Predictions in Environmental Hydrodynamics Using the Finite Element Method I. Theoretical Development

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Differential equation descriptions for specific three-dimensional environmental hydrodynamical flowfields are established. The parabolic Navier-Stokes system is applicable to predominant direction steady flowfields. An integral transform formulation of the transient Navier-Stokes system is applicable to recirculating flowfields in lakes, rivers, and tide water regions. A finite element numerical solution algorithm is established for each of these developed systems including complete nonlinearity and tensor turbulent transport phenomena. The algorithm directly utilizes nonuniform computational meshes and nonregular solution domain closures, upon which boundary condition constraints may be readily applied.

Nomenclature

a = boundary coefficient
A = coefficient; area; one-dimensional matrix prefix
b = boundary coefficient
B = body force; coefficient; two-dimensional matrix prefix
c = specific heat
D = binary diffusion coefficient; determinant
Ec = Eckert Number
f = Coriolis force; function of known argument
F = Coriolis force
Fr = Froude Number
g = gravity constant; function of known argument
h = static enthalpy; cross-sectional depth
H = stagnation enthalpy
k = thermal conductivity
K = shear stress constant; generalized diffusion tensor
l = length
L = reference length; functional
m = mass flow
M = total finite elements of the discretization
n = unit normal vector; dimensionality of finite element space; nodes per finite element
N = differential operator
p = static pressure
Pr = Prandtl Number
q = generalized dependent variable
Q = transformed generalized dependent variable
r = position vector
R = shear Reynolds number; solution domain
Re = Reynolds Number
S = mass source term
Sc = Schmidt Number
t = time; thickness of finite element
T = temperature
u = velocity
U = velocity
x_i = Cartesian coordinate system
x, y, z = Cartesian reference basis
Y = mass fraction
α = direction cosine
β = inverse sidereal day
δ = Kronecker delta; small parameter
Δ = increment
∂R = closure of solution domain
ε = eddy viscosity; unit vector
η = surface description; differential operator
$\dot{\theta}$ = angular velocity
κ = coefficient
λ = multiplier
ν = effective or kinematic viscosity
ξ = surface description
ρ = density
σ = surface integral kernel
τ = shear stress; domain integral kernel
ϕ = latitude; shear function
Φ = dissipation function
χ = initial value differential operator
Ψ = streamfunction
Ω = vorticity
{ } = column matrix
[ ] = matrix

Superscripts and Subscripts

$*$ = reference value; approximate solution
$'$ = scalar components after coordinate transformation; ordinary derivative
e = effective value
w = at the boundary
α = species
$\hat{}$ = unit vector
$\tilde{}$ = stress reference value
$\bar{}$ = constrained to domain closure
i, j, k, l = tensor indices
m = pertaining to mth subdomain (finite element)
o = initial reference value
T = turbulent reference parameter; matrix transpose
∞ = reference condition
$,i$ = derivative

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Introduction

AN accurate prediction capability for the complex flows characteristic of environmental hydrodynamics is required to evaluate fully the ecological impact of man's design and construction decisions upon coastal and inland waterways. For example, a river or lake can no longer be considered an infinite sink for thermal or waste water discharge, since such negligent action is amply proved to unbalance the contained ecosystem and destroy the usefulness of the waterway as anything other than a sewer. The complexity of such flows has generally hindered application of detailed analytical and/or numerical analysis techniques to model the complete flow systems. Instead, complex and expensive hydrodynamically scaled flow models have been utilized to perform parameter studies, and field measurements have provided "after the fact" data. The development of an accurate theoretical flow model for environmental systems, and reduction of theory to practice within a viable computer program system capable of readily simulating the nonregularity of practical flow geometries, would provide a valuable research and analysis tool. The capability to theoretically predict turbulent dispersion of pollutants in estuaries and rivers should provide insight into the fundamental mechanisms of natural hydrodynamical transport. Numerical predictions also could provide detailed information on shear stress distributions on natural or artificial containment devices, and thus provide the engineer with important design criteria.

The problem class to which these problems belong mathematically is governed by the transient, three-dimensional Navier-Stokes equations. Rarely is solution of this system of initial-valued, nonlinear elliptic boundary value equations either attempted or required. Several levels of approximation are available to render solutions for specific problem categories considerably more tractable. The parabolic Navier-Stokes system is applicable to three-dimensional steady flows characterized by a predominant flow direction. The system includes the conventional boundary-layer equations as a subset. Numerical results for pollutant dispersion in two-dimensional estuaries using "law of the wall and wake" boundary-layer velocity profiles have been reported.[1] The employment of a boundary-layer similar solution, for thermal waste discharge into a river has been explored.[2] Observations verifying the requirement for a more rigorous accounting of dispersion in the transverse plane, than can be obtained using boundary-layer concepts, have been reported,[3] as well as the need to account for the nonisotropy of the diffusion coefficient.[4] The influence of the surface wind shear load on scalar dispersion has been shown to be important.[5] A second simplification, that is applicable to nontrivial problems, is to apply an integral transform to the full Navier-Stokes equations that averages behavior over one dimension, and retains the transient description. For this case, recirculation regions in the flow can be computed. No general results are reported but exploratory concepts have been evaluated.[6–7] The influence of stream meandering and depth distribution on scalar dispersion has been studied.[8]

Even with these simplifications, solution of the resultant nonlinear equation systems represents a formidable task, due in large part to the irregularity of the solution domain closure and the need to apply complex combinations of boundary conditions on these surfaces. The finite element method has been employed for many years for solution of linear boundary value problems, particularly in structural mechanics, and the ease with which complex boundary specifications can be handled is a distinct feature. Recent developments have rendered the finite element technique of numerical solution applicable to a much broader problem class including the Navier-Stokes equations. Solutions have been reported for simple two-dimensional,[9,10] as well as transient flows[11] for an incompressible fluid. Extension to compressible two-dimensional flows has also been documented.[12] Solutions for a class within the parabolic Navier-Stokes for binary turbulent mixing in supersonic compressible flow are published.[13]

In all cases, the governing differential equation systems retain their nonlinear elliptic boundary value character. This paper presents the theoretical development of the finite element solution procedure for the general problem class, including complete nonlinearity and generalized tensor turbulent transport coefficient distributions for all dependent variables, for the transient and parabolic Navier-Stokes equations for multiple-species flows of environmental character. Both solutions are adapted to accept a solution domain with variable cross-sectional depth, as occurs in natural waterways, as well as the effects of the Coriolis body force. Numerical solutions illustrating the versatility of the analysis procedure for practical problems are reported in Part II.

