{1}}{du}\right)_{k+1/2*}_{n,m-1/2}}{2} \right] + \frac{\Delta t}{2\Delta \alpha_{1}^{2}(\mu_{1})_{m}} \left[ \frac{\left(\frac{\alpha_{1}}{dK_{x}}\right)_{n,m+1/2}_{n,m+1/2}}{(\mu_{1})_{m+1/2}} + \frac{\left(\frac{\alpha_{1}}{dK_{x}}\right)_{n,m-1/2}_{n,m-1/2}}{(\mu_{1})_{m-1/2}} \right]$$
(2.7)

Collecting all results we obtain the following interior equation for the X-Sweep

$$a_{n,m-1} s_{n,m-1}^{k+1/2*} + a_{n,m} s_{n,m}^{k+1/2*} + a_{n,m+1} s_{n,m+1}^{k+1/2*} = B_{m}$$
 (2.8)

The approximations for the Y-Sweep may now be written as follows:

$$\delta_{t}^{k+1/2*}(d_{\theta}) + \frac{\Delta t \, \delta_{\alpha_{2}}}{2\Delta \alpha_{2}(\mu_{2})_{n}} \left( \frac{\alpha_{2}}{d^{k+1}} \frac{\alpha_{2}}{s^{k+1}v^{k+1}} \right) - \frac{\Delta t \, \delta_{\alpha_{2}}}{2\Delta \alpha_{2}^{2}(\mu_{2})_{n}} \left[ \frac{\alpha_{2}}{d^{k+1}} \kappa_{\alpha_{2}}^{k+1} \frac{\delta_{\alpha_{2}}(s^{k+1})}{(\mu_{2})_{n}} \right]$$

$$+ \frac{\Delta t \, \delta_{\alpha_{1}}}{2\Delta \alpha_{1}(\mu_{1})_{m}} \left( \frac{\alpha_{1}}{d^{k+1/2*}} \frac{\alpha_{1}}{s^{k+1/2*}u^{k+1/2*}} \right) - \frac{\Delta t \, \delta_{\alpha_{1}}}{2\Delta \alpha_{1}^{2}(\mu_{1})_{m}} \left[ \frac{\alpha_{1}}{d^{k+1/2*}} \kappa_{\alpha_{1}}^{k+1/2*} \frac{\delta_{\alpha_{1}}(s^{k+1/2*})}{(\mu_{1})_{m}} \right] = 0 \quad \text{at (n,m)}$$

$$(2.9)$$

Expanding (2.9) by employing (1.18) and collecting terms at time level k+1 on the left hand side and leaving terms at time level k+1/2\* on the right hand side the following interior equation for the Y-Sweep is obtained.

$$a_{n-1,m} s_{n-1,m}^{k+1} + a_{n,m} s_{n,m}^{k+1} + a_{n+1,m} s_{n+1,m}^{k+1} = B_n$$
 (2.10)

where  $(K_x \equiv K_{\alpha_1}, K_y \equiv K_{\alpha_2})$ 

$$-a_{n-1,m} = \frac{\Delta t \left(\frac{\alpha_2}{d}\right)_{k+1}}{2\Delta \alpha_2(\mu_2)_n} \left[\frac{v_{n-1/2,m}^{k+1}}{2} + \frac{(K_y)_{n-1/2,m}^{k+1}}{\Delta \alpha_2(\mu_2)_{n-1/2}}\right] \quad (2.11)$$

$$a_{n+1,m} = \frac{\Delta t \left(\frac{\alpha_2}{d}\right)_{k+1}}{2\Delta \alpha_2(\mu_2)_n} \left[\frac{v_{n+1/2,m}^{k+1}}{2} - \frac{(K_y)_{n+1/2,m}^{k+1}}{\Delta \alpha_2(\mu_2)_{n+1/2}}\right] \quad (2.12)$$

$$a_{n,m} = d_{n,m}^{k+1} + \frac{\Delta t}{2\Delta \alpha_2(\mu_2)_n} \left[ \frac{\left(\frac{\alpha_2}{dv}\right)_{k+1}}{2} - \frac{\left(\frac{\alpha_2}{dv}\right)_{k+1}_{n-1/2,m}}{2} \right]$$

(2.13)

$$+ \frac{\Delta t}{2\Delta \alpha_2^2(\mu_2)_n} \left[ \frac{\left(\frac{\alpha_2}{dK_y}\right)_{n+1/2,m}^{k+1}}{(\mu_2)_{n+1/2}} + \frac{\left(\frac{\alpha_2}{dK_y}\right)_{n-1/2,m}^{k+1}}{(\mu_2)_{n-1/2}} \right]$$

$$B_{n} = (ds)_{n,m}^{k+1/2*} - \frac{\Delta t}{2(u_{1})_{m}\Delta \alpha_{1}} \left[ \left( \frac{\alpha_{1}}{ds} \right)_{n,m+1/2}^{k+1/2*} u_{n,m+1/2}^{k+1/2*} - \left( \frac{\alpha_{1}}{ds} \right)_{n,m-1/2}^{K+1/2*} u_{n,m-1/2}^{k+1/2*} \right] + \frac{\Delta t}{2(u_{1})_{m}(\Delta \alpha_{1})^{2}} \left[ \left( \frac{\alpha_{1}}{dK} \right)_{n,m+1/2}^{k+1/2*} \frac{\left( s_{n,m+1}^{k+1/2*} - s_{n,m}^{k+1/2*} \right)}{(u_{1})_{m+1/2}} - \left( \frac{\alpha_{1}}{dK} \right)_{n,m-1/2}^{k+1/2*} - \frac{\left( s_{n,m-1}^{k+1/2*} - s_{n,m-1/2}^{k+1/2*} \right)}{(u_{1})_{m+1/2}} \right]$$

$$(2.14)$$

# 3. Leendertse FTUS Multioperational Scheme

The following finite difference equation is considered as an approximation to the nonlinear transport equation (1.17):

$$\delta_{t}^{'k}(ds) + \frac{\Delta t}{2\Delta \alpha_{1}(\mu_{1})_{m}} \delta_{\alpha_{1}} \left( \frac{\alpha_{1}}{d^{k+1} u_{s_{1}}^{k+1} u^{k+1}} + \frac{\alpha_{1}}{d^{k} u_{s_{1}}^{k} u^{k}} \right) \\ + \frac{\Delta t}{2\Delta \alpha_{2}(\mu_{2})_{n}} \delta_{\alpha_{2}} \left( \frac{\alpha_{2}}{d^{k+1} u^{k+1} u^{k+1}} + \frac{\alpha_{2}}{d^{k} u^{k} u^{k}} + \frac{\alpha_{2}}{d^{k} u^{k} u^{k}} \right) \\ - \frac{\Delta t}{2(\Delta \alpha_{1})^{2}(\mu_{1})_{m}} \delta_{\alpha_{1}} \left[ \frac{\alpha_{1}}{d^{k+1} u^{k+1} u^{k+1} u^{k+1} u^{k+1} u^{k+1} u^{k+1} u^{k+1} u^{k} u^{k}$$

The following upwind difference operators used in the above equation are defined at (n,m) as follows:

$$\frac{f_{s_{1}}^{k}}{s_{1}^{k}} = \begin{cases} s_{n,m-1/2}^{k} & f_{n,m}^{k} \ge 0 \\ s_{n,m+1/2}^{k} & f_{n,m}^{k} < 0 \end{cases}$$

$$\frac{f_{s_{2}}^{k}}{s_{2}^{k}} = \begin{cases} s_{n-1/2,m}^{k} & f_{n,m}^{k} \ge 0 \\ s_{n+1/2,m}^{k} & f_{n,m}^{k} < 0 \end{cases}$$
(3.2)

For the linear case  $[(\mu_1)_m = (\mu_2)_n = 1.0$ ,  $K_{\alpha_1}$ ,  $K_{\alpha_2}$ , u, v, and d constant], the constituent intermediate time level in the multioperational approach, may be eliminated. The difference equation obtained is consistent with the linear transport equation and equals the above difference equations plus some higher order in time factorization terms. For the nonlinear case considered here, it is not possible to eliminate the constituent intermediate time level. Therefore the exact form of the factorization terms may not be determined. However, their numerical effect may be assessed.

