MIKE 3

Estuarine and Coastal Hydraulics and Oceanography

Short Description

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1 INTRODUCTION

MIKE 3 is a generalised mathematical modelling system designed for a wide range of applications in areas such as:

- oceanography
- coastal regions
- estuaries and lakes

The system is fully three-dimensional solving the momentum equation and continuity equations in the three Cartesian directions.

MIKE 3 simulates unsteady flow taking into account density variations, bathymetry and external forcing such as meteorology, tidal elevations, currents and other hydrographic conditions.

MIKE 3 can be applied to:

- oceanographic studies
- coastal circulation studies
- water pollution studies
- environmental impact assessment studies
- heat and salt recirculation studies
- sedimentation studies

MIKE 3 is composed of three fundamental modules: The hydrodynamic (HD) module, the turbulence module and the advection-dispersion (AD) module. Various features such as free surface description, laminar flow description and density variations are optionally invoked within the three fundamental modules.

A number of application modules have been implemented and can be invoked optionally. These are advection-dispersion of conservative or linearly decaying substances, a water quality (WQ) module describing BOD-DO relations, nutrients and hygienic problems, an eutrophication (EU) module simulating algae growth and primary production, and a mud transport (MT) module simulating transport along with erosion and deposition of cohesive material. A Lagrangian based particle (PA) module can also be invoked for simulating e.g. tracers, sediment transport or the spreading and decay of E-Coli bacteria.

The modelling system is based on the conservation of mass and momentum in three dimensions of a Newtonian fluid. The flow is decomposed into mean quantities and turbulent fluctuations. The closure problem is solved through the Boussinesq eddy viscosity concept relating the Reynold stresses to the mean velocity field. To handle density variations, the equations for conservation of salinity and temperature are included. An equation of state constitutes the relation between the density and the variations in salinity and temperature and – if the MT calculations are invoked – mud concentration.

In the hydrodynamic module, the prognostic variables are the velocity components in the three directions and the fluid pressure. The model equations are discretised in an implicit, finite difference scheme on a staggered grid and solved non-iteratively by use of the alternating directions' implicit technique. A phase and amplification analysis neglecting effects of viscosity, convective terms, rotation, density variations, etc. has been performed. Under these circumstances, the finite difference scheme is unconditionally stable.

The transport of scalar quantities, such as salinity and temperature, is solved in the advection-dispersion module using an explicit, finite difference technique based on quadratic upstream interpolation in three dimensions. The finite difference scheme, which is accurate to fourth order, has attractive properties concerning numerical dispersion, stability and mass conservation.

The decomposition of the prognostic variables into a mean quantity and a turbulent fluctuation leads to additional stress terms in the governing equations to account for the non-resolved processes both in time and space. By the adoption of the eddy viscosity concept these effects are expressed through the eddy viscosity, which is optionally determined by one of the following five closure models:

- a constant eddy viscosity
- the Smagorinsky sub-grid (zero-equation) model
- the *k*- (one-equation) model
- the standard *k*-ε (two-equation) model
- a combination of the Smagorinsky model for the horizontal direction and a *k*-ε model for the vertical direction

The turbulence models are all solved in an explicit manner except for the one-dimensional (vertical) *k*-ε model, which is solved by an implicit scheme.

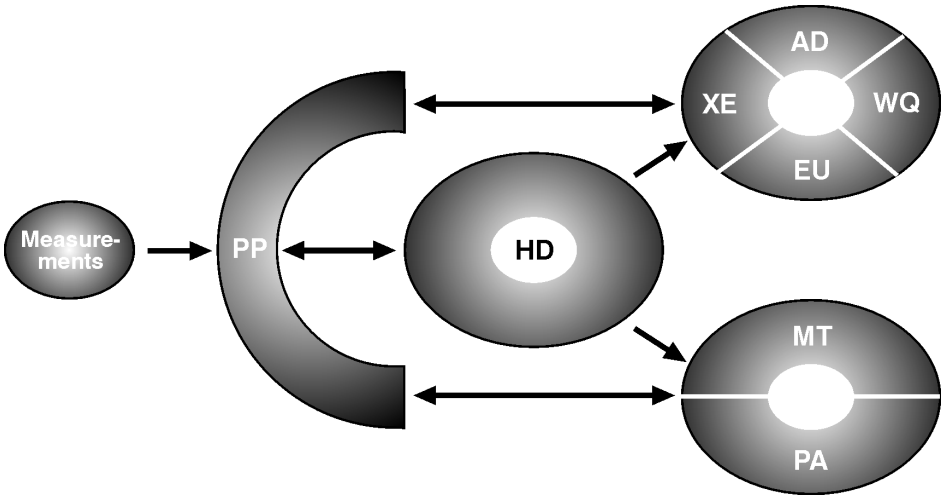


Figure 1.1 Design structure of the three-dimensional modelling system, called MIKE 3

2 GOVERNING EQUATIONS

In a three-dimensional hydrodynamic model for flow of Newtonian fluids, the following elements are required:

- mass conservation
- momentum conservation
- conservation of salinity and temperature
- equation of state relating local density to salinity, temperature and pressure as well as to possible mud concentration

Thus, the governing equations consist of seven (possibly eight) equations with seven (eight) unknowns.

