Water Quality Models: Types, Issues, Evaluation
Major Model Types

- Finite Difference
- Finite Element
- Harmonic Models
- Methods of Characteristics (Eulerian-Lagrangian Models)
- Random Walk Particle Tracking
Finite Difference

- Differential eq. $\Rightarrow$ difference eqn.
- Choices of grids in horizontal and vertical (orthogonal)
- Different orders of approximation in space and time
- Large matrices, solved interatively

MWRA, 1996
Example Codes

- **3-D**
  - Princeton Ocean Model
  - Regional Ocean Modeling System (ROMS)
  - GLLVHT Model
  - EFDC
- **2-D depth averaged**
  - WI FM-SAL
- **2-D laterally averaged**
  - LARM
- **1-D Cross-sectional-averaged**
  - QUAL2E
- **1-D Horizontally-averaged**
  - DYRESM
  - WQRRS
  - MI TEMP
Grids

- **Horizontal**
  - Rectangular
  - Orthogonal

- **Vertical**
  - Stair-stepped (z coordinate)
  - Bottom fitting (σ coordinate)

Also isopycnal models
Finite Difference (1-D examples)

\[ \frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2} \]

\[ \frac{c_i^{n+1} - c_i^n}{\Delta t} = -u_i \frac{c_i - c_{i-1}}{\Delta x} + E \left( \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} \right) \]

B from conservative (control volume) form of eqn
Time stepping

- **Explicit** (evaluate RHS at time $n$)
  \[
  a \frac{c_i^{n+1}}{\Delta x} = c_i^n \left[ 1 - \frac{u_i \Delta t}{\Delta x} - \frac{2E \Delta t}{\Delta x^2} \right] + c_{i-1}^n \left[ \frac{u_i \Delta t}{\Delta x} + \frac{E \Delta t}{\Delta x^2} \right] + c_{i+1}^n \frac{E \Delta t}{\Delta x^2}
  \]

- **Implicit** (evaluate RHS at time $n+1$)
  \[
  [ - \frac{u_i \Delta t}{\Delta x} - \frac{E \Delta t}{\Delta x^2} ] c_{i-1}^{n+1} + [1 + \frac{u_i \Delta t}{\Delta x} + \frac{2E \Delta t}{\Delta x^2}] c_i^{n+1} - \frac{E \Delta t}{\Delta x^2} c_{i+1}^{n+1} = c_i^n
  \]

Solution involves tri-diagonal matrix
Time stepping (cont’d)

- Mixed schemes
  - e.g., Crank-Nicholson wts n, n+1 50% each

Numerical accuracy and stability depend on

\[ \frac{u \Delta t}{\Delta x} \] Courant Number
\[ \frac{E \Delta t}{\Delta x^2} \] Diffusion Number

being less than critical values (~1)
Finite Element

- Information stored at element nodes
- Approx sol’n to differential eqn.
- Large matrices, solved iteratively
- More flexible than FD
- Somewhat more overhead
Example Codes

- **3-D**
  - RMA-10 and -11

- **2-D Horizontal Average**
  - EDF
  - ADCIRC
  - RMA-2 and -4
Finite Element (1-D example)

\[ \frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - E \frac{\partial^2 c}{\partial x^2} = 0 \]

\[ c(x, t) \approx \hat{c}(x, t) = \sum_{j=1}^{N_T} \alpha_j(t) \phi^j(x) \]

real c \quad discrete c \quad unknowns interpolation fns

\[ \phi^{j-1} \quad \alpha_{j-1} \quad 1 \quad \alpha_j \quad \alpha_{j+1} \quad \phi^{j+1} \]

j-1 \quad j \quad j+1
Finite Element (1-D example)

R = residual = discrete equation - real equation

\[ R = \frac{\partial \hat{c}}{\partial t} + u \frac{\partial \hat{c}}{\partial x} - E \frac{\partial^2 \hat{c}}{\partial x^2} \]

W = weighted residual

\[ W = \int_0^L wRdx = 0 \]

weighting functions \( \phi \)

Account for boundary conditions as well
Different element dimensions

- Finite element grid (RMA10/11) for Delaware R
- 1-D, 2-D and 3-D elements

PSEG, 2000
Harmonic Models

- Periodic motion outside $\Rightarrow$ periodic motion inside
- Plus harmonics
- Transient problem $\Rightarrow$ steady problem
- Best for tidally-dominated flows