Differential Equation Systems Governing Three-Dimensional Environmental Hydrodynamics

The description of the state point in hydrodynamics is contained within the solution of a system of coupled nonlinear second-order partial differential equations enforcing local conservation of species mass, total mass, linear momentum, and energy. Closure of this system requires identification of constitutive laws; for laminar flow, transport properties such as viscosity and thermal conductivity are describable in terms of molecular behavior. For turbulent flows, the time-averaged Navier-Stokes equation system appears similar to the laminar flow equations after identification of turbulence parameters which are expressed by the kinematics of the flowfield. Assuming a general tensor transport property description, and utilizing Cartesian tensor notation with summation over repeated indices (unless underscored), the three-dimensional Navier-Stokes equations for an incompressible fluid take the form

$$0 = u_{k,k} \tag{1}$$

$$u_{j,t} = -\left[u_k u_j - \frac{p}{\rho}\delta_{jk} - \frac{1}{Re}\tau_{jk}\right]_{,k} + \frac{1}{Fr}B_j \tag{2}$$

$$H_{,t} = -\left[u_k H - \frac{Ec}{Re}\tau_{ik}u_i - \frac{1}{Re\,Pr}\nu_{ik}{}^e H_{,i}\right]_{,k} + Ec\frac{p_{,t}}{\rho} \tag{3}$$

$$Y^\alpha_{,t} = -\left[u_k Y^\alpha - \frac{1}{Re\,Sc}\nu_{ik}{}^e Y^\alpha_{,i}\right]_{,k} + S^\alpha \tag{4}$$

The dependent variables appearing in Eqs. (1–4) have their usual fluid dynamic interpretation with u_i the velocity vector, p the pressure, τ_{ij} the stress tensor, H the stagnation enthalpy, Y^α the mass fraction of the α species, B_i the body force, and S the source term for the α species. The stress-strain-rate law for the generalized description can be written as

$$\tau_{ij} = \nu_{jk}{}^e(u_{i,k}+u_{k,i}) \tag{5}$$

where $\nu_{jk}{}^e$ is the combined effective transport coefficient defined in terms of ν, the laminar kinematic viscosity, as

$$\nu_{jk}{}^e = (\nu\delta_{jk}+\varepsilon_{jk}) \tag{6}$$

where ε_{jk} is the turbulent eddy viscosity tensor. Note that the combination of Eqs. (5) and (6) will reduce to Stokes viscosity law for laminar incompressible flow. The nondimensional groupings of fluid dynamic parameters in Eqs. (1–4) are defined as

$$Re \equiv U_\infty L/\nu^e \tag{7}$$

$$Pr \equiv c\rho\nu^e/k \tag{8}$$

$$Sc \equiv \nu^e/\rho D \tag{9}$$

$$Ec \equiv U_\infty{}^2/cT_\infty \tag{10}$$

$$Fr \equiv U_\infty{}^2/Lg \tag{11}$$

In Eqs. (7–9), ν^e is the magnitude of the effective diffusion coefficient, i.e., the square root of the inner product of Eq. (6), and the nondimensional groupings are algebraic combinations of the effective laminar and turbulent contributions; for example,

$$\nu_{jk}{}^e/Re \equiv \nu\delta_{jk}/Re + \varepsilon_{jk}/Re_T \tag{12}$$

where the subscript, T refers to the turbulent reference parameter. The mass coefficient, D, in Eq. (9) is defined for essentially binary diffusion.

Two simplications to the general Navier-Stokes equation system have been studied for application to problems in environmental hydrodynamics. The parabolic Navier-Stokes equations result for steady flows wherein a predominant flow direction is uniformly discernible and the stress tensor contribution to momentum transport in that direction is negligible. Flows in essentially straight sections of rivers and channels fall into this category. Align the x_1 coordinate with the direction of predominant flow and select the x_3 coordinate to lie in the plane formed by x_1 and the local gravity vector. Constraining summation over repeated indices to 2 and 3, the parabolic Navier-Stokes approximation to the equation system (1–6) is

$$u_1 u_{j,1} = \left[\frac{\nu_{ik}{}^e}{Re}(u_{j,i}+u_{i,j})\right]_{,k} - u_k u_{j,k} - \frac{p_{,j}}{\rho} + \frac{1}{Fr}[\varepsilon_{jik} f_i u_k - g_j] \tag{13}$$

$$u_1 H_{,1} = \left[\frac{\nu_{ik}{}^e}{Re\,Pr}H_{,i}\right]_{,k} - u_k H_{,k} - \Phi \tag{14}$$

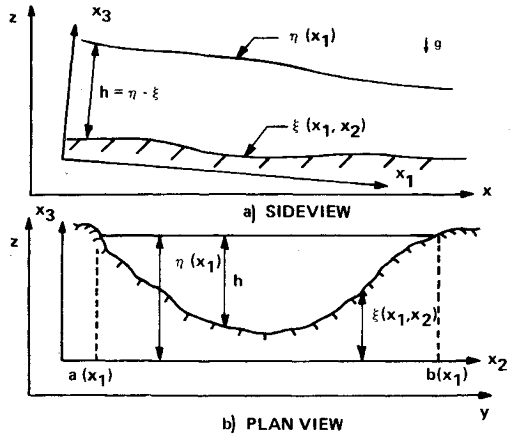

Fig. 1 Definition of waterway coordinate systems.