The mathematical foundation is the Reynolds-averaged Navier-Stoke's equations in three dimensions, including the effects of turbulence and variable density, together with the mass conservation equation:

$$\frac{\partial u_i}{\partial t}+\frac{\partial u_i u_j}{\partial x_j}+2\Omega_{ij}u_j=-\frac{1}{\rho}\frac{\partial P}{\partial x_i}+g_i+\frac{\partial}{\partial x_j}\left(\nu_T\left\{\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right\}-\frac{2}{3}\delta_{ij}k\right)$$

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho u_j\right)=0$$

where ρ is the local density of the fluid, u_i the velocity in the x_i-direction, Ω_{ij} the Coriolis tensor P the fluid pressure, g_i the gravitational vector, ν_T the turbulent eddy viscosity, δ_{ij} Kronecker's delta, k the turbulent kinetic energy, and t denotes the time.

Coast contours and depth contours are described as accurately as possible with the selected grid size. The transport equations for salt and temperature are used together with an equation of state for the density of the water:

$$\frac{\partial S}{\partial t}+\frac{\partial}{\partial x_j}(u_j S) = \frac{\partial}{\partial x_j}\left(D_s\frac{\partial S}{\partial x_j}\right)$$

$$\frac{\partial T}{\partial t}+\frac{\partial}{\partial x_j}(u_j T) = \frac{\partial}{\partial x_j}\left(D_T\frac{\partial T}{\partial x_j}\right)+Q_H$$

where S is the salinity, T the temperature and Q_H the heat exchange with the atmosphere. D_s and D_T are the dispersion coefficients for salt and temperature, respectively. There are several types

of equations of state for the density of seawater. In MIKE 3, the definition given by UNESCO has been adopted relating local density to salinity, temperature and pressure.

Heat exchange with the atmosphere is implemented with basis in the four physical processes:

- sensible heat flux (convection)
- latent heat flux (vaporisation)
- net short wave radiation
- net long wave radiation

The mass and momentum equations cannot be solved by a computer as they express a continuous change in both time and space. Thus, the equations need to be reformulated in terms of discrete changes in both time and space. A number of techniques for this reformulation are used in computational fluid dynamics of which the finite volume and finite difference are the most popular techniques.

Traditionally, the finite difference technique is used in the field of hydraulics, and thus it is also used in (almost) all existing models developed throughout the years at DHI.

Before discretising the differential equations into a finite difference scheme, a spatial grid is required. The actual grid that has been adopted is the so-called Arakawa C staggered grid, see Figure 2.1.

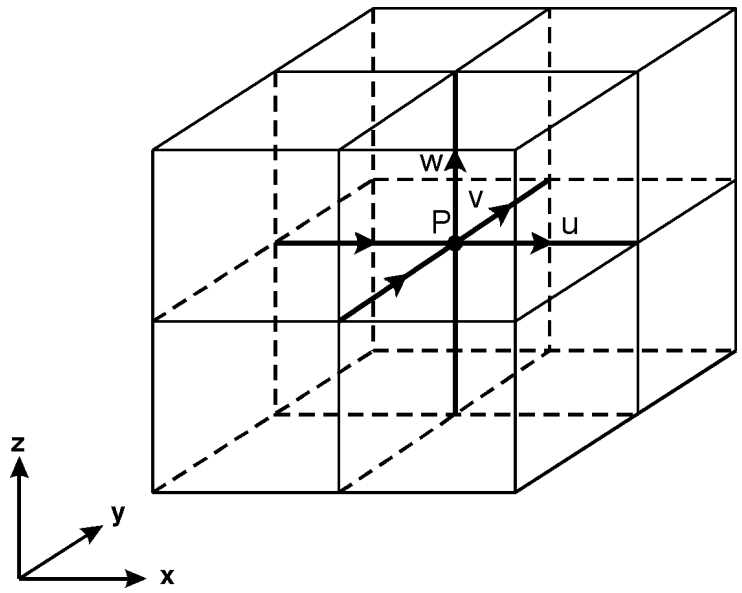


Figure 2.1 The staggered grid adopted in MIKE 3

The mesh size (or grid spacing) is defined as the distance between two nodes.

The velocities u, v and w are defined between the nodes, whereas scalar quantities such as the pressure, salinity, temperature, etc. are defined in the nodes. The prognostic variables used in the hydrodynamic part of MIKE 3 are shown in the Figure 2.2.

The adopted staggered grid allows for the spatial discretisation of the differential equations. The mass equation is space centred in every node, whereas the momentum equations are space centred in the corresponding velocity 'nodes' to form a huge set of equations. However, the time derivatives imply the definition of certain time levels, also, leading to either explicit or implicit schemes. In general, all prognostic variables in implicit schemes are defined at the same time level and then an iterative technique is applied to inverse the matrix to advance the solution one time step.