$\eta, u, v$
Example Codes

- 3-D
  - Lynch et al. (Dartmouth)

- 2-D Horizontal
  - Tidal Embayment Analysis (MIT)
Harmonic Decomposition

\[ \eta(x, y, t) = A_\eta(x, y) \cos(\omega t + \phi_\eta) = A_\eta^* e^{i\omega t} \]

\[ u(x, y, t) = A_x^* e^{i\omega t} \]

\[ v(x, y, t) = A_y^* e^{i\omega t} \]

Ex.

\[ \frac{\partial \eta}{\partial t} = A_\eta^* (i\omega) e^{i\omega t} \]

\[ h \frac{\partial u}{\partial x} = h \frac{\partial A_x^*}{\partial x} e^{i\omega t} \]

\[ h \frac{\partial v}{\partial y} = h \frac{\partial A_y^*}{\partial y} e^{i\omega t} \]

\[ i\omega A_n^* e^{i\omega t} + h \frac{\partial A_x^*}{\partial x} e^{i\omega t} + h \frac{\partial A_y^*}{\partial y} e^{i\omega t} = 0 \]
TEA-Basic Equations

\[
\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} (uh) + \frac{\partial}{\partial y} (vh) = -\frac{\partial}{\partial x} (u \eta) - \frac{\partial}{\partial y} (v \eta)
\]

\[
\frac{\partial u}{\partial t} + g \frac{\partial \eta}{\partial x} - f v + \frac{\lambda u}{h} - \tau_x^s = -u \frac{\partial u}{\partial x} - v \frac{\partial u}{\partial y} - \frac{\tau_{x, nl}^b}{\rho h}
\]

\[
\frac{\partial v}{\partial t} + g \frac{\partial \eta}{\partial y} + f u + \frac{\lambda v}{h} - \tau_y^s = -u \frac{\partial v}{\partial x} - v \frac{\partial v}{\partial y} - \frac{\tau_{y, nl}^b}{\rho h}
\]

Linear Terms \hspace{2cm} \text{Non-Linear Terms}

Westerink et al. (1985)
Non-linear Terms

Products of sine/cosine functions produce new sine/cosine functions with sums and differences of frequencies

\[ \cos \alpha \cos \beta = \frac{1}{2} \cos(\alpha - \beta) + \frac{1}{2} \cos(\alpha + \beta) \]

Ex:

\[ M_2 \text{ tide} \quad (T = 12.4 \text{ hr}) \]
\[ M_4 \text{ tide} \quad (T/2 = 6.2 \text{ hr}) \]

Non-linear forcing terms determined by iteration.
Eulerian-Lagrangian Analysis (ELA)

- Baptista (1984, 1987)
- Uses “quadratic” triangles
- Split-operator approach
  - Method of characteristics (advection)
  - FEM (diffusion/reaction)
- Puff routine
- Ideal with periodic HM input
Method of Characteristics

- Backward tracking of characteristic lines
- Interpolation among nodes at feet of characteristics
- Avoids difficulties with advection-dominated flows

Baptista et al. (1984)
Diffusion

- Diffusion/simple reaction uses implicit Galerkin FEM under stationary conditions
- No stability limit on $\Delta t$
- Not intrinsically mass conserving
- Linearity facilitates source/receptor calculations

Baptista et al. (1984)
ELA-Basic Equation

\[ \frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = \frac{1}{h} \frac{\partial}{\partial x_i} \left( hD_{ij} \frac{\partial c}{\partial x_j} \right) + Q \]

Advection      Dispersion      Reaction

\[ \frac{\partial c}{\partial t} + u_i^* \frac{\partial c}{\partial x_i} = D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} + Q \]

\[ u_i^* = u_i - \frac{1}{h} \frac{\partial}{\partial x_j} (hD_{ij}) \]

Baptista et al. (1984)
Operator Splitting

\[
\frac{\partial c}{\partial t} + u_i^* \frac{\partial c}{\partial x_i} = D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} + Q
\]

\[
\frac{c^{n+} - c^n}{\Delta t} + \left\{ u_i^* \frac{\partial c}{\partial x_i} \right\}_n = 0
\]

\[
\frac{c^{n+1} - c^{n+}}{\Delta t} = \left\{ D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} \right\}_{n+1} + \left\{ Q \right\}_{n+1}
\]
Puff Algorithm

- Gaussian puffs distributed backwards in time over near field
- Advected/diffused over intermediate field
- Projected to grid after sufficient diffusion (hybrid model)
- Or, self-contained model (Transient Plume Model)
Lagrangian Models

Particle Models

Forward Puffs

Backward Puffs

Figure by MIT OCW.