This scheme is similar to the standard ADI technique except that upwind differencing is employed for the advective terms. The necessary modifications for the X-Sweep are shown in Table VII while those employed for the Y-Sweep are given in Table VIII.

Thus the FTUS scheme may be obtained from the FTCS scheme programming with only modest programming modification. In CRAY-I FORTRAN three vector functions may be employed to define the FTUS modifications as follows:

CVMGP 
$$(x_1, x_2, x_3) = x_1 \quad x_3 \ge 0$$
 (3.3)  
 $x_2 \quad x_3 < 0$ 

AMAXI 
$$(x_1, x_2) = x_1 \qquad x_1 \ge x_2$$
  
 $x_2 \qquad x_1 < x_2$  (3.4)

AMINI 
$$(x_1, x_2) = x_1 \qquad x_1 \le x_2$$
 (3.5)  
 $x_2 \qquad x_1 > x_2$ 

These functions eliminate the need for IF type statements.



### Table VII. X-Sweep Modifications FTUS

Equation	FTCS	FTUS
2.11	$\frac{v^{k+1}_{n-1/2,m}}{2}$	max $(0., v_{n-1/2,m}^{k+1})$
2.12	v <sup>k+1</sup> <u>n+1/2,m</u> 2	min $(0., v_{n+1/2,m}^{k+1})$
2.13	$\frac{\left(\frac{\alpha_2}{dv}\right)_{k+1}}{2}$	$\max\left[0., \left(\frac{\alpha_2}{dv}\right)_{n+1/2, m}^{k+1}\right]$
2.13	$\frac{\binom{\alpha_2}{dv}_{k+1}_{n-1/2,m}}{2}$	$\min\left[0., \left(\frac{\alpha_2}{dv}\right)_{n-1/2, m}^{k+1}\right]$
2.14	$\left(\frac{\alpha_1}{ds}\frac{\alpha_1}{n}\right)_{n,m-1/2}^{k+1/2*}$	$\frac{\alpha_{1}}{dk+1/2*} = \frac{k+1/2*}{n,m+1/2} = 0$
		$\frac{\alpha_{1}}{d_{n,m+1/2}} \times \frac{k+1/2}{n,m+1} \qquad u_{n,m+1/2}^{k+1/2} < 0$
2.14	$ \begin{pmatrix} \frac{\alpha_1}{ds} & \frac{\alpha_1}{s} \\ n, m-1/2 \end{pmatrix} $ k+1/2*	$\frac{a_{1}}{d_{n,m-1/2}} + \frac{1}{s_{n,m-1}} + \frac{1}{s_{n,m-1}} + \frac{1}{s_{n,m-1}} + \frac{1}{s_{n,m-1/2}} + \frac{1}{s$
		$\frac{a_{1}}{d_{n,m-1/2}} + \frac{k+1/2}{a_{n,m}} + \frac{k+1/2}{a_{n,m-1/2}} < 0$

# Table VIII. Y-Sweep Modifications FTUS

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# 4. The Spread Time Derivative STCS Scheme

Using previous notation, the approximations for the X-Sweep may now be written as follows

$$\frac{2}{3}\delta_{t}^{k}(ds) + \frac{\mu_{x}}{3} (ds)^{k+1/2*} - \frac{\mu_{y}}{3} (ds)^{k} + \frac{\Delta t \ \delta_{\alpha_{1}}}{2\Delta\alpha_{1}(\mu_{1})_{m}} \left[ \left( \frac{\alpha_{1}}{ds} \frac{\alpha_{1}}{ds} \right)^{k+1/2*} \frac{k+1/2*}{s} \right] \\ - \frac{\Delta t \ \delta_{\alpha_{1}}}{2\Delta\alpha_{1}^{2}(\mu_{1})_{m}} \left[ \frac{\alpha_{1}}{d}^{k+1/2*} \ \kappa_{\alpha_{1}}^{k+1/2*} \frac{\delta_{\alpha_{1}}(s)^{k+1/2*}}{(\mu_{1})_{m}} \right] + \frac{\Delta t \ \delta_{\alpha_{2}}}{2(\mu_{2})_{n}\Delta\alpha_{2}} \left[ \left( \frac{\alpha_{2}}{ds} \frac{\alpha_{2}}{2} \right)^{k} \right]$$

$$- \frac{\Delta t \ \delta_{\alpha_{2}}}{2\Delta\alpha_{2}^{2}(\mu_{2})_{n}} \left[ \frac{\alpha_{1}}{d}^{k} \ \kappa_{\alpha_{2}}^{k} \frac{\delta_{\alpha_{2}}(s^{k})}{(\mu_{2})_{n}} \right] = 0 \ \text{at } (n,m)$$

If we place all terms at time level k+1/2\* on the left-hand side of the equation and expand we obtain (2.3) if

$$\frac{2}{3} (ds)_{n,m}^{k+1/2*} + \frac{(ds)_{n,m+1}^{k+1/2*} + (ds)_{n,m-1}^{k+1/2*}}{6} \equiv (ds)_{n,m}^{k+1/2*}$$
(4.2)

and (2.4) for

$$\frac{2}{3} (ds)_{n,m}^{k} + \frac{(ds)_{n+1,m}^{k} + (ds)_{n-1,m}^{k}}{6} \equiv (ds)_{n,m}^{k}$$
(4.3)

All other terms in (2.3) and (2.4) remain the same. Equation (4.2) necessitates the following modifications to (2.5)-(2.7).

$$-a_{n,m-1} \equiv -a_{n,m-1} - \frac{d_{n,m-1}^{k+1/2*}}{6}$$
 (4.4)

$$a_{n,m+1} \equiv a_{n,m+1} + \frac{d_{n,m+1}^{k+1/2*}}{6}$$
 (4.5)

$$a_{n,m} \equiv a_{n,m} - \frac{\frac{d^{k+1/2*}}{n,m}}{3}$$
 (4.6)

The approximations for the Y-Sweep are as follows

$$\delta_{t}^{k+1/2*}(ds) + \frac{\mu_{y}(ds)^{k+1}}{3} - \frac{\mu_{x}(ds)^{k+1}}{3} + \frac{\Delta t \delta_{\alpha_{2}}}{2\Delta\alpha_{2}(\mu_{2})_{n}} \left[ \left( \frac{\alpha_{2}}{ds} \frac{\alpha_{2}}{ds} \right)^{k+1} v^{k+1} \right]$$
$$- \frac{\Delta t \delta_{\alpha_{2}}}{2\Delta\alpha_{2}^{2}(\mu_{2})_{n}} \left[ \frac{\alpha_{2}}{dt} + 1 v^{k+1} \frac{\delta_{\alpha_{2}}(s^{k+1})}{(\mu_{2})_{n}} \right] + \frac{\Delta t \delta_{\alpha_{1}}}{2\Delta\alpha_{1}(\mu_{1})_{m}} \left[ \left( \frac{\alpha_{1}}{ds} \frac{\alpha_{1}}{s} \right)^{k+1/2*} v^{k+1/2*} \right]$$
$$- \frac{\Delta t \delta_{\alpha_{1}}}{2\Delta\alpha_{1}^{2}(\mu_{1})_{m}} \left[ \frac{\alpha_{1}}{dt} + 1/2* v^{k+1/2*} \frac{\delta_{\alpha_{1}}(s^{k+1/2*})}{(\mu_{1})_{m}} \right] = 0 \text{ at } (n,m)$$

If we place all terms at time level k+1 on the left-hand side of (4.7) and expand we obtain relations similar to (2.11)-(2.14).