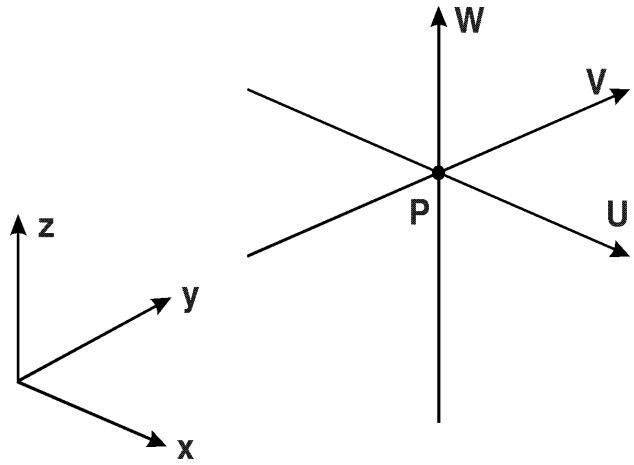


Figure 2.2 Definition of the prognostic variables used in the hydrodynamic part of MIKE 3

This inversion may be performed on the entire matrix in one step, which, due to the size of the matrix, is a costly way. Alternatively, the inversion may be split into three operations according to the three directions. In each operation, only the prognostic variables directly associated with the directions are considered as prognostic, whereas the other direction variables are locked, e.g. only the pressure and u-velocities during a x-direction operation. This technique is known as the Alternating Directions Implicit (ADI) algorithm.

In almost all of the modelling systems developed at DHI, the ADI-technique has been adopted to inverse the matrices. Usually, iterative methods are required for the inversion of the matrices due to the non-linear terms in the momentum equations. However, applying two special techniques allows for a non-iterative ADI algorithm to be adopted. The first of these two techniques is called the 'fractioned-step' technique.

Basically, the 'fractioned-step' technique is a time staggering of the prognostic variables. This technique has been described in detail by Leendertse (1967).

The second special technique is called 'side-feeding' and is basically a semi-linearisation of the non-linear terms. Details on this side-feeding technique are given by Abbott (1979).

The primitive equations, as listed above, will mathematically form an ill-posed problem whenever the fluid pressure and the velocities constitute the prognostic variables due to a weak coupling between the pressure and the velocities. *This is the key issue in three-dimensional modelling*. The system is said to be stiff as both slow and fast processes are present, which inherently cause difficulties in the numerical algorithm. In free surface flows, however, only the slow processes are of interest and usually the fast processes (like shock waves) have no

substantial influence on the slow processes (like the free surface waves) suggesting that they may be removed without loss of information. The fast processes are easily eliminated by replacing the time derivative of the density in the mass conservation equation with the pressure term in the equation of state, whereby a compressibility of the fluid is introduced. The fast processes are then subsequently eliminated through an artificial compressibility whereby the system has become hyperbolic dominated. This approach is known as the artificial compressibility approach and was first proposed by Chorin, 1967.

Alternatively, so-called pressure correcting methods can be applied in which the divergence-free continuity equation is enforced through the solution of a Poisson equation for the pressure (cf. Ferziger, 1987 and Patankar, 1980).

It is the artificial compressibility method that has been adopted in MIKE 3.

3 ADVECTION - DISPERSION

MIKE 3 is applicable to flow problems in which density variations and turbulence are important features. The mathematical modelling of such flows requires the solution of partial differential equations of the advective-diffusive type.

The flow modelling will require the solution of the transport equation for:

- salinity
- temperature (heat)
- turbulent kinetic energy (k-equation)
- dissipation of turbulent kinetic energy (ε-equation).

The latter two equations form the well-known k and k-ε turbulence models, see Section on Turbulence. For the k-model and the standard k-ε model, the non-linear transport equations are solved by explicit UPWIND scheme. The one-dimensional (vertical) k-ε model essentially forms two one-dimensional diffusion equations, which are efficiently solved by an implicit scheme.

The partial differential equations describing transport of salinity and temperature as well as transport of concentrations of substances, water quality and eutrophication components and mud concentration are all linear advective-diffusive type equations, and accordingly the same solution scheme is applied to all these components.

A large number of methodologies for solving the advection-diffusion problem are reported in the literature. However, in order to be consistent with the HD module, a finite difference approach was chosen.

The QUICKEST (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms, Leonard (1979)) is applied. The method is based on a conservative control-volume formulation. Upstream interpolation is used to determine higher order derivatives. This procedure avoids the stability problems of central differencing while remaining free of the inaccuracies of numerical diffusion associated with the usual upstream differencing.

The extension of this scheme to two and three dimensions is given in Justesen et al (1989), Ekebjærg and Justesen (1991) and Vested et al (1992). For use in situations where resolution of steep fronts are important, the scheme has been further improved by implementation of an exponential interpolation at steep fronts, the so-called QUICKEST-SHARP scheme, see also Leonard (1988).

Alternatively, the so-called QUICKEST-ULTIMATE scheme, using operator splitting, may optionally be invoked, see e.g. Leonard (1991). This scheme is advantageous in cases with more than one advection-diffusion component, since in MIKE 3 it has been implemented such that the CPU time consumption is practically independent of the number of components.