Israelsson et al. (2006)
Hybrid Random Walk Particle Tracking/Grid Based Model

Use finer grid to visualize intermediate-field concentrations

Project particles onto OGCM grid

far-field concentrations
Application to Larval Entrainment at Coastal Power Plants

- Millstone Station on Long Island Sound
- Winter flounder larvae entrained at station intakes
- How many, what age, what proportion of local & LIS populations?
2-D Simulations

Each larva may:

- die or mature
- be entrained
- be flushed

\[
\Delta x_i = \left[ u + \frac{\partial E_x}{\partial x} + \frac{E_x}{h \partial x} \right] \Delta t
+ \sqrt{2E_x \Delta t p_i + S / S}
\]

\[
\Delta y_i = \left[ v + \frac{\partial E_y}{\partial y} + \frac{E_y}{h \partial y} \right] \Delta t
+ \sqrt{2E_y \Delta t p_i + S / S}
\]

Dimou and Adams (1989)
Dye study calibration

- Dye released at Niantic River mouth
- ~20% recovered at station intake
- Accounting for mortality ~17% of larvae exiting Niantic R are being entrained

Dimou and Adams (1989)
Entrained larval lengths (10^6): observed Vs simulated

Conclusion: most larvae imported (Connecticut and Thames Rivers)

Supported by studies using Mitochondrial DNA and trace metal accumulation

Dimou et al. (1990)
Contemporary Issues in Surface Water Quality Modeling

- Open boundary conditions
- Inverse modeling
- Data assimilation: integrating data and model output
- Problems of spatial scale: interfacing near and far field models
- Problems of time scale: coupling hydrodynamic and water quality models
Model Performance Evaluation
aka verification, validation, confirmation, quantitative skill assessment, etc.

Who is evaluating?

- **Model Developer**
  - Evaluates whether simulated processes matches real world behavior

- **Model User**
  - Output-oriented
  - Ability to accurately simulate conditions at specific location(s) under variety of extreme and design conditions

- **Decision makers**
  - Reliability, cost-effectiveness
Model Performance Evaluation*

- Problem Identification
- Relationship of model to problem
- Solution scheme examination
- Model response studies
- Model calibration
- Model validation

*Ditmars, et al., 1987,
Model Performance Evaluation*

- Natural System
- Conceptual Model
- Algorithmic Implementation
- Software Implementation

*Dee, 1995
Problem Identification

What are the important processes and what are their space and time scales?

Ex: If biogeochemical transformations are quicker than the hydraulic residence time, then perhaps steady state is OK
Relationship of model to problem

- Does model do what you concluded was important?
- Direct simulation or parameterization?
- Are data adequate to resolve the processes, initial conditions and boundary conditions?
Solution scheme examination

- Is scheme consistent with differential equations?
- Are mass, vorticity, etc. preserved?
- Choice of grid scheme, time and space steps as they affect stability and accuracy.
- Is model well documented?
Model response studies

- Does model behave as expected for simple cases?
- Does model match analytical solutions (some call this and previous step verification, connoting truth)
- Provides sensitivity to be used in model calibration.
Model calibration

- Best model fit against a known data set.
- Make sure output is appropriate
  - tidal currents vs amplitude
  - residual vs instantaneous currents
- Only tweak appropriate input parameters/coefficients.
  - physically relevant
  - those requiring least change relative to expected range of variation.
Model validation

- Comparison against independent data set (or a different period of time) without changing model parameters/coefficients.
- Choice of appropriate metrics (mean error, rms error, etc).
- Perfect agreement not possible; but are results believable? (Validity connotes legitimacy)
- Oreskes et al. (1994) refers to model confirmation
Additional Comments

- **Absolute vs Relative accuracy**
  - Latter is easier as uncertainties may cancel when comparing options under same conditions

- **Uncertainty (as measured by output variation) during sensitivity tests**
  - Usually underestimated because of unknown unknowns

- **Generic versus site-specific models**
  - Will model be used at different site?
Additional Comments

 Purpose of models is insight

 - they book keep what we already think we know