In fact for (2.11)-(2.13)

$$-a_{n-1,m} \equiv -a_{n-1,m} - \frac{d_{n-1,m}^{k+1}}{6}$$
 (4.8)

$$a_{n+1,m} \equiv a_{n+1,m} + \frac{d_{n+1,m}^{k+1}}{6}$$
 (4.9)

$$a_{n,m} \equiv a_{n,m} - \frac{d_{n,m}^{k+1}}{3}$$
 (4.10)

In Equation (2.14), we employ (4.2),

$$(ds)_{n,m}^{k+1/2*} \equiv \frac{2(ds)_{n,m}^{k+1/2*}}{3} + \frac{(ds)_{n,m+1}^{k+1/2*} + (ds)_{n,m-1}^{k+1/2*}}{6}$$
(4.11)

We therefore note that the spread time derivative scheme may be obtained from the standard scheme with only minor modifications.

#### 5. Flux-Corrected Transport

As in the linear case, both higher and lower order in space schemes are employed. For the nonlinear case, the following flux format is needed.

$$\mathbf{d}_{n,m}^{k+1}\mathbf{s}_{n,m}^{I} = \mathbf{d}_{n,m}^{k}\mathbf{s}_{n,m}^{k} - \left[\Delta\alpha_{1}(\mu_{1})_{m}\Delta\alpha_{2}(\mu_{2})_{n}\right]^{-1} \left(\mathbf{F}_{n+1/2,m}^{I} - \mathbf{F}_{n+1/2,m}^{I} + \mathbf{F}_{n,m+1/2}^{I} - \mathbf{F}_{n,m-1/2}^{I}\right)$$
(5.1)

where  $t = k\Delta t$ ,  $x = \sum_{i} (\mu_{1})_{i}\Delta\alpha_{1}$ ,  $y = \sum_{i} (\mu_{2})_{i}\Delta\alpha_{2}$   $S_{n,m}^{k} \equiv \text{concentration at location (n,m) at time level k}$   $\Delta\alpha_{1}(\mu_{1})_{m} \equiv x$  space step at m  $\Delta\alpha_{2}(\mu_{2})_{n} \equiv y$  space step at n I  $\equiv$  general index at time level k+1, which we set to H or L for the higher or lower scheme, respectively  $F_{n+1/2,m+1/2}^{I} \equiv$  fluxes through the appropriate cell faces of cell (n,m). Form dependent upon the finite difference formulation,

We observe from (5.1) that the difference between the higher and lower

order scheme at (n,m) may be written as follows:

$$\left( s_{n,m}^{H} - s_{n,m}^{L} \right) = - \left[ \Delta \alpha_{1} (\mu_{1})_{m} \Delta \alpha_{2} (\mu_{2})_{n} d_{n,m}^{k+1} \right]^{-1} \left[ \left( F_{n+1/2,m}^{H} - F_{n+1/2,m}^{L} \right) - \left( F_{n-1/2,m}^{H} - F_{n-1/2,m}^{L} \right) + \left( F_{n,m+1/2}^{H} - F_{n,m+1/2}^{L} \right) \right]$$

$$- \left( F_{n,m-1/2}^{H} - F_{n,m-1/2}^{L} \right)$$

$$- \left( F_{n,m-1/2}^{H} - F_{n,m-1/2}^{L} \right)$$

$$(5.2)$$

Note this difference may be expressed as an array of fluxes between adjacent grid points. We next develop the flux expressions for the higher ( $F^H$ ) and lower ( $F^L$ ) order schemes. In order to aid in notation, we make the following definition for an arbitrary variable, F.

$$F_{n,m}^{k+1/2} = \left(F_{n,m}^{k+1} + F_{n,m}^{k}\right) / 2.$$
 (5.3)

For the higher order scheme we employ the FTCS scheme written in (2.1) in which the factorization terms developed in the multioperational method are not shown. Equation (2.1) may be written in the form of (5.1), where the total fluxes are presented as the sum of advective and diffusive fluxes as given in Part II (7.4) with  $\ell = n$ .

From Equation (2.1) one then obtains for the advective fluxes:

$$F_{n\pm1/2,m}^{H} = v_{n\pm1/2,m}^{k+1/2} \Delta t(\mu_{1})_{m} \Delta \alpha_{1} \left[ \left( \frac{s^{H} + s^{k}}{2} \right)_{n\pm1,m} d_{n\pm1,m}^{k+1/2} + \left( \frac{s^{H} + s^{k}}{2} \right)_{n,m} d_{n,m}^{k+1/2} \right] / 2.$$
(5.4)

$$F_{n,\underline{m+1/2}}^{H_{A}} = u_{n,\underline{m+1/2}}^{k+1/2} \Delta t (\mu_{2})_{n} \Delta \alpha_{2} \left[ \left( \frac{s^{H} + s^{k}}{2} \right)_{n,\underline{m+1}} d_{n,\underline{m+1}}^{k+1/2} + \left( \frac{s^{H} + s^{k}}{2} \right)_{n,\underline{m}} d_{n,\underline{m}}^{k+1/2} \right] / 2.$$
(5.5)

The diffusive fluxes are then given by the following relations.  

$$(K_{x} \equiv K_{\alpha_{1}}, K_{y} \equiv K_{\alpha_{2}})$$

$$F_{n\pm1/2,m}^{H_{0}} = \pm K_{y_{n\pm1/2,m}}^{k+1/2} \frac{\Delta t(\mu_{1})_{m}\Delta \alpha_{1}}{2}$$

$$\times \frac{\left[(S^{H} + S^{k})_{n,m} - (S^{H} + S^{k})_{n\pm1,m}\right]}{\Delta \alpha_{2}(\mu_{2})_{n\pm1/2}} \frac{\left(d_{n\pm1,m}^{k+1/2} + d_{n,m}^{k+1/2}\right)}{2}$$
(5.6)

$$F_{n,\underline{m+1/2}}^{H_{0}} = \frac{+\kappa_{x_{n,\underline{m+1/2}}}^{k+1/2}}{\sum_{n,\underline{m+1/2}}^{\Delta t (\mu_{2})_{n} \Delta \alpha_{2}}} \frac{\Delta t (\mu_{2})_{n} \Delta \alpha_{2}}{2}}{\sum_{n,\underline{m+1/2}}^{\Delta t (\mu_{2})_{n} \Delta \alpha_{2}}} \frac{\left(d_{n,\underline{m+1}}^{k+1/2} + d_{n,\underline{m}}^{k+1/2}\right)}{2}$$
(5.7)

For the lower order scheme, the FTUS scheme written in (3.1) is employed. Factorization terms generated by the multioperational method are not considered. Equation (3.1) is written in the form of (5.1). The total fluxes are presented as the sum of advective and diffusive fluxes.