The equation to be solved in the AD model can be written as:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(uc) + \frac{\partial}{\partial y}(vc) + \frac{\partial}{\partial z}(wc) \quad =$$

$$\frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z}\right)$$

$$+ \quad SOURCE \ / \ SINK$$

Considering the grid point (x_j, y_k, z_l), the explicit, finite difference approximation for the equation above is written for the associated control volume:

$$\left(x_j - \tfrac{1}{2}\Delta x,\ x_j + \tfrac{1}{2}\Delta x;\quad y_k - \tfrac{1}{2}\Delta y,\ y_k + \tfrac{1}{2}\Delta y;\quad z_l - \tfrac{1}{2}\Delta z,\ z_l + \tfrac{1}{2}\Delta z\right)$$

$$\begin{aligned} c_{j,k,l}^{n+1} \quad = \quad c_{j,k,l}^{n} \quad & - \frac{\Delta t}{\Delta x} \quad \left\{T_x(j,k,l) - T_x(j-1,k,l)\right\} \\ & - \frac{\Delta t}{\Delta y} \quad \left\{T_y(j,k,l) - T_y(j,k-1,l)\right\} \\ & - \frac{\Delta t}{\Delta z} \quad \left\{T_z(j,k,l) - T_z(j,k,l-1)\right\} \end{aligned}$$

It is computationally more convenient and efficient to express the scheme by the use of transports. The transports through the control surface are the velocity perpendicular to the surface multiplied by the surface concentrations. These concentrations are located between nodes and have to be interpolated.

With the QUICKEST-SHARP scheme, eight points are used to calculate the transport through each control surface. With the QUICKEST-ULTIMATE scheme, three points are used corresponding to down-stream, up-stream and very-up-stream positions relative to each control surface. The interpolation weights are determined in such a way that truncation error terms up to third order are cancelled.

4 TURBULENCE

Today, calculations of mean flow properties of turbulent flows in 2D and 3D can be accomplished with a number of different mathematical models to provide closure, e.g. the k-ε model. Such calculations are now standard in many industrial applications. Furthermore, in the scientific community, results of laboratory experiments are often compared with results from mathematical models. In such simulations it is usually possible to make a distinction between the 'mean flow' and the superimposed 'turbulent fluctuations' in an unambiguous way.

In geophysical systems, on the other hand, a variety of interacting motions at different time scales exist. The terms' grid scale processes and subgrid scale processes therefore apply to different physical phenomena depending upon the grid on which the system is resolved.

In Table 4.1, a number of processes are listed according to their time scale. The spectral window indicates the resolved time scales, whereas the smaller scale processes are given as filtered out processes. It is seen that depending upon which process one wants to resolve, a different, smaller scale process may be the most important to model.

Of course, there is a length scale associated with each of the time scales in Table 4.1. It is observed that a larger time scale will generally correspond to a larger length scale.

Table 4.1 Time Scales in Oceanography. From Nihoul et al (1989)

Time scale	**Frequency s^{-1}**	**Spectral windows (highlighted processes)**	**Smaller scale fluctuations (filtered out processes)**
1 second	1	**Microscale processes**	Molecular diffusion
		3D "eddy" turbulence (+surface waves)	
1 minute	10^{-2}	**Mesialscale processes**	Eddy turbulence
		Internal waves Vertical microstructure "Bliny" inhibited turbulence	
1 hour	10^{-4}	**Mesoscale processes**	"Bliny turbulence"
		Inertial oscillations Tides, storm surges	
1 day	10^{-5}	Diurnal variations	
1 week	10^{-6}	**Synoptiscale processes**	Mesoscale variability
		Frontal currents Meanders, "rossby" turbulence	
1 month	10^{-7}	**Seasonalscale processes**	"Rossby turbulence"
1 year	10^{-8}	**Globalscale processes**	Seasonal variability
		Climatic processes	
		(Paleo) climaticscale processes	

Furthermore, Table 4.1 makes it apparent that the term turbulence model is inappropriate, because this model has to include the effects of processes that are usually not referred to as turbulence. Such processes include mesialscale and mesoscale processes such as internal waves, tides and surges. Generally, these motions would be placed at the 'mean flow' level, but in reality this will depend on the temporal resolution!

4.1 Smagorinsky model

A turbulence closure model must prove its validity through the model calibration and the associated comparisons with measured data. Good turbulence models have extensive universality without being too complex. The most popular model for the subgrid scale eddy viscosity was proposed by Smagorinsky (1963). Here, the eddy viscosity is linked to the filter size (grid spacing) and the large eddy strain rate, i.e. velocity gradients of the resolved flow field,

$$\nu_T = \ell^2 \sqrt{2 S_{ji} S_{ij}}$$

in which

$$S_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

is the stress tensor and ℓ is a characteristic length scale.

4.2 k model

The first important improvement of the mixing-length theory is to determine the velocity scale from a transport equation rather than from the mean flow field.

It is physically most reasonable to utilise $\sqrt{k}$ as the velocity scale. k is a direct measure of the intensity of the turbulent fluctuations in all three directions (the turbulent kinetic energy). Since this energy is contained in the large-scale eddies, $\sqrt{k}$ becomes a velocity scale for the large-scale motion.

Now, using this velocity scale together with a prescribed length scale ℓ, the eddy viscosity can be expressed as

$$\nu_T = c_\mu' \sqrt{k\ell}$$

This expression is known as the Kolmogorov-Prandtl relation. The distribution of k has to be deduced from the solution of a transport equation for k. c_μ' is an empirical constant to be determined from experiments.

Turbulence models that consist of the flow equation, the transport equation for *k*, and a specified length scale are called one-equation models of turbulence and are normally based on the eddy viscosity concept.