$$u_1 Y_{,1}^{\alpha} = \left[\frac{\nu_{ik}^{e}}{Re\,Sc} Y_{,i}^{\alpha}\right]_{,k} - u_k Y_{,k}^{\alpha} + S^{\alpha} \tag{15}$$

$$\eta(x_1, x_2) = f(u_{k,k}) \tag{16}$$

In Eq. (13), ε_{jik} is the Cartesian alternating tensor, and the term containing f_i is the Coriolis body force. The viscous dissipation term, Φ is defined as

$$\Phi \equiv \frac{1}{Re}\left[\frac{Ec}{2}\left(\frac{1-Pr}{Pr}\right)\nu_{jk}^{e}(u_i u_i)_{,k} + \left(\frac{Sc-Pr}{Pr\,Sc}\right)\nu_{jk}^{e}\sum_{\alpha} h^{\alpha} Y_{,k}^{\alpha}\right]_{,j} \tag{17}$$

where h^{α} is the static enthalpy of the α species, which is related to the stagnation enthalpy as

$$H \equiv \sum_{\alpha} h^{\alpha} Y^{\alpha} + \tfrac{1}{2} u_k u_k \tag{18}$$

In Eq. (16), $\eta(x_1, x_2)$ is the description of the waterway surface, solution of which is established via the continuity equation. Integrate Eq. (1) over the transverse plane (x_2, x_3), (see Fig. 1), to yield an expression for the total mass flow rate, $m(x_1)$. Considering the general case where mass may be added or subtracted through external sources, e.g., merging of a secondary stream, the integrated continuity equation is given by

$$m_{,1} = \dot{m}^{i} \tag{19}$$

where $\dot{m}^{i}$ is a specified mass addition rate and

$$m(x_1) = \int_{a(x_1)}^{b(x_1)} \int_{\xi(x_1,x_2)}^{\eta(x_1)} \rho u_1 \, dx_3 \, dx_2 \tag{20}$$

It is assumed that $\eta = \eta(x_1)$ is a reasonable approximation for the problems considered, i.e., the river elevation is constant in the x_2 direction. A mass balance across the increment, Δx_1, gives

$$m(x_1 + \Delta x_1) = m(x_1) + \dot{m}^{i} \Delta x \tag{21}$$

The finite element numerical integration algorithm used to compute $m(x_1 + \Delta x_1)$ can be reduced to a form

$$m(x_1 + \Delta x_1) = A \Delta\eta + B \tag{22}$$

where A and B are expressed explicitly in terms of the finite element size, location, and velocity field. The change in η with x_1, $\Delta\eta$, is obtained directly from Eqs. (21) and (22), as

$$\Delta\eta = [m(x_1) + \dot{m}^{i} \Delta x_1 - B]/A \tag{23}$$

The new river height is then estimated from

$$\eta(x_1 + \Delta x_1) = \eta(x_1) + \Delta\eta \tag{24}$$

A second useful simplification to the Navier-Stokes equation system (1–4) exists for hydrodynamical flows in lakes, rivers, and the tide water regions wherein a predominant flow direction does not exist but wave motion is of secondary importance. Assuming the bottom profile of the water body is a prescribed function $\xi(x_i)$ and that $\eta(x_i)$ describes the water surface, integrate Eqs. (1–4) in the x_3 direction parallel to the local gravity vector. Now constraining summation of repeated indices to 1 and 2, applying known boundary conditions at the end points of integration and noting that the Coriolis force is conveniently written as

$$f_i = 2\beta \sin\phi\, \delta_{i3} \tag{25}$$

where ϕ is latitude and β is an inverse day, the integral transformation of three-dimensional Navier-Stokes equations for isoenergetic flow takes the form

$$\int_{\xi}^{\eta} [u_{k,k}] \, dx_3 = -u_3(\eta) \tag{26}$$

$$\int_{\xi}^{\eta} \left\{ u_{1,t} + u_k u_{1,k} - \frac{1}{Fr}\left(f u_2 - \frac{1}{\rho} p_{,1}\right) - \left[\frac{\nu_{jk}^{e}}{Re}(u_{1,j} + u_{j,1})\right]_{,k} \right\} dx_3 = \frac{\nu_{j3}^{e}}{Re} u_{1,j}\Big|_{\xi}^{\eta} + \frac{\nu_{33}^{e}}{Re} u_{1,3}\Big|_{\xi}^{\eta} - u_3 u_1(\eta) \tag{27}$$

$$\int_{\xi}^{\eta} \left\{ u_{2,t} + u_k u_{2,k} + \frac{1}{Fr}\left(f u_1 + \frac{1}{\rho} p_{,2}\right) - \left[\frac{\nu_{jk}^{e}}{Re}(u_{2,j} + u_{j,2})\right]_{,k} \right\} dx_3 = \frac{\nu_{j3}^{e}}{Re} u_{2,j}\Big|_{\xi}^{\eta} + \frac{\nu_{33}^{e}}{Re} u_{2,3}\Big|_{\xi}^{\eta} - u_3 u_2(\eta) \tag{28}$$

$$\int_{\xi}^{\eta} \left\{ u_{3,t} + u_k u_{3,k} - \left[\frac{\nu_{jk}^{e}}{Re}(u_{3,j} + u_{j,3})\right]_{,k} \right\} dx_3 = -\left(\frac{p}{\rho} + gz\right)\Big|_{\xi}^{\eta} + \frac{\nu_{i3}^{e}}{Re} u_{3,i}(\eta) - u_3 u_3(\eta) \tag{29}$$

$$\int_{\xi}^{\eta} \left\{ Y_{,t}^{\alpha} + u_k Y_{,k}^{\alpha} - \left[\frac{\nu_{jk}^{e}}{Re\,Sc} Y_{,j}^{\alpha}\right]_{,k} - S^{\alpha} \right\} dx_3 = \frac{\nu_{i3}^{e}}{Re\,Sc} Y_{,i}^{\alpha}\Big|_{\xi}^{\eta} \tag{30}$$