From Equation (3.1) one obtains the following set of advective fluxes.

$$F_{n+1/2,m}^{L} = \begin{cases} v_{n+1/2,m}^{k+1/2} \ge 0 & v_{n+1/2,m}^{k+1/2} \Delta t(\mu_{1})_{m} \Delta \alpha_{1} \left( \frac{s^{L} + s^{k}}{2} \right)_{n,m} d_{n,m}^{k+1/2} \\ & & \\ v_{n+1/2,m}^{k+1/2} < 0 & v_{n+1/2,m}^{k+1/2} \Delta t(\mu_{1})_{m} \Delta \alpha_{1} \left( \frac{s^{L} + s^{k}}{2} \right)_{n+1,m} d_{n+1,m}^{k+1/2} \end{cases}$$
(5.8)

$$F_{n-1/2,m}^{L} = \begin{cases} v_{n-1/2,m}^{k+1/2} \ge 0 & v_{n-1/2,m}^{k+1/2} \Delta t(\mu_{1})_{m} \Delta \alpha_{1} \left(\frac{s^{L} + s^{k}}{2}\right)_{n-1,m} d_{n-1,m}^{k+1/2} \\ v_{n-1/2,m}^{k+1/2} < 0 & v_{n-1/2,m}^{k+1/2} \Delta t(\mu_{1})_{m} \Delta \alpha_{1} \left(\frac{s^{L} + s^{k}}{2}\right)_{n,m} d_{n,m}^{k+1/2} \end{cases}$$
(5.9)

$$F_{n,m+1/2}^{L_{A}} = \begin{cases} u_{n,m+1/2}^{k+1/2} \ge 0 & u_{n,m+1/2}^{k+1/2} \Delta t (u_{2})_{n} \Delta \alpha_{2} \left( \frac{s^{L} + s^{k}}{2} \right)_{n,m} d_{n,m}^{k+1/2} \\ & & \\ u_{n,m+1/2}^{k+1/2} < 0 & u_{n,m+1/2}^{k+1/2} \Delta t (u_{2})_{n} \Delta \alpha_{2} \left( \frac{s^{L} + s^{k}}{2} \right)_{n,m+1} d_{n,m+1}^{k+1/2} \end{cases}$$
(5.10)

$$F_{n,m-1/2}^{L_{A}} = \begin{cases} u_{n,m-1/2}^{k+1/2} \ge 0 & u_{n,m-1/2}^{k+1/2} \Delta t(\mu_{2})_{n} \Delta \alpha_{2} \left( \frac{s^{L} + s^{k}}{2} \right)_{n,m-1} d_{n,m-1}^{k+1/2} \\ & & \\ u_{n,m-1/2}^{k+1/2} < 0 & u_{n,m-1/2}^{k+1/2} \Delta t(\mu_{2})_{n} \Delta \alpha_{2} \left( \frac{s^{L} + s^{k}}{2} \right)_{n,m} d_{n,m}^{k+1/2} \end{cases}$$
(5.11)

The diffusive fluxes are obtained from relations (5.6) and (5.7) with H replaced by L.

The Zalesak flux-correction procedure as reported in [3] for the linear case proceeds analogously as follows:

First, the anti-diffusive fluxes are computed.

$$A_{n+1/2,m} = F_{n+1/2,m}^{H_A} - F_{n+1/2,m}^{L_A} + F_{n+1/2,m}^{H_O} - F_{n+1/2,m}^{L_O}$$
(5.12)

$$A_{n,\underline{m+1/2}} = F_{n,\underline{m+1/2}}^{H_{A}} - F_{n,\underline{m+1/2}}^{L_{A}} + F_{n,\underline{m+1/2}}^{H_{O}} - F_{n,\underline{m+1/2}}^{L_{O}}$$
(5.13)

In computing the difference between the diffusive fluxes (third and fourth terms in the above expressions), note that the terms with  $S_{n,m}^k$  may be completely eliminated.

The above anti-diffusive fluxes are screened in the following manner.

$$A_{n+1/2,m} = 0 \quad \text{if} \quad A_{n+1/2,m} \left( S_{n+1,m}^{L} - S_{n,m}^{L} \right) < 0$$
  
and either  $A_{n+1/2,m} \left( S_{n+2,m}^{L} - S_{n+1,m}^{L} \right) < 0$  (5.14)  
or  $A_{n+1/2,m} \left( S_{n,m}^{L} - S_{n-1,m}^{L} \right) < 0$ 

$$A_{n,m+1/2} = 0 \quad \text{if} \quad A_{n,m+1/2} \left( s_{n,m+1}^{L} - s_{n,m}^{L} \right) < 0$$
  
and either 
$$A_{n,m+1/2} \left( s_{n,m+2}^{L} - s_{n,m+1}^{L} \right) < 0 \quad (5.15)$$
  
or 
$$A_{n,m+1/2} \left( s_{n,m}^{L} - s_{n,m-1}^{L} \right) < 0$$

Next the maximum and minimum cell values are determined.

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$$S_{n,m}^{a} = \max(S_{n,m}^{k}, S_{n,m}^{L})$$
  $S_{n,m}^{b} = \min(S_{n,m}^{k}, S_{n,m}^{L})$  (5.16)

$$S_{n,m}^{\max} = \max\left(S_{n-1,m}^{a}, S_{n,m}^{a}, S_{n+1,m}^{a}, S_{n,m-1}^{a}, S_{n,m+1}^{a}\right)$$
(5.17a)

$$S_{n,m}^{\min} = \min\left(S_{n-1,m}^{b}, S_{n,m}^{b}, S_{n+1,m}^{b}, S_{n,m-1}^{b}, S_{n,m+1}^{b}\right)$$
 (5.17b bis)

The author has also employed only quantities at time level k , obtaining the following alternative relations:

$$S_{n,m}^{\max} = \max\left(S_{n-1,m}^{k}, S_{n,m}^{k}, S_{n+1,m}^{k}, S_{n,m-1}^{k}, S_{n,m+1}^{k}\right)$$
(5.18a)

$$S_{n,m}^{\min} = \min\left(S_{n-1,m}^{k}, S_{n,m}^{k}, S_{n+1,m}^{k}, S_{n,m-1}^{k}, S_{n,m+1}^{k}\right)$$
(5.18b)

Next the sum of all anti-diffusive fluxes into cell (n,m),  $P_{n,m}^+$ , is determined.

$$P_{n,m}^{T} = \max(0, A_{n-1/2,m}) - \min(0, A_{n+1/2,m})$$

$$+ \max(0, A_{n,m-1/2}) - \min(0, A_{n,m+1/2})$$
(5.19)

The maximum allowable mass into the cell,  $Q_{n,m}^+$ , is then computed.

$$Q_{n,m}^{+} = \left(S_{n,m}^{\max} - S_{n,m}^{L}\right) \left[ (\mu_{1})_{m} \Delta \alpha_{1} (\mu_{2})_{n} \Delta \alpha_{2} d_{n,m}^{k+1} \right]$$
(5.20a)

Note  $S_{n,m}^{max}$  is as given by (5.17a). The author has employed two alternative formulations.

$$Q_{n,m}^{+} = \left(S_{n,m}^{\max} - S_{n,m}^{L}\right) \left[ (\mu_{1})_{m} \Delta \alpha_{1} (\mu_{2})_{n} \Delta \alpha_{2} d_{n,m}^{k+1} \right]$$
(5.20b)
where  $S_{n,m}^{max}$  is now given by (5.18a).