The inclusion of the memory effect in the turbulence represents one step forward in comparison with the zero-equation models. However, when the effects of convection and diffusion are important, a transport equation for either the length scale or a related quantity must be added to the turbulence model. This may be relevant in recirculating flows or rapidly changing flows.

4.3 Standard k-ε model

The length scale specification inherent in the one-equation model can be replaced by a transport equation for a turbulent quantity

$$z = k^m \ell^n$$

where m and n can be any numbers. Several of these combinations have been proposed and tried so far. Little success has been gained using the length scale itself, see e.g. Launder and Spalding (1972). Instead, the isotropic energy dissipation rate has been used extensively:

$$\varepsilon = C_D \frac{k^{3/2}}{\ell}$$

A two-equation turbulence model may consist of the flow equation, the transport equation for the turbulent kinetic energy, the transport equation for the dissipation rate, and the Kolmogorov-Prandtl expression

$$\nu_T = c_\mu \frac{k^2}{\varepsilon}$$

to link the quantities together. Such a model is usually referred to as a *k*-ε model in the literature.

Within the framework of the eddy viscosity concept it is the most advanced turbulence model that can be established. In many flows, however, when the individual Reynolds stresses play very important roles, transport equations can be derived that eliminate the need for the eddy viscosity.

4.4 Mixed 2D Smagorinsky, 1D k-ε model

Due to the large aspect ratio Δx/Δz often used in applications of MIKE 3, different formulations are appropriate for the horizontal and the vertical directions. In the mixed Smagorinsky/k-ε model, the horizontal eddy viscosity is determined as described above for the pure Smagorinsky model. For the vertical direction, the 1D k-ε model described by Burchard and Baumert (1995) is

applied. This model uses transport equations for two quantities to describe the turbulent motion: the turbulent kinetic energy, *k*, and the dissipation rate of turbulent kinetic energy, ε.

The Kolmogorov-Prandtl expression:

$$\nu_T = c_\mu \frac{k^2}{\varepsilon}$$

couples the mean flow equations to the state variables of the turbulence model. The basic assumption of the present k-ε model is that vertical motions are mainly turbulent fluctuations and the mean component can be neglected. Due to the coarse horizontal resolutions, it is further assumed that advective processes are insignificant compared to the local balance. The transport equation for k and for ε then reads:

$$\frac{\partial k}{\partial t} = \frac{\partial}{\partial z}\left(\frac{\nu_T}{\sigma_k}\frac{\partial k}{\partial z}\right) + P + G - \varepsilon$$

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial z}\left(\frac{\nu_T}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right) + c_{1\varepsilon}\frac{\varepsilon}{k}\left(P + c_{3\varepsilon}G\right) - c_{2\varepsilon}\frac{\varepsilon^2}{k}$$

where

$$P = \nu_T\left\{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2\right\}$$

is the production term due to velocity shear, and

$$G = \frac{g}{\rho}\frac{\nu_T}{\sigma_T}\frac{\partial \rho}{\partial z}$$

is the production term due to buoyancy, u and v are the horizontal velocity components, ν_T is the effective eddy viscosity, g the gravity, ρ the density, and σ_T the Prandtl number. c_μ , σ_k , σ_ε , $c_{1\varepsilon}$, $c_{2\varepsilon}$ and $c_{3\varepsilon}$ are empirical parameters.

4.5 Buoyancy Effects

A very important aspect of turbulence modelling is to incorporate the effects of buoyancy in a correct way. Although turbulence modelling has been a research area for more than 20 years,

there is no universal modification for buoyancy, which can be applied to the existing turbulence models in all cases. This is mainly due to the fact that stratified flows in oceanography are often governed by instabilities and countergradient transport phenomena. Usually, turbulence models are based on gradient diffusion/ transport models, which will fail in such cases.

When a density gradient is present in e.g. the mixing layer in a stratified flow, the diffusion coefficient is damped. This means that entrainment and mixing will be overpredicted if the model does not account for this effect. The simplest way of introducing this is to reduce the eddy viscosity in areas with density gradients. The problem is how to parameterise the dampening.

Various suggestions on how to modify the Smagorinsky formulation of the eddy viscosity have been given. From the research on stratified flows, see e.g. Pedersen (1980), it has been established that such a dampening must be a function of the Richardson gradient number, Ri given by

$$Ri = -\frac{g}{\rho}\frac{\partial \rho}{\partial z} \Big/ \sqrt{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2}$$

For stable stratification, the Smagorinsky eddy viscosity can optionally be reduced as

$$\frac{\nu_T}{\nu_{T0}} = \frac{1}{(1+\psi\, Ri)^{\alpha}}$$

where ψ and α are dimensionless constants. The Smagorinsky formulation of the eddy viscosity and modified to handle buoyancy effect has been implemented in an explicit manner.

In the *k*-ε closure model, the Prandtl number σ_T, which appears in the transport equations for *k* and ε, is modified explicitly by the expression:

$$\sigma_T = \left\{ \frac{\left(1+\frac{10}{3}Ri\right)^3}{1+10Ri} \right\}^{1/2}$$

for stable stratification, while σ_T equals unity for unstable stratification. The eddy viscosity is modified implicitly through the *k*-ε equations and the Kolmogorov-Prandtl expression.