In establishing Eqs. (26–30), at $x_3 = \xi(x_1, x_2)$, the velocity vector vanishes while at the water surface, $x_3 = \eta(x_1, x_2)$, the u_3 component of velocity is established as

$$u_3 = x_{3,t} = u_1 \eta_{,1} + u_2 \eta_{,2} \tag{31}$$

For a large number of practical hydrodynamical flows, the hydrostatic approximation for pressure is valid. This occurs for all terms in Eq. (29) vanishing except for the exact integral balance of pressure and the gravity body force. Assuming u_1 and u_2 and the derivatives in the corresponding directions are of order unity, this balancing occurs for u_3 and derivatives on x_3 being of order $\delta \ll 1$. Referring to Eq. (31), the x_1 and x_2 derivatives of the surface η must also be of order δ. For this simplification, Eq. (29) can be directly integrated to yield

$$p = \rho g[\eta(x_1, x_2) - x_3] + p_o \tag{32}$$

where p_o is atmospheric pressure, at the surface $\eta(x_1, x_2)$. Equation (32) can then be differentiated to obtain the required derivatives of pressure as

$$1/\rho\, p_{,1} = g\eta_{,1} \tag{33}$$

$$1/\rho\, p_{,2} = g\eta_{,2} \tag{34}$$

The desired computational form for the parent differentiation equation system occurs for definition of a new set of dependent variables. Considering Q as a generalized dependent variable, identify

$$Q \equiv \int_{\xi}^{\eta} q \, dx_3 \tag{35}$$

Using Liebnitz' formula, a scalar component of the gradient of Q takes the form

$$Q_{,i} = \int_{\xi}^{\eta} q_{,i} \, dx_3 + q(\eta)\eta_{,i} - q(\xi)\xi_{,i} \tag{36}$$

Using Eqs. (36) and (31), the continuity equation (26) for this three-dimensional flow becomes transformed to the conventional two-dimensional form as

$$U_{1,1} + U_{2,2} = U_{i,i} = 0 \tag{37}$$

Therefore, in the integral transform (capitalized) variables, the velocity field is divergenceless in the two scalar components of velocity normal to the local gravity vector. This in turn allows specification of a vector potential function with a single scalar component which automatically ensures conservation of mass as

$$U_i \equiv \varepsilon_{3ik} \Psi_{,k} \tag{38}$$

where Ψ is the integral transform two-dimensional streamfunction. Having Eq. (38), it remains to define the curl of the velocity vector to completely specify the velocity field. Neglecting terms involving u_3 and derivatives by 3, combine Eqs. (27) and (28) into a single vector equation of the form

$$U_{j,t}+(U_k U_j)_{,k} = g(\eta-\xi)\eta_{,j}-\varepsilon_{3jk}(fU_k)+\frac{1}{Re}[v_{ik}{}^e(U_{j,k}+U_{k,j})]_{,i}+\frac{v_{i3}{}^e}{Re}U_{j,i}\Big|_\xi^\eta \quad (39)$$

Upon identifying the x_3 scalar component of the vorticity vector potential function as,

$$\Omega \equiv \varepsilon_{3ik} U_{k,i} \quad (40)$$

the curl of Eq. (39) can be directly written as

$$\Omega_{,t}+(U_k\Omega)_{,k} = -(fU_k)_{,k}+g\varepsilon_{3ij}\eta_{,j}(\eta-\xi)_{,i}+\frac{1}{Re}[v_{kj}{}^e\Omega_{,j}-v_{kl,j}{}^e\Psi_{,jl}]_{,k}-\frac{1}{Re}[v_{,ik}(\Omega\delta_{ik}+\Psi_{,ik})]+\varepsilon_{3ik}\left[\left(\frac{v_{j3}{}^e}{Re}U_{k,j}\right)\Big|_\xi^\eta\right]_{,i} \quad (41)$$

Upon expanding the term involving gravity, obtain

$$g\varepsilon_{3ij}\eta_{,j}(\eta-\xi)_{,i} = g\varepsilon_{3ij}(\eta_{,i}\xi_{,j}) \quad (42)$$

Substituting Eq. (38) for the terms involving velocity, the required equation cast entirely in terms of computational variables and parameters becomes

$$\Omega_{,t} = \varepsilon_{3ik}\left[(\Omega\Psi_{,i})_{,k}+g\eta_{,i}\xi_{,k}-\frac{1}{Fr}\Psi_{,k}f_{,i}\right]+\frac{1}{Re}[(v_{kl}{}^e\Omega_{,l}+v_{kl,j}{}^e\Psi_{,jl})_{,k}-v_{,ik}(\Omega\delta_{ik}+\Psi_{,ik})]+\frac{\varepsilon_{3ik}}{Re}[v_{j3}{}^eU_{k,j}]_{,i}\Big|_\xi^\eta \quad (43)$$

The nonviscous contributions to vorticity generation, Eq. (43), are respectively the convection of vorticity, pressure contributions due to variations in waterway profile, and the curl of the Coriolis force. The final term accounts for shear loads impressed upon the solution domain by the bottom contour and the wind load at the surface.

Solution of the hydrodynamic flowfield is completed by combining Eqs. (38) and (40) to yield the vorticity-streamfunction compatibility equation

$$-\Omega = \Psi_{,kk} \quad (44)$$

Finally, solution of Eq. (30) for mass fraction is directly transformed to terms involving the computational variables as

$$Y_{,t}^\alpha = \varepsilon_{3ik}(Y^\alpha\Psi_{,i})_{,k}+S^\alpha+\left[\frac{v_{kl}{}^e}{Re\,Sc}Y_{,k}^\alpha\right]_{,l}+\frac{v_{i3}{}^e}{Re\,Sc}Y_{,i}^\alpha\Big|_\xi^\eta \quad (45)$$

where Y^α defined in Eq. (45) is the integrated variable defined by Eq. (35).

The original three-dimensional equation system, Eqs. (1), (2), and (4), has thus been transformed via Eq. (35), to solution of the two-dimensional incompressible flow equations cast in terms of integral-transform streamfunction and vorticity, Eqs. (43–45). Closure of this system requires specification of the turbulent eddy viscosity tensor, $v_{kl}{}^e$, and a modeling of the contribution to vorticity stemming from shear loads applied at the surfaces, η and ξ, Eq. (43). Some clarification occurs for a scalar turbulent eddy viscosity. In this instance, $v_{kl}{}^e$ becomes $v^e\delta_{kl}$, and the lead viscosity term in Eq. (43) becomes

$$[v_{kl}{}^e\Omega_{,l}+v_{kl}{}^e\Psi_{,jl}]_{,k} = (v^e\Omega_{,k})_{,k}+v_{,k}{}^e\Omega_{,k}-v_{,ij}{}^e\Psi_{,ij} \quad (46)$$