The second formulation considered is given by:

$$Q_{n,m}^{+} = \left(S_{n,m}^{\max} - S_{n,m}^{n}\right) \left[ (\mu_{1})_{m} \Delta \alpha_{1} (\mu_{2})_{n} \Delta \alpha_{2} d_{n,m}^{k+1} \right] \quad (5.20c \text{ bis})$$

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where  $S_{n,m}^{max}$  is given by (5.18a).

Similarly, the sum of all anti-diffusive fluxes out of cell (n,m),  $P_{n,m}^{-}$  , is determined.

$$P_{n,m}^{-} = \max(0, A_{n+1/2,m}) - \min(0, A_{n-1/2,m}) + \max(0, A_{n,m+1/2}) - \min(0, A_{n,m-1/2})$$
(5.21)

The maximum allowable mass to leave the cell,  $Q_{n,m}^{-}$ , is then computed.

$$Q_{n,m}^{-} = \left(S_{n,m}^{L} - S_{n,m}^{\min}\right) \left[ (\mu_{1})_{m} \Delta \alpha_{1} (\mu_{2})_{n} \Delta \alpha_{2} d_{n,m}^{k+1} \right]$$
(5.22a)

Note  $S_{n,m}^{\min}$  is as given by (5.17b).

As in the case of  $Q_{n,m}^+$ , the author has employed two corresponding alternatives. Under the first alternative, (5.22a) is employed with  $S_{n,m}^{\min}$  now given by (5.18b). Under the second alternative,

$$Q_{n,m}^{-} = \left(S_{n,m}^{n} - S_{n,m}^{\min}\right) \left[ (\mu_{1})_{m} \Delta \alpha_{1} (\mu_{2})_{n} \Delta \alpha_{2} d_{n,m}^{k+1} \right]$$
(5.22b)

with  $S_{n,m}^{\min}$  given by (5.18b).

The following ratios are next computed for use in determining the limiting coefficients.

$$R_{n,m}^{+} = \begin{cases} \min(1,Q_{n,m}^{+}/P_{n,m}^{+}) & P_{n,m}^{+} > 0 \\ 0 & P_{n,m}^{+} = 0 \end{cases}$$
(5.23)

$$R_{n,m}^{-} = \begin{cases} \min(1, Q_{n,m}^{-} / P_{n,m}^{-}) & P_{n,m}^{-} > 0 \\ 0 & P_{n,m}^{-} = 0 \end{cases}$$
(5.24)

The limiting coefficients are then given by

$$C_{n+1/2,m} = \begin{cases} \min(R_{n+1,m}^+, R_{n,m}^-) & A_{n+1/2,m} \ge 0 \\ \min(R_{n,m}^+, R_{n+1,m}^-) & A_{n+1/2,m} < 0 \end{cases}$$
(5.25)

$$C_{n,m+1/2} = \begin{cases} \min(R_{n,m+1}^{+}, \bar{R_{n,m}}) & A_{n,m+1/2} \ge 0 \\ \min(R_{n,m}^{+}, \bar{R_{n,m+1}}) & A_{n,m+1/2} < 0 \end{cases}$$

The anti-diffusive fluxes in (5.12) and (5.13) are limited by multiplying by the limiting coefficients and the solution is advanced to the next time level.

$$s_{n,m}^{k+1} = s_{n,m}^{L} - \left[ \Delta \alpha_{1}(\mu_{1})_{m} \Delta \alpha_{2}(\mu_{2})_{n} d_{n,m}^{k+1} \right]^{-1} (c_{n+1/2,m} A_{n+1/2,m}$$

$$(5.26)$$

$$- c_{n-1/2,m} A_{n-1/2,m} + c_{n,m+1/2} A_{n,m+1/2} - c_{n,m-1/2} A_{n,m-1/2}$$

We observe that for  $C_{n\pm 1/2,m} = C_{n,m\pm 1/2} = 0$ ,  $S_{n,m}^{k+1} = S_{n,m}^{L}$  and for  $C_{n\pm 1/2,m} = C_{n,m\pm 1/2} = 1.0$ ,  $S_{n,m}^{k+1} = S_{n,m}^{H}$ .

6. Additional Flux-Corrected Transport Limiters

In conjunction with (5.18a), one could insist  $S_{n,m}^{\min} = \max(0.0, S_{n,m}^{\min})$ , where  $S_{n,m}^{\min}$  on the right hand side is as determined in (5.18b). Equation (5.22a) would be employed for  $Q_{n,m}^{-}$ , where  $S_{n,m}^{\min}$  would be replaced by  $S_{n,m}^{\min}$ .

As another alternative, one could consider the following relations for  $S_{n,m}^{max}$  and  $S_{n,m}^{min}$ .

$$s_{n,m}^{\max} = \max\left(s_{n-1,m}^{k}, s_{n,m}^{k}, s_{n+1,m}^{k}, s_{n,m-1}^{k}, s_{n,m+1}^{k}, s_{n,m}^{k+1}\right)$$
(5.27a)

$$S_{n,m}^{\min} = \min\left(S_{n-1,m}^{k}, S_{n,m}^{k}, S_{n+1,m}^{k}, S_{n,m-1}^{k}, S_{n,m+1}^{k}, S_{n,m}^{k+1}\right)$$
(5.27b)

These relations could be employed with (5.20a) and (5.22a).

As an additional alternative, one could employ the second alternate limiter of the previous section; e.g., (5.18a), (5.18b), (5.20c) and (5.22b), on the first time step and the original Zalesak limiter on subsequent time steps.

Clearly, many different forms of the limiter are possible. We have presented these additional limiters to outline the direction of possible future research.

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#### PART IV: ADDITIONAL NUMERICAL CONSIDERATIONS

In order to develop a numerical model it is necessary to develop the necessary approximations near both open and closed boundaries. This then leads to a discussion of the tridiagonal matrix solution scheme necessary for each sweep.

The development of flow field influence on the effective dispersion coefficients is presented to close the numerical model. This closure is by no means perfect; however, it is sufficiently general to permit model calibration. Additional approaches may be necessary to incorporate wind effects. The approach followed here allows a determination of the anticipated range of physical dispersion. In general, the numerical scheme will also produce dispersion. The model should be calibrated by adjusting the dispersion coefficients to values within the acceptable physical range.

#### 1. Approximations Near Solid Boundaries

In the hydrodynamic equations, the convective acceleration terms and the eddy viscosity terms must be modified in the vicinity of the boundaries. This is due to the fact, that if the standard differencing formulae at the boundary are used points are referenced outside the grid. No modifications are necessary for the continuity equation. Since the transport equation is nothing more than a constituent continuity equation, we would anticipate no need to modify the formula. This is indeed the case, for the difference formulae for continuity are cell centered; namely, fluxes are evaluated at each cell face. The fluxes are merely set to zero in the standard formulae for no flow conditions across the

appropriate faces. Let us investigate this procedure in turn for each difference scheme. In the X or  $\alpha_1$  sweep each column in the grid is swept from top to bottom stating and ending at a boundary. In the Y or  $\alpha_2$  sweep each row is swept from left to right again starting and ending with a boundary.

Let us consider Equation (2.8) of Part III, which we rewrite below as the standard equation for the  $X-\alpha_1$  sweep .

$$a_{n,m-1} s_{n,m-1}^{k+1/2*} + a_{n,m} s_{n,m}^{k+1/2*} + a_{n,m+1} s_{n,m+1}^{k+1/2*} = B_{m}$$
 (1.1)

TOP BOUNDARY

1. FTCS Scheme

In (2.5) of Part III  $u_{n,m-1/2}^{k+1/2*} = K_{x_{n,m-1/2}}^{k+1/2*} = 0$ ; i.e., there is no mass transfer through the solid boundary. Therefore  $a_{n,m-1} = 0$ , and one obtains

$$a_{n,m} s_{n,m}^{k+1/2*} + a_{n,m+1} s_{n,m+1}^{k+1/2*} = B_{m}$$
 (1.2)

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2. FTUS Scheme

Exactly the same conditions hold for this scheme and (1.2) is again obtained.