5 WATER QUALITY AND EUTROPHICATION

5.1 Modelling of BOD/DO

The main factors affecting the Dissolved Oxygen (DO) budget in polluted waters are the oxygen consuming degradation of organic matter, expressed as the Biological Oxygen Demand (BOD) in both water and bed sediments, the naturally occurring oxygen production/consumption of photosynthetic algae and plants, the Sediment Oxygen Demand (SOD), and the reaeration of oxygen at the sea surface. The Biological Oxygen Demand expresses the amount of organic material degradable by living organisms (bacteria, etc.) whereas the parallel term Chemical Oxygen Demand (COD) is the total amount of degradable organic material by chemical agents. The BOD is a more relevant measure of the degradable components in the environment than COD, since the living organisms (in this case bacteria) have to biologically degrade the substances in the environment.

Pollution can affect the natural process of photosynthetic oxygen production due to high water turbidity which will result in reduced light transparency and hence reduced photosynthetic oxygen production, e.g. in the pelagiale and by bed vegetation.

Oxygen conditions could become a problem in an area where the BOD loads from domestic and industrial sewage are significant. BOD loads in storm water can also be of importance in many cases.

Low oxygen concentrations and oxygen depletion can, besides affecting the environment (especially fish, but also organisms living at the bed), be the direct cause of aesthetic problems like nasty smells and bad aesthetic conditions, which can be very problematic in areas of a touristic value.

Oxygen model calculations serve the following main purposes:

- to determine or predict concentrations of pollutants and of oxygen to be compared with international or national water quality standards
- to investigate the consequences of the development of the human environment in the area, for example new sewage outlet schemes with respect to environmental problems caused by BOD pollution and resulting oxygen depletion

The relationship between BOD-loadings (organic material measured as biodegradable oxygen demand) and the concentration of dissolved oxygen is described in a specific module (WQ) in the 3D model. The system incorporates the processes shown in Figure 5.1.

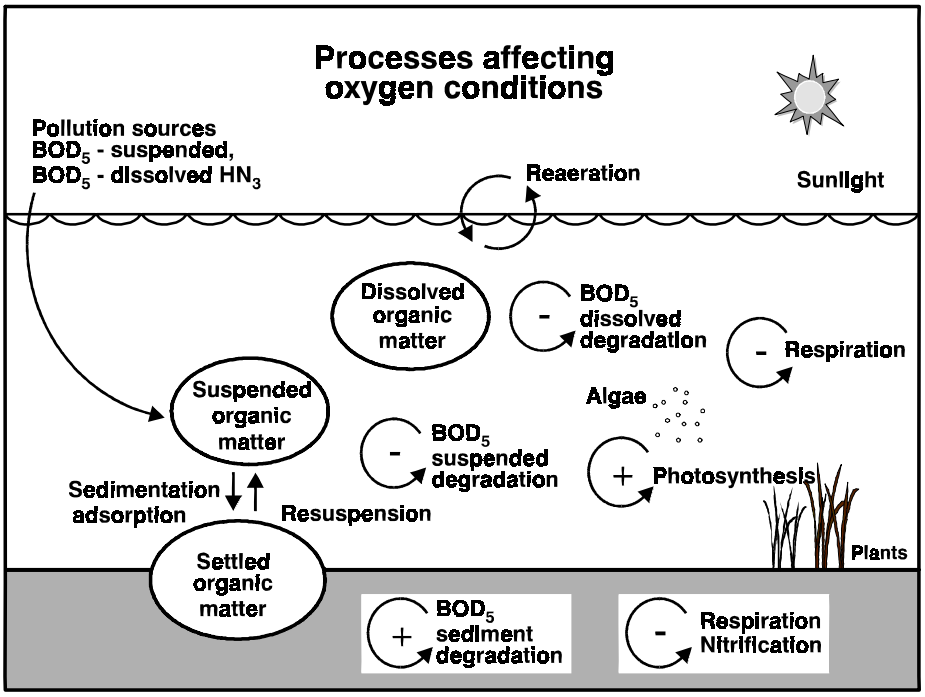


Figure 5.1 Principle sketch of BOD/DO model

The dissolved oxygen concentration depends on a number of processes of which the following main processes are included in the model:

- reaeration, e.g. the exchange between water and air
- the natural oxygen production and respiration from photosynthetic activity
- oxygen consumption from naturally occurring organic material
- oxygen consumption in the bottom waters from the sediment oxygen demand
- biological oxygen demand caused by degradation of discharged organic material from sewage outlets
- nitrification, i.e. oxidation of ammonia
- horizontal and vertical transport of oxygen

The MIKE 3 WQ model can also include modelling of the nutrients: ammonia, nitrite, nitrate and phosphate. The ammonia and phosphate come from municipal and industrial wastewater and are released at the degradation of organic matter (BOD decay). Nitrite and nitrate are the products of the nitrification. Denitrification changes nitrate into elementary nitrogen. All the nutrients but especially nitrate are transported to the coastal areas via rivers. The ammonia and phosphate are assimilated at photosynthesis.

The description of the photosynthetic activity is very simple in this model and not comparable to the approach used in general eutrophication models (see 'Modelling of eutrophication').