Similarly, neglecting spatial variations in $v_{j3}{}^e$, a clarification of the shear load term in Eq. (43) accrues by completing the differentiation to yield

$$\phi(v^e, U_k, \eta, \xi) \equiv \frac{v_{j3}{}^e}{Re}\Omega_{,j}\Big|_\xi^\eta \quad (47)$$

At the surface η, Eq. (47) provides a means for modeling the wind shear applied to the surface of the body of water. Since circulation in many large water bodies is predominantly wind driven, an accurate modeling of Eq. (47) is of paramount importance. At the surface, the vorticity of the wind is simply $\dot{\theta}$, the local angular velocity. An approximation for the wind shear function ϕ, is then

$$\phi(\eta) = \frac{v^a}{Re\,l_\theta}\left[\dot{\theta}-\frac{\Omega}{(\eta-\xi)}\right] \quad (48)$$

where v^a is the turbulent (or laminar) viscosity of the air, the square bracket contains the average difference between the angular velocities of the air and the water, and l_θ is an empirically determined measure of the mean distance over which the frequency difference occurs. At the surface ξ, the function, $\phi(\xi)$, measures the mean dissipation of vorticity due to interaction of the motion of the water over the bed and is directly related to the cross stream gradient of the shear stress. The approach of Patankar and Spalding[14] is suggested to evaluate empirically the shear stress in terms of a Reynolds number, R, as

$$\tau = K^2\rho\tilde{U}^2(R_*{}^{-1}-0.1561R_*{}^{-0.45}+0.08723R_*{}^{-0.3}+0.03713R_*{}^{-0.18}) \quad (49)$$

where K is an empirical constant (equal to 0.435), $R_* = K^2R$ and $R = \tilde{U}\tilde{x}_3/v$. The length scale $\tilde{x}_3$ represents the thickness of the narrow region just above the waterway floor where convective flow effects are negligible, i.e., the constant shear stress region. Similarly, $\tilde{U}$ represents the streamwise velocity component at the edge of the constant shear region. Values for $\tilde{U}$ and $\tilde{x}_3$ are obtained by assuming the streamwise velocity may be expressed by a similarity profile, e.g., for turbulent flows a logarithmic velocity distribution with the van Driest laminar damping factor employed. The vorticity dissipation function at the surface $\xi(x_1, x_2)$ then becomes

$$\phi(\xi) = \tau/Re \quad (50)$$

It remains to establish the boundary conditions for these developed equation systems. No confusion exists for the parabolic Navier-Stokes system, since solutions are determined in physical variables. At points of injection, the velocity vector, U_j, stagnation enthalpy, H, and species mass fractions, Y^α, are directly specified. The riverbed is typically impervious to both H and Y^α, hence the normal gradient would vanish, as would the velocity vector itself. At the interface with the atmosphere, the normal gradient of all dependent variables would vanish. It is necessary to derive equivalent boundary condition statements for streamfunction and vorticity in the integral-transform Navier-Stokes system. The vorticity equivalent of a no-slip wall is obtained from Eq. (44). In the near vicinity of an impervious boundary, Eq. (44) can be approximated as an ordinary differential equation relating differential coupling in the direction normal to the surface. Integrating this equation twice,[12] the vorticity at the wall is related to the near-vicinity streamfunction distribution as

$$\Omega_w = -\left[\frac{3(\Psi-\Psi_w)}{l^2}+\frac{\Omega}{2}\right] \quad (51)$$

In Eq. (51), the subscript w refers to values at the wall, while the remaining variables are evaluated at an interior point lying a distance l from the wall. From its basic definition, Eq. (44), streamfunction measures the mass flux across a boundary. The change in streamfunction is simply the velocity perpendicular to the boundary times the flow cross-sectional area, A; hence

$$\Delta\Psi = AU_{in} \quad (52)$$

If the detailed velocity distribution is unknown, as at outflow for example, the vanishing normal gradient of streamfunction is appropriate if the flow is approximately parallel. On an impervious boundary, streamfunction is a constant.

Finite Element Solution Algorithm

The developed parabolic- and integral-Navier-Stokes equation systems governing three-dimensional hydrodynamical flows, are uniformly initial-boundary value problems of mathematical physics, i.e., each of the partial differential equations, Eqs. (13),

Table 1 Coefficients in generalized equation for parabolic Navier-Stokes

Eq. No.	q	k	K_{ij}	f	g
(13)	u_j	Re^{-1}	$v_{ik}{}^e$	$-u_k u_{j,k} - \frac{1}{\rho} p_{,j} + \frac{1}{Fr}[\varepsilon_{jik} f_i u_k - g_j]$	$u_1 u_{j,1}$
(14)	H	$(Re\,Pr)^{-1}$	$v_{ik}{}^e$	$-u_k H_{,k} - \Phi$	$u_1 H_{,1}$
(15)	Y^α	$(Re\,Sc)^{-1}$	$v_{ik}{}^e$	$-u_k Y_{,k}{}^\alpha + S^\alpha$	$u_1 Y_{,1}{}^\alpha$

(14), (15), (43), (44), and (45), is a special case of the general second-order, nonlinear partial differential equation

$$N(q) \equiv \kappa[K_{ij}(q)q_{,i}]_{,j} + f(q, q_{,i}, x_i) - g(q, \chi) = 0 \tag{53}$$

where q is a generalized dependent variable identifiable with each computational dependent variable. In Eq. (53), f and g are specified functions of their arguments, wherein χ is identified with x_1 or t, respectively, for the parabolic- and integral-descriptions, and x_i are coordinates for which second-order derivatives exist in the lead term. In Eq. (53), $N(q)$ is assumed uniformly parabolic within a bounded open domain R, i.e., the lead term in Eq. (53) is assumed uniformly elliptic within its domain R, with closure ∂R, where

$$R = Rx(\chi_o, \chi) \tag{54}$$

wherein $\chi_o \leqq \chi < \infty$. Table 1 lists the functions f and g, as well as the appropriate parameters, for Eq. (53) identified with the parabolic Navier-Stokes equations. Table 2 contains similar information for the integral description.