3. STCS Scheme

In this scheme referring to (4.4) of Part III  $-a_{n,m-1} \equiv -a_{n,m-1} - \left(\frac{d^{k+1/2*}_{n,m-1}}{d^{k+1/2*}_{n,m-1}}\right) / 6$  and  $a_{n,m-1} = \left(\frac{d^{k+1/2*}_{n,m-1}}{d^{k+1/2*}_{n,m-1}}\right) / 6$ . For a true land boundary  $\left(\frac{d^{k+1/2*}_{n,m-1}}{d^{k+1/2*}_{n,m-1}}\right) / 6 = 0$  and again (1.2) is obtained. For the case of

a flux restriction only at a barrier,  $\binom{k+1/2}{n,m-1}/6 \neq 0$  and for this scheme a barrier may not form the end of a computational segment. BOTTOM BOUNDARY

All statements previously made regarding the top boundary hold directly if (n,m-1) is replaced by (n,m+1). Equation (1.1) now becomes

$$a_{n,m-1} s_{n,m-1}^{k+1/2*} + a_{n,m} s_{n,m}^{k+1/2*} = B_{m}$$
 (1.3)

Let us consider (2.10) of Part III, which we rewrite below as the standard equation for the  $Y{-}\alpha_2$  sweep .

$$a_{n-1,m} s_{n-1,m}^{k+1} + a_{n,m} s_{n,m}^{k+1} + a_{n+1,m} s_{n+1,m}^{k+1} = B_n$$
 (1.4)

LEFT BOUNDARY

1. FTCS Scheme

In (2.11) of Part III  $v_{n-1/2,m}^{k+1} = K_{y_{n-1/2,m}}^{k+1} = 0$ ; i.e., there is no mass transfer through the solid boundary. Therefore  $a_{n-1,m} = 0$ , and one obtains

$$a_{n,m} s_{n,m}^{k+1} + a_{n+1,m} s_{n+1,m}^{k+1} = B_n$$
 (1.5)

2. FTUS Scheme

 $a_{n-1,m} = 0$  and (1.5) is again obtained.

3. STCS Scheme

$$a_{n-1,m} = \left( \frac{d^{k+1}}{n-1,m} \right) / 6$$
 and (1.5) is obtained for a land boundary.

#### RIGHT BOUNDARY

All statements previously made regarding the left boundary hold directly if (n-1,m) is replaced by (n+1,m). Equation (1.5) now becomes

$$a_{n-1,m} s_{n-1,m}^{k+1} + a_{n,m} s_{n,m}^{k+1} = B_n$$
 (1.6)

# 2. Approximations Near Open Boundaries

In the hydrodynamic equations, convective and eddy viscosity terms in both motion equations must be modified in the vicinity of these type boundaries. No modifications are necessary for the continuity equation nor for the transport equation. However fluxes must be specified across the appropriate cell faces. Let us investigate this procedure for each sweep in each scheme.

TOP (-) AND BOTTOM (+) BOUNDARIES

1. FTCS and FTUS Schemes

 $u_{n,m_{\mp}^{-1/2}}^{k+1/2*}$  and  $K_{x,m_{\mp}^{-1/2}}^{k+1/2*}$  must be specified. In (2.8) of Part III

 $S_{n,m_{\mp}1}^{k+1/2*}$  must also be given.

2. STCS Scheme

 $u_{n,m_{+}^{-1/2}}^{k+1/2*}$ ,  $K_{x_{n,m_{+}^{-}1/2}}^{k+1/2*}$  and  $d_{n,m_{+}^{-1}}^{k+1/2*}$  must be specified. In (2.8)

of Part III  $S_{n,m_{\mp}1}^{k+1/2*}$  must also be given.

As a result, Equations (1.2) and (1.3) are again obtained. LEFT (-) AND RIGHT (+) BOUNDARIES

1. FTCS and FTUS Schemes

 $v_{n_{\mp}1/2,m}^{k+1}$  and  $K_{y_{n_{\mp}1/2,m}}^{k+1}$  must be specified. In (2.10) of

Part III  $s_{n_{\pm}^{\pm}1,m}^{k+1}$  must also be given.

2. STCS Scheme

 $v_{n_{\pm}^{1/2},m}^{k+1}$ ,  $K_{y_{n_{\pm}^{-1/2},m}}^{k+1}$ , and  $d_{n_{\pm}^{-1},m}^{k+1}$  must be specified. In (2.10)

of Part III  $s_{n_{\mp}^{-1},m}^{k+1}$  must also be given. As a result, Equations (1.5) and (1.6) are again obtained.

The specification of s deserves further attention. In the general case, s must be given as a function of time over the period of concern. However, in estuarine type (oscillating) flows, it is possible to compute s based upon the values at interior points during ebb tide. The following procedure due to Leendertse [1] is presented subsequently with reference to Figure 3. Diffusion is allowed only on one face of the boundary cell.

TOP (-) AND BOTTOM (+) BOUNDARIES

$$s_{n,m_{\mp}^{k+1/2*}}^{k+1/2*} = s_{n,m_{\mp}^{1}}^{k} + u_{n,m_{\mp}^{1}^{1/2}}^{k+1/2*} \frac{\left(s_{n,m}^{k} - s_{n,m_{\mp}^{1}}^{k}\right)}{\Delta \alpha_{1}^{(\mu_{1})} m_{\mp}^{-1/2}} \frac{\Delta t}{2}$$

$$+ \kappa_{n,m_{\mp}^{1/2}}^{k+1/2*} \frac{\left(s_{n,m}^{k} - s_{n,m_{\mp}^{1}}^{k}\right)}{\left[(\mu_{1})_{m_{\mp}^{1}} \Delta \alpha_{1}\right]^{2}} \frac{\Delta t}{2}$$
(2.1)

LEFT (-) AND RIGHT (+) BOUNDARIES

$$s_{n+1,m}^{k+1} = s_{n+1,m}^{k+1/2*} + v_{n+1/2,m}^{k+1} \frac{\left(s_{n,m}^{k+1/2*} - s_{n+1,m}^{k+1/2*}\right)}{\Delta \alpha_2(\mu_2)_{n+1/2}} \frac{\Delta t}{2}$$

$$\frac{1}{4} \kappa_{y_{n+1/2,m}}^{k+1} \frac{\left(s_{n,m}^{k+1/2*} - s_{n+1,m}^{k+1/2*}\right)}{\left[(\mu_2)_{n+1} \Delta \alpha_2\right]^2} \frac{\Delta t}{2}$$
(2.2)



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Figure 3. Open boundary specification of S

Consider at an arbitrary boundary location b, ebb flow conditions to endure over N time steps. Compute at each time step of length  $\Delta t$  the following variables.

$$Me_{i} = Se_{b}^{i} Ve_{b}^{i} \qquad Ve_{b}^{i} = \Delta t (\overline{Vd})^{i}$$
(2.3)

where

 $Me_i \approx mass flux across boundary face during time step i$  $<math>Ve_b^i \approx volume$  through boundary face during time step i  $Se_b^i \approx concentration$  at the boundary face during time step i  $(\overline{Vd})^i \approx average$  discharge through boundary face during time step i Compute totals over the ebb flow period as follows

$$M_{ebb} = \sum_{i=1}^{N} Me_{i} \quad V_{ebb} = \sum_{i=1}^{N} Ve_{b}^{i}$$
 (2.4)

where

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M<sub>ebb</sub> = total mass flux across boundary face during ebb
V<sub>ebb</sub> = total volume across boundary face during ebb
For the next M time steps occurring during the flood period, compute
the following quantities.