The chlorophyll concentration resulting from the photosynthetic activity can be calculated by the model.

The WQ module simulates the state variables simultaneously (coupled), e.g. the concentration of BOD and oxygen, because they are in nature interactively coupled. The BOD changes will have an influence on the changes in the oxygen concentration and vice versa, e.g. the oxygen concentration can at low values affect the decay rate of BOD because the degrading bacteria are affected at low oxygen levels.

The water quality model of MIKE 3 can furthermore simulate the distribution and decay of total and faecal coliform bacteria.

The water quality module is integrated with the advection-dispersion module of MIKE 3, which describes the physical transport processes at each grid-point covering the area of interest.

The forcing functions of the water quality model are the temperature and the irradiation, the latter in order to describe the influence of the light on the coliform bacteria decay. Detailed descriptions of the process equations used in the 3D WQ modelling are available in the 'Scientific Description of MIKE 3 WQ'. These process descriptions are similar to the ones implemented in the 3D model.

5.2 Modelling of eutrophication

The applied model includes a description of the pelagic system and the benthic vegetation. The state variables in the eutrophication (EU) module are:

PC	:	phytoplankton carbon
PN	:	phytoplankton nitrogen
PP	:	phytoplankton phosphorus
CH	:	chlorophyll concentration
ZC	:	zooplankton carbon
DC	:	detritus carbon
DN	:	detritus nitrogen
DP	:	detritus phosphorus
IN	:	inorganic nitrogen
IP	:	inorganic phosphorus
DO	:	dissolved oxygen
BC	:	benthic vegetation carbon

The model describes the dynamics of the first and second step of the basic food chain in the pelagic part of the ecosystem, for example the primary production by phytoplankton (the first step) and the grazing of phytoplankton by zooplankton (the second step). Additionally, the primary production by benthic vegetation can be modelled.

This means that 11 of the 12 included state variables constitute the pelagic system and 1 constitutes the benthic vegetation. The model describes the seasonal and spatial variations of these variables within a given area.

The seasonal variations depend on a number of forcing functions:

- water exchange
- influx of light
- water temperature
- water turbidity
- nutrient loadings
- conditions in the surrounding areas (boundary conditions)

The processes described by the standard EU-module are:

Phytoplankton	:	production, uptake of nutrients, sedimentation, grazing
Macrophytes	:	growth, nutrient uptake, decay
Zooplankton	:	production, death, respiration, excretion
Detritus	:	mineralisation (release of nutrients), sedimentation
Sediment	:	mineralisation
Oxygen	:	reaeration, production by phytoplankton and macrophytes, consumption by zooplankton, detritus and sediment mineralisation (SOD)
Nitrogen	:	uptake of inorganic nitrogen in phytoplankton and macro algae, respiration, e.g. release of nitrogen from detritus and bed sediment
Phosphorus	:	uptake in phytoplankton and macro algae, respiration, e.g. release of phosphorus from detritus and bed sediment

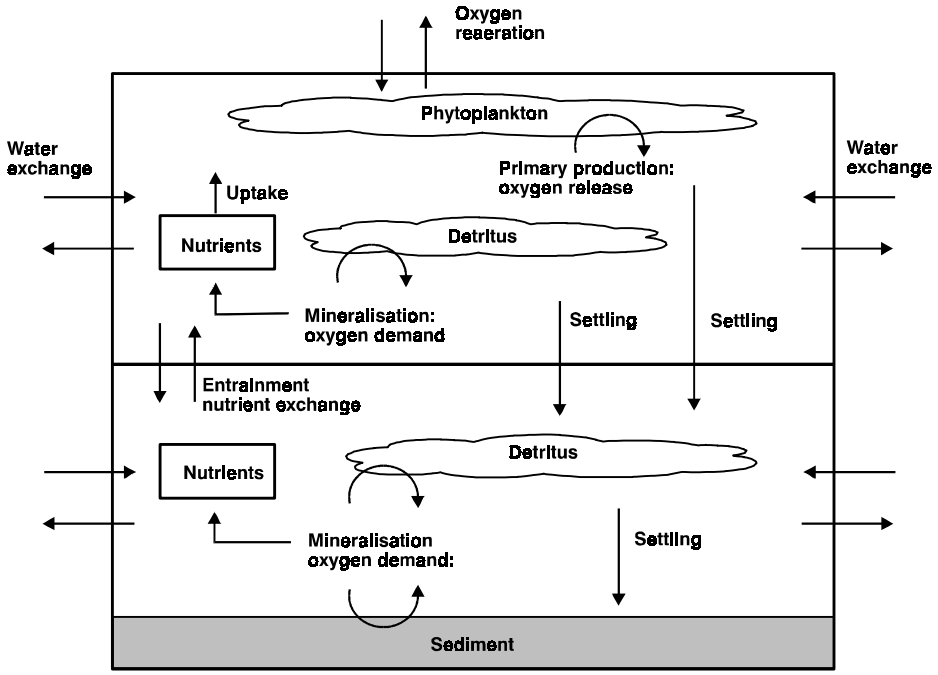
The principle of carbon and nutrient flows is illustrated in Figure 5.2.