Since Eq. (53) is assumed uniformly parabolic, unique solutions are obtained after specification of boundary constraints on ∂R. The most general form relates the function and its normal derivative everywhere on the closure as

$$\eta(q) \equiv a^{(1)}(\bar{x}_i, \chi) q(\bar{x}_i, \chi) + a^{(2)} K_{ij} q(\bar{x}_i, \chi)_{,i} n_j - a^{(3)}(\bar{x}_i, \chi) = 0 \tag{55}$$

In Eq. (55), the $a^{(i)}(\bar{x}_i, \chi)$ are user-specified coefficients, the superscript bar notation constraints x_i to ∂R, and n_k is the local outward pointing unit normal vector. For g nonvanishing in Eq. (53), an initial distribution is also required; hence, assume given throughout R and on ∂R at the initial station χ_o,

$$q(x_i, \chi_o) = q_o(x_i) \tag{56}$$

Formation of the finite element solution for both Navier-Stokes equation systems is thus obtained by establishing the algorithm for the equation system (53–56). The theoretical foundation is the method of weighted residuals (MWR) applied on a local basis.[11,12] Since Eq. (53) is valid throughout R, it is valid within disjoint interior subdomains R_m called "finite elements," wherein the aggregate sum of R_m is the domain R. Form an approximate solution to q within R_m, called $q_m{}^*(x_i, \chi)$, by expansion into a series solution of the form

$$q_m{}^*(x_i, \chi) \equiv \{L(x_i)\}^T \{Q(\chi)\}_m \tag{57}$$

wherein the functionals $L_k(x_i)$ are members of a function set complete in R_m, and the unknown expansion coefficients, $Q_k(\chi)$, represent the χ-dependent values of $q_m{}^*(x_i, \chi)$ at specific points called "nodes," interior to R_m and on the closure, ∂R_m. Equation (57) is a scalar, and introduces the column matrix notation and its transpose (superscript T), and the method of selection of the L_k is user specifiable and may be problem class dependent. To establish the values taken by the expansion coefficients in Eq. (57), require that the local error in the approximate solution to both the differential, $N(q_m{}^*)$, and the boundary condition statement, $\eta(q_m{}^*)$, if applicable (i.e., a boundary segment of the finite element, ∂R_m coincides with the global solution domain boundary ∂R) be orthogonal to the functional set in Eq. (57). This is accomplished by enforcing the local variant of Galerkin criterion of classical MWR, and integration over the respective domains. Employing an unknown multiplier, λ, these equation sets can be combined to give the constraint equation system

$$\int_{R_m} \{L(x_i)\} N(q_m{}^*) d\tau - \lambda \int_{\partial R_m} \{L(x_i)\} \eta(q_m{}^*) d\sigma \equiv 0 \tag{58}$$

The number of Eq. (58) is identical to the number of node points of the finite element, R_m, i.e., the number of elements in the column matrix $\{Q(\chi)\}_m$.

Equation (58) forms the basic operation within the finite element solution procedure. Establishment of the global solution algorithm, and determination of λ, is accomplished by evaluating Eq. (58) in each of the M finite elements of the discretized solution domain, R, and column-wise addition of these $M \times n$ equations into a global matrix system. The rank of the global system is less than $M \times n$ by connectivity of the finite element domains as well as those boundary condition statements on ∂R where the term $a^{(2)}$ in Eq. (55) vanishes identically. The lead term in Eq. (53) can be integrated by parts to yield

$$\int_{R_m} \{L(x_i)\} \kappa [K_{ij} q_{m,i}{}^*]_{,j} d\tau = \kappa \oint_{\partial R_m} \{L(x_i)\} K_{ij} q_{m,i}{}^* n_j d\sigma - \kappa \int_{R_m} \{L(x_i)\}_{,j} K_{ij} q_{m,i}{}^* d\tau \tag{59}$$

For ∂R_m intersecting ∂R, Eq. (59), the corresponding segment of the closed surface integral will cancel the boundary condition contribution, Eq. (58), by identifying $\lambda a^{(2)}$ with κ of Eq. (53). The contributions from the closed surface integral, Eq. (59), where ∂R_m does not intersect ∂R can be made to vanish (Ref. 12). Hence, combining Eqs. (53–59), the globally assembled finite element solution algorithm for the representative partial differential equation system description for the Navier-Stokes equations becomes

$$\sum_m \left[-\kappa \int_{R_m} \{L\}_{,j} K_{ij} q_{m,i}{}^* d\tau + \int_{R_m} \{L\} (f_m{}^* - g_m{}^*) d\tau - \kappa \int_{\partial R_m} \{L\} [a_m{}^{(1)} q_m{}^* - a_m{}^{(3)}] d\sigma = \{0\} \right] \tag{60}$$

where it is understood that the surface integral contribution has meaning only when ∂R_m coincides with ∂R.

The rank of the global equation system (60) is identical to the total number of node points within the solution domain R, and on the closure ∂R, at which the dependent variable requires solution. Equation (60) is either a first-order ordinary differential or algebraic equation system dependent upon whether the term g, in Eq. (53), vanishes identically. In either event, the equation system is large order and the matrix structure is sparse and banded, with bandwidth a function of both selected discretization and the order of the employed approximation function, Eq. (57). Solution of the algebraic system can be obtained by direct inverse or equation solver techniques. The ordinary differential equation solution can be directly obtained using an appropriate numerical integration algorithm.

Table 2 Coefficients in generalized equation for integral Navier-Stokes

Eq. No.	q	k	K_{ij}	f	g
(43)	Ω	$(Re)^{-1}$	$v_{kl}{}^e$	$\varepsilon_{3ik}\left[(\Omega\Psi_{,i})_{,k} + g\eta_{,i}\xi_{,k} - \frac{1}{Fr}\Psi_{,k} f_{,i}\right] + \phi + \frac{1}{Re}[(v_{kl,j}{}^e \Psi_{,jl})_{,k} - v_{,ik}(\Omega\delta_{ik} + \Psi_{,ik})]$	$\Omega_{,t}$
(44)	Ψ	1	1	$-\Omega$	0
(45)	Y^α	$(Re\,Sc)^{-1}$	$v_{kl}{}^e$	$\varepsilon_{3ik}(Y^\alpha \Psi_{,i})_{,k} + \frac{1}{(Re\,Sc)} v_{i3}{}^e Y_{,i}{}^\alpha \Big\vert_\xi^\eta + S^\alpha$	$Y_{,t}{}^\alpha$