$$Vf_{1} = V_{ebb} \qquad Mf_{1} = M_{ebb}$$

$$Vf_{1} = V_{ebb} - \sum_{k=1}^{i-1} Ve_{b}^{N-k} \qquad Mf_{i} = M_{ebb} - \sum_{k=1}^{i-1} Me_{N-k} \qquad i \ge 2$$
(2.5)

Then the boundary concentration during the flood period is given by

$$St_{b}^{i} = \begin{cases} \frac{(1 - r_{b})Mf_{i}}{Vf_{i}} + r_{b}c_{b}, & Vf_{i} \ge 0\\ \\ c_{b} & & , Vf_{i} < 0 \end{cases}$$
(2.6)

where

 $Sf_b^i \equiv$  boundary concentration during flood for time step i  $Mf_i \equiv$  mass in ebb storage remaining prior to time step i  $Vf_i \equiv$  ebb volume remaining prior to time step i  $r_b \equiv$  exchange ratio for the boundary ( $0 \le r_b \le 1$ )  $c_b \equiv$  ocean background concentration

The method above represents one approach toward specifying s during the flood period. Other approaches similar in concept are available. Usually one must select individually the most appropriate approach for each area to be modelled.

# 3. Tridiagonal Matrix Solution

Consider the following system of equations, which is termed a tridiagonal system. We note from our previous sections on boundary conditions that this system of equations is obtained.

$b_1v_1 + c_1v_2$	= d <sub>1</sub>	
$a_2v_1 + b_2v_2 + c_2v_3$	= d <sub>2</sub>	
$a_{3}v_{2} + b_{3}v_{3} + c_{3}v_{4}$	= d <sub>3</sub>	(3,1)
$a_i v_{i-1} + b_i v_i + c_i v_{i+1}$	= d <sub>i</sub>	(311)
$a_{N-1}v_{N-2} + b_{N-1}v_{N-1} + c_{N-1}v_{N}$	= d <sub>N-1</sub>	
$a_N v_{N-1} + b_N v_N$	= d <sub>N</sub>	

A numerically effective approach in solving this system is forward elimination and backward substitution. Each step is discussed in turn. Forward elimination

$$v_1 = \frac{d_1}{b_1} - \frac{c_1}{b_1} v_2$$
 (3.2)

Substituting (3.2) into the second equation in (3.1)

$$a_2\left(\frac{d_1}{b_1} - \frac{c_1}{b_1}v_2\right) + b_2v_2 + c_2v_3 = d_2$$

(3.3)  
$$\mathbf{v}_{2} = \frac{\mathbf{d}_{2} - \mathbf{a}_{2} \frac{\mathbf{d}_{1}}{\mathbf{b}_{1}} - \mathbf{c}_{2} \mathbf{v}_{3}}{\mathbf{b}_{2} - \frac{\mathbf{a}_{2}^{c} \mathbf{1}}{\mathbf{b}_{1}}}$$

Let us define  $\beta_1 = b_1$  and  $\gamma_1 = d_1/\beta_1$  then we note (3.2) may be written as  $v_1 = \gamma_1 - (c_1/\beta_1)v_2$  and (3.3) may be written as

$$\mathbf{v}_{2} = \frac{(\mathbf{d}_{2} - \mathbf{a}_{2}\gamma_{1}) - \mathbf{c}_{2}\mathbf{v}_{3}}{\mathbf{b}_{2} - \mathbf{a}_{2}\frac{\mathbf{c}_{1}}{\mathbf{b}_{1}}} \qquad \mathbf{v}_{2} = \gamma_{2} - \frac{\mathbf{c}_{2}}{\beta_{2}}\mathbf{v}_{3}$$
(3.4)

$$\beta_2 = \beta_2 - \alpha_2 \frac{c_1}{\beta_1}$$
  $\gamma_2 = \frac{d_2 - \alpha_2 \gamma_1}{\beta_2}$ 

Let us suppose that for equation i, we have the following quantities

$$\beta_{i} = b_{i} - \frac{a_{i}c_{i-1}}{\beta_{i-1}} \qquad \gamma_{i} = \frac{d_{i} - a_{i}\gamma_{i-1}}{\beta_{i}}$$
and
$$v_{i} = \gamma_{i} - \frac{c_{i}}{\beta_{i}} v_{i+1}$$
(3.5)

For the (i+1) equation we have,

$$a_{i+1}v_i + b_{i+1}v_{i+1} + c_{i+1}v_{i+2} = d_{i+1}$$
 (3.6)

Substituting for  $\ \mathbf{v}_{i}$  , we obtain

$$a_{i+1}\left(\gamma_{i} - \frac{c_{i}}{\beta_{i}} v_{i+1}\right) + b_{i+1}v_{i+1} + c_{i+1}v_{i+2} = d_{i+1}$$

$$v_{i+1} = \frac{d_{i+1} - a_{i+1}\gamma_{i} - c_{i+1}v_{i+2}}{b_{i+1} - \frac{a_{i+1}c_{i}}{\beta_{i}}} = \gamma_{i+1} - \frac{c_{i+1}}{\beta_{i+1}} v_{i+2}$$
(3.7)

where

$$\gamma_{i+1} = \frac{d_{i+1} - a_{i+1}\gamma_i}{\beta_{i+1}} \qquad \beta_{i+1} = b_{i+1} - \frac{a_{i+1}c_i}{\beta_i}$$

Therefore we have obtained the general form of the recursion relations. For proceeding to N from N-1  $\,$ 

$$\mathbf{v}_{N-1} = \gamma_{N-1} - \frac{c_{N-1}}{\beta_{N-1}} \mathbf{v}_{N} \qquad \gamma_{N-1} = \frac{d_{N-1} - a_{N-1}\gamma_{N-2}}{\beta_{N-1}}$$
(3.8)

$$\beta_{N-1} = b_{N-1} - \frac{a_{N-1}c_{N-2}}{\beta_{N-2}}$$

Substituting the above relation for  $v_{N-1}$  into equation N we obtain:

$$a_{N}\left(\gamma_{N-1} - \frac{c_{N-1}}{\beta_{N-1}} v_{N}\right) + b_{N}v_{N} = d_{N}$$

$$d_{N} - a_{N}\gamma_{N-1}$$

$$\mathbf{v}_{\mathrm{N}} = \frac{\mathbf{a}_{\mathrm{N}} - \mathbf{a}_{\mathrm{N}} \mathbf{v}_{\mathrm{N-1}}}{\mathbf{b}_{\mathrm{N}} - \frac{\mathbf{a}_{\mathrm{N}} \mathbf{c}_{\mathrm{N-1}}}{\beta_{\mathrm{N-1}}}} = \mathbf{v}_{\mathrm{N}}$$

(3.9)

where  $\beta_N = b_N - (a_N c_{N-1} / \beta_{N-1})$ . This completes the forward elimination step. The  $\gamma_i$ ,  $\beta_i$  are computed for i = 1, N as summarized below.

$$\beta_{1} = b_{1} \qquad \gamma_{1} = \frac{d_{1}}{\beta_{1}} \qquad \beta_{i} = b_{i} - \frac{a_{i}c_{i-1}}{\beta_{i-1}}$$

$$\gamma_{i} = \frac{d_{i} - a_{i}\gamma_{i-1}}{\beta_{i}} \qquad i = 2, N$$
(3.10)

Backward substitution

We note  $v_N = \gamma_N$  and it is therefore possible to then employ

$$v_{i-1} = \gamma_{i-1} - \frac{c_{i-1}}{\beta_{i-1}} v_i$$
 for  $i = N, \dots 2$  (3.11)

thereby computing  $v_{N-1}, \dots v_1$  employing the previously computed values  $\gamma_{N-1}$ ,  $\beta_{N-1} \dots \gamma_1$ ,  $\beta_1$  on the forward elimination step.