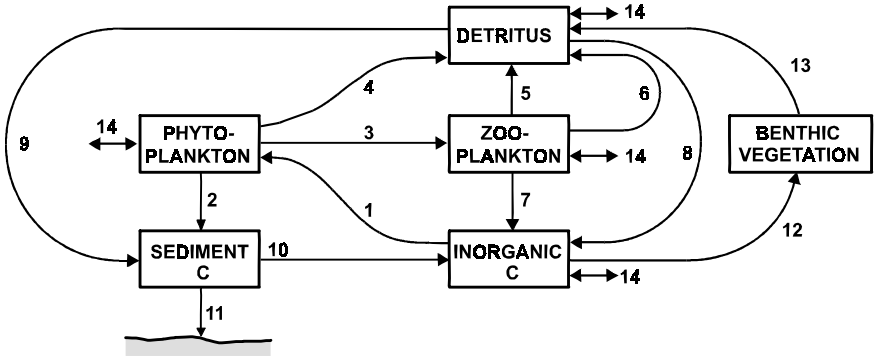
The pelagic system is described by the growth of phytoplankton, grazing of phytoplankton, and the transformation of living phytoplankton and grazers to dead organic material (detritus) (process numbers 1, 3, 4, 5 and 6 of Figure 5.2). In addition, phytoplankton and detritus are subject to sedimentation (process numbers 2 and 9).

The release of nutrients from the degradation of organic matter in the water and sediment and the corresponding oxygen demand are also included (process number 10). The growth of phytoplankton depends on light conditions, water temperature, water turbidity, and nutrient concentrations. The nutrient dynamics in phytoplankton are expressed by internal pools of nitrogen and phosphorus. This means that algae growth can take place even though the nutrient concentrations in the water are very low.

The special conditions related to eutrophication in stratified environments can be summarised as follows: the phytoplankton and detritus in the upper water masses will settle to the bottom waters and here be degraded, for example create an oxygen demand. The sediment can also hold a potential oxygen demand due to degradation of settled material. Because of the stratification, virtually no oxygen or other dissolved substances are transported from one layer to the other. The oxygen demand in the bottom layer can thus potentially lower the oxygen concentration here to critical levels.

Additionally, high concentrations of nutrients in the bottom waters can, because of the mixing induced transport over the interface, contribute to the nutrient limited algae production in the upper water masses.





1. production, phytoplankton
2. sedimentation, phytoplankton
3. grazing
4. extinction, phytoplankton
5. excretion, zooplankton
6. extinction, zooplankton
7. respiration, zooplankton
8. mineralisation of detritus
9. sedimentation of detritus
10. mineralisation of sediment
11. accumulation in sediment
12. production, benthic vegetation
13. extinction, benthic vegetation
14. exchange with surrounding waters

Figure 5.2 *Processes and state variables in the ecological model, exemplified by the carbon cycle*

6 MUD TRANSPORT

Mud is typically defined as a fluid-sediment mixture consisting of saltwater, sands, silts, clays and organic materials. In the environment, a layered mud structure is often observed with a suspension layer near the surface, a fluid mud layer below and finally the settled mud bed, see Table 6.1. The fluid mud layer is defined as having a dry density from 10 g/l to 325 g/l. This division is made due to the following reasons:

- mud with dry densities higher than 10 g/l shows beginning non-Newtonian behaviour, i.e. changing viscous properties
- mud with dry densities higher than 325 g/l will be 'frame-work supported' (an effective stress is present) and shows plastic behaviour

Table 6.1 An overview of the division of fluid-sediment mixtures used in this document, see also van Rijn (1993)

Name	Dry density (g/l)	Wet density (g/l)	Consolidation stage	Rheological behaviour
Suspension	0-10	----	----	'Newtonian'
Fluid mud	10-100	----	freshly consolidated (1 day)	dilute fluid mud
	100-250	----	weakly consolidated (1 week)	fluid mud (Bingham)
	250-325	1150-1200	medium consolidated (1 month)	dense fluid mud (Bingham)
Soft settled mud bed	325-400	1200-1250	medium consolidated (1 month)	dense fluid mud (Bingham)
	400-550	1250-1350	highly consolidated (1 year)	fluid-solid
	550-650	1350-1400	stiff mud (10 years)	solid
Hard	>650	>1400	hard mud (100 years)	solid

The mud suspension shows Newtonian behaviour and may be approached by classical fluid mechanics, i.e. be immediately included in the hydrographic description. The fluid mud layer shows non-Newtonian behaviour and may be approached by fluid mechanics using the relevant rheologic constitutive equation. The (hard) settled mud bed may be approached by continuum mechanics (i.e. soil mechanics).

The mud transport module is coupled with the hydrodynamic module in MIKE 3. The suspended mud influences the hydrodynamics by changing the density and the kinematic viscosity of the mixture. The density of the mixture is by definition related to the concentration as follows:

$$\rho_m = \rho_{wat} + c\left(\frac{\rho_{sed} - \rho_{wat}}{\rho_{sed}}\right)$$

where ρ_m [g/l] is the density of the mixture, ρ_{wat} [~1000 g/l] is the density of the water, c [g/l] is the sediment concentration, and ρ_{sed} [~2600 g/l] is the density of the sediment. By altering the density due to suspended material damping of turbulence at lutoclines