Finite Element Matrix Generation

Implementation of the finite element theory into a computer code involves evaluation of Eq. (60) for the required dependent variables, hence evaluation within each finite element of the

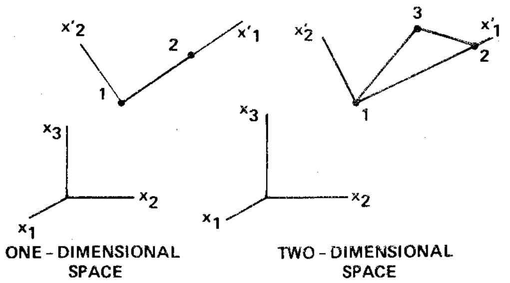

Fig. 2 Intrinsic finite element domains for simplex approximation functions.

discretized solution domain. Use of finer discretizations employing linear (simplex) approximation functionals, Eq. (57) aids conceptual clarity. The intrinsic finite element shapes for one- and two-dimensional spaces, spanned by simplex functionals, are the line and triangle, see Fig. 2. Accurate determination of the element matrices of Eq. (60) is mandatory, and involves evaluation of various-order moment distributions over the domain of the finite element. Simplex natural coordinate functions are suggested[15]; they are a linearly dependent set of normalized functions that are orthogonal to the respective closure segments of the finite element domain. For an n-dimensional space, there are $n+1$ simplex natural coordinate functions. Table 3 contains the implicit definition of these functions in their respective spaces. The natural coordinate functions vanish at all node points of the finite element except one where the value is unity; hence, these functions are the elements of the approximation functional matrix, $\{L\}$, Eq. (57). Integration of arbitrary-order products of scalar components of the $\{L\}$, over the domain of the finite element, are analytically evaluable in terms of the exponent distribution, Table 4.

Both Navier-Stokes equation descriptions require moment generation in Euclidean space spanned by a rectangular Cartesian basis. All computations are performed in the local (primed) coordinate system, Fig. 2, defined by the tensor transformation law

$$x_i' = \alpha_{ij} x_j + r_i \tag{61}$$

Table 3 Implicit definition of simplex natural coordinate functions

Dimensions	Element	Nodes	Natural Coordinate Definition[a]
1	Line	2	$\begin{bmatrix} 1 & 1 \\ x_1^{(1)} & x_1^{(2)} \end{bmatrix} \begin{Bmatrix} L_1 \\ L_2 \end{Bmatrix} = \begin{Bmatrix} 1 \\ x_1 \end{Bmatrix}$
2	Triangle	3	$\begin{bmatrix} 1 & 1 & 1 \\ x_1^{(1)} & x_1^{(2)} & x_1^{(3)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} \end{bmatrix} \begin{Bmatrix} L_1 \\ L_2 \\ L_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ x_1 \\ x_2 \end{Bmatrix}$

[a] Superscripts in parentheses refer to node number.

Table 4 Integrals of natural coordinate function products over finite element domains

Dimensions	Integrals[a]
1	$\int_R L_1^{n_1} L_2^{n_2}\, d\sigma = D \dfrac{n_1!\, n_2!}{(n+n_1+n_2)!}$
2	$\int_R L_1^{n_1} L_2^{n_2} L_3^{n_3}\, d\tau = D \dfrac{n_1!\, n_2!\, n_3!}{(n+n_1+n_2+n_3)!}$

[a] D = Determinant of coefficient matrix defining the natural coordinate system, see Table 3.
n = Dimensionality of the finite element space.

Table 5 Standard finite element matrix forms for simplex functionals in two-dimensional space

Matrix Name	Matrix Function	Matrix Evaluation
$\{B10\}$	$\int_{R_m} \{L\}\, d\tau$	$\dfrac{A^m t^m}{3} \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}$
$[B11]$	$[L]_{,k}$	$\begin{bmatrix} L_{1,1} & L_{2,1} & L_{3,1} \\ L_{1,2} & L_{2,2} & L_{3,2} \end{bmatrix}$
$\{B11\}$	$\{L\}_{,k}$	$\hat{\varepsilon}_1 \begin{Bmatrix} L_1 \\ L_2 \\ L_3 \end{Bmatrix}_{,1} + \hat{\varepsilon}_2 \begin{Bmatrix} L_1 \\ L_2 \\ L_3 \end{Bmatrix}_{,2}$
$[B200S]$	$\int_{R_m} \{L\}\{L\}^T\, d\tau$	$\dfrac{A^m t^m}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$
$[B3000S]$	$\int_{R_m} \{L\}\{L\}\{L\}^T\, d\tau$	$\dfrac{A^m t^m}{60} \begin{bmatrix} \begin{Bmatrix} 6 \\ 2 \\ 2 \end{Bmatrix} & \begin{Bmatrix} 2 \\ 2 \\ 1 \end{Bmatrix} & \begin{Bmatrix} 2 \\ 1 \\ 2 \end{Bmatrix} \\ \begin{Bmatrix} 2 \\ 2 \\ 1 \end{Bmatrix} & \begin{Bmatrix} 2 \\ 6 \\ 2 \end{Bmatrix} & \begin{Bmatrix} 1 \\ 2 \\ 2 \end{Bmatrix} \\ \begin{Bmatrix} 2 \\ 1 \\ 2 \end{Bmatrix} & \begin{Bmatrix} 1 \\ 2 \\ 2 \end{Bmatrix} & \begin{Bmatrix} 2 \\ 2 \\ 6 \end{Bmatrix} \end{bmatrix}$
$[B211A]$	$\varepsilon_{3ki}\{L\}_{,i}\{L\}_{,k}^T$	$\dfrac{1}{2A^m} \begin{bmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}$
$[A200S]$	$\int_{\partial R_m} \{L\}\{L\}^T\, d\sigma$	$\dfrac{t^m l^m}{6} \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
$\{A10\}$	$\int_{\partial R_m} \{L\}\, d\sigma$	$\dfrac{t^m l^m}{2} \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix}$

where r_i is the position vector to the origin of the primed coordinate system, and the α_{ij} are the direction cosines of the coordinate transformation. The integration kernels for two-dimensional space, Eq. (60), are

$$d\tau = t^m dx_1' dx_2' \tag{62}$$

$$d\sigma = t^m dx_1' \tag{63}$$

where t^m is the thickness ($\eta - \xi$ or unity) of the mth finite element. The first term in Eq. (60) is standard for all dependent variables in both equation systems. Assuming the generalized diffusion tensor is distributed over the element as a dependent variable, obtain

$$\kappa \int_{R_m} \{L\}_{,j} K_{ij}^m q_{m,i}^* \, d\tau = \kappa \int_{R_m} \{L\}_{,j} \{L\}^T \{K_{jk}\}_m \{L\}_{,j}^T \{Q\}_m \, d\tau$$
$$= \kappa [B11]_m^T \{B10\}^T [K]_m [B11]_m \{Q\}_m \tag{64}$$