Let us make the following variable assignments in anticipation of coding efforts.

$$Q_{i} \equiv \gamma_{i}$$

$$P_{i} \equiv \frac{c_{i}}{\beta_{i}}$$

$$(3.12)$$

Thus we may reformulate our solution procedures as indicated in Table IX. Mitchell and Griffiths [5] report that in order for this algorithm to be implemented on a digital computer the following characteristics must be possessed by the coefficient matrix elements.

 $a_{i} < 0$ ,  $b_{i} > 0$ ,  $c_{i} < 0$  i = 1, N

(3.13)

 $b_{i} \ge - (a_{i} + c_{i})$ 

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In this case  $|P_i| \leq 1$  for i = 1, N and the growth of errors will be eliminated. The values of  $\beta$ , P, and Q may be output during preliminary computations to check the numerical formulation.

### 4. Hydrodynamic Interface

Within the hydrodynamics program, a three time-level stabilizing correction scheme is employed to compute the field variables  $\eta$ , u, and v at each time step. Within the two time-level transport scheme, u and v are employed at k, k+1/2\*, and k+1. Two approaches suggest themselves for interfacing the two schemes.

### Approach 1

- 1. Employ  $\Delta t_T$  in the transport scheme equal to  $\Delta t_H$  in the hydrodynamic scheme. Define  $u^{k+1/2*} = (u^{k+1} + u^k)/2$ . and  $v^{k+1/2*} = (v^{k+1} + v^k)/2$ .
- Perform one sweep in the transport scheme for each sweep in the hydrodynamic scheme.

#### Approach 2

1. Employ  $\Delta t_{T}$  in the transport scheme as twice  $\Delta t_{H}$  in the

Forward Elimination	Backward Substitution
$ \left[ \begin{array}{c} P_{1} = \frac{c_{1}}{b_{1}} & Q_{1} = \frac{d_{1}}{b_{1}} \\ & & \end{array} \right] $	$v_N = Q_N$
$\beta_2 = b_2 - a_2 P_1$	$\mathbf{v}_{N-1} = \mathbf{Q}_{N-1} - \mathbf{P}_{N-1}\mathbf{v}_{N}$
$P_2 = \frac{c_2}{\beta_2}$	$v_1 = Q_1 - P_1 v_2$
$Q_2 = \frac{d_2 - a_2 Q_1}{\beta_2}$	
• • •	
$ \begin{pmatrix} \beta_k = b_k - a_k P_{k-1} \end{pmatrix} $	
$\begin{cases} P_{k} = \frac{c_{k}}{\beta_{k}} \\ k = 1, \dots N \end{cases}$	
$\left(Q_{k} = \frac{d_{k} - a_{k}Q_{k-1}}{\beta_{k}}\right)$	

Table IX. Tridiagonal Matrix Solution Procedure

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hydrodynamic scheme. Thereby obtain  $u_T^{k+1/2*} = u_H^k$ ,  $u_T^k = u_H^{k-1}$ ,  $u_T^{k+1} = u_H^{k+1}$ .

Approach 2 would certainly be the more economical of the two approaches. Approach 1 may be more accurate. Numerical testing may be necessary to determine the most suitable approach.

#### 5. Dispersion Coefficient Determination

The effective dispersion coefficients in Equation (1.1) Part II must be related to the flow properties to close the numerical approximations. This represents an active area of research with several alternate approaches available.

Elder [6] has determined the longitudinal dispersion coefficient in the open channel flow experiments to be given by the following relation.

$$K_v = 5.93 h u^*$$
 (5.1)

where

K = longitudinal dispersion coefficient h = water depth (hydraulic radius) u\* = shear velocity

For open channel flow  $u^* = \sqrt{ghS_e}$  and from the Chezy relation  $u = c\sqrt{hS_e}$ . As a result, we obtain

$$u_{\star} = \sqrt{g} \frac{u}{c}$$
(5.2)

where

u = velocity

g = gravity

c = Chezy coefficient

Therefore, Equation (5.1) becomes

$$K_{x} = 5.93\sqrt{g} \frac{un}{c}$$
(5.3)

Taylor [7] has conducted pipe flow experiments to determine the longitudinal dispersion coefficient. By assuming the hydraulic radius as half the pipe radius in the pipe experiments and equal to the water depth in a uniform steady flow open channel, the coefficient in (5.1) and (5.3) is determined to be 20.2 rather than 5.93. As a result, we would expect a general relationship of the following form to hold.

$$K_{x} = c_{x}\sqrt{g} \frac{uh}{c}, c_{x} \in (5.93, 20.2)$$
 (5.4)

Wind and wave effects will increase the effective dispersion coefficients. The relationships are not well known. However, Swain [8] has suggested the addition of the following term to (5.4) to account for wind effects

$$KW_{x} = \frac{\kappa \sqrt{g}}{6c} u_{w} h\beta$$
 (5.5)

where

 $KW_{\downarrow} \equiv wind effect addition$ 

$$\beta \equiv$$
 ratio of sediment mass transfer coefficient ( $\varepsilon_s$ ) to turbu-  
lent transfer coefficient ( $\varepsilon_m$ ) ( $1 \le \beta \le 5$ )  
 $\zeta_m \equiv$  wind velocity

- c ∃ Chezy coefficient
- $h \equiv$  water depth

 $\kappa \equiv \text{von Karman's constant (.41)}$ 

Elder [6] has reported a lateral dispersion coefficient similar to (5.1) with 5.93 replaced by 0.23. For a general model formulation, the following relations will be initially considered.

$$K_{x} = c_{x}\sqrt{g} \frac{uh}{c} + cw \frac{(u_{w})_{x}h}{c} + K'_{x}$$
 (5.6)

$$K_{y} = c_{y}\sqrt{g} \frac{vh}{c} + cw \frac{(u_{w})_{y}h}{c} + K'_{y}$$
 (5.7)

where  $c_x$ ,  $c_y \in (5.93, 20.2)$  or 0.23 and are spatially variable, cw equals ( $\kappa \sqrt{g} \beta/6$ ),  $K'_x$ ,  $K'_y$  are additional constants.

The above relations represent a first approach toward describing the dispersion mechanisms. Additional approaches may need to be considered to develop suitable results in Mississippi Sound.

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# APPENDIX A: LEENDERTSE 1-DIMENSIONAL CASE

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# APPENDIX B: 2-DIMENSIONAL CASE, WITH Pe = 10



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# APPENDIX C: 2-DIMENSIONAL CASE, WITH Pe = 108


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Will Kt.         Mill Ht.	<u> </u>	<u> </u>		Ļ			?	-	<u> </u>			Ļ	<u> </u>	Ļ			·					C3		1		1				 <u> </u>	
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## APPENDIX D: PROGRAM LISTING

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•	EPVELD=GAPS(LANDALLE). PHAGE(L)=ATAN2(L]MAG(L_)).FEAL(LANDA(LL)).15%./PI CGUTANE	
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