In Eq. (64), the matrices with B prefixes are standard two-dimensional forms, see Table 5, the diffusion tensor matrix, $[K]_m$, is defined as

$$[K]_m \equiv \begin{bmatrix} \{K'_{11}\} & \{K'_{12}\} \\ \{K'_{21}\} & \{K'_{22}\} \end{bmatrix}_m \tag{65}$$

with individual matrix elements comprised of node point values of the diffusion tensor in the primed coordinate system, determined via Eqs. (65) and (61), as

$$K'_{ij} = \alpha_{ik} \alpha_{jl} K_{kl} \tag{66}$$

All but the streamfunction compatibility Eq. (44) contain a convection term and an initial-value operator as dominant terms. For the parabolic Navier-Stokes equation description, the finite element equivalent for convection is

$$\int_{R_m} \{L\} u_k{}^* q_{,k}{}^* \, d\tau = \int_{R_m} \{L\}\{L\}^T\{U_k'\}_m\{L\}_{,k}{}^T\{Q\}_m \, d\tau$$
$$= [B200S]\{U'\}_m\{B11\}^T\{Q\}_m \quad (67)$$

where the elements of the vector, $\{U'\}$, are nodal values of the planar flow velocity transformed to the local coordinate system via Eqs. (67) and (61) as

$$U_k' = \alpha_{kj} U_j \quad (68)$$

The initial-value operator, which comprises the mainstream convection term, similarly becomes

$$\int_{R_m} \{L\} u_1{}^* q_{,1}{}^* \, d\tau = \int_{R_m} \{L\}\{L\}^T\{U1\}_m\{L\}^T\{Q\}_{m,1} \, d\tau$$
$$= \{U1\}_m{}^T[B3000S]\{Q\}_m' \quad (69)$$

where the matrix elements of $[B3000S]$ are column matrices, see Table 5, and the superscript prime exterior to a matrix denotes an ordinary derivative.

In a similar manner, for the integral Navier-Stokes system, the finite element equivalent for convection becomes

$$\int_{R_m} \{L\} \varepsilon_{3ki} \Psi_{,i}{}^* q_{m,k}{}^* \, d\tau =$$
$$\int_{R_m} \{L\}\{\Psi\}_m{}^T\{L\}_{,i}\, \varepsilon_{3ki}\{L\}_{,k}{}^T\{Q\}_m \, d\tau$$
$$= \{B10\}\{\Psi\}_m{}^T[B211A]\{Q\}_m \quad (70)$$

The acceleration expression is

$$\int_{R_m} \{L\} q_{m,t}{}^* \, d\tau = \int_{R_m} \{L\}\{L\}^T\{Q\}_{,t} \, d\tau = [B200S]\{Q\}_m' \quad (71)$$

Evaluation of the remaining terms in the particular differential equations is straightforward. For example, in Eq. (43), the Coriolis body force term becomes

$$\frac{1}{Fr}\int_{R_m} \{L\} \varepsilon_{3ik} \Psi_{,k}{}^* f_i{}^* \, d\tau =$$
$$\frac{1}{Fr}\int_{R_m} \{L\}\{\Psi\}_m{}^T \varepsilon_{3ik}\{L\}_{,k}\{L\}_{,i}{}^T\{F\}_m \, d\tau =$$
$$\frac{1}{Fr}\{B10\}\{\Psi\}_m{}^T[B211A]\{F\}_m \quad (72)$$

For the same expression in the x_1 component of Eq. (13), obtain

$$\frac{1}{Fr}\int_{R_m} \{L\} \varepsilon_{1ik} f_i{}^* u_k{}^* \, d\tau =$$
$$\frac{1}{Fr}\int_{R_m} \{L\}\varepsilon_{132}\{L\}^T\{F\}_m\{L\}^T\{U2\}_m \, d\tau =$$
$$\frac{1}{Fr}\{F\}^T[B3000S]\{U2\}_m \quad (73)$$

using Eq. (25) and assuming x_3 and the local gravity vector are parallel. The vorticity source term for Eq. (44) becomes

$$\int_{R_m} \{L\}\Omega_m{}^* \, d\tau = \int_{R_m} \{L\}\{L\}^T\{\Omega\}_m \, d\tau = [B200S]\{\Omega\}_m \quad (74)$$

The boundary condition matrices in Eq. (60) are directly evaluated. Using prefix A to denote a matrix resulting from integration over a one-dimensional element,

$$\kappa\int_{\partial R_m} \{L\} a_m{}^{(1)} q_m{}^* \, d\sigma = \kappa a_m{}^{(1)}[A200S]\{Q\}_m \quad (75)$$

$$\kappa\int_{\partial R_m} \{L\} a_m{}^{(3)} \, d\sigma = \kappa a_m{}^{(3)}\{A10\} \quad (76)$$

where the $a_m{}^{(i)}$ are user-specified boundary condition constraints.

Conclusion

A finite element solution algorithm has been derived for two equation systems covering a wide range of practical three-dimensional flowfields in environmental hydrodynamics. The solution procedure explicitly assumes tensor turbulent transport properties. It accepts nonregular solution domain closures upon which complicated combinations of boundary condition constraints are routinely specifiable, and can employ specifiably nonuniform computational meshes for solution economy. Applications of the computational procedure to analysis of representative problems in environmental hydrodynamics, employing both developed equation systems, are presented in Part II.[16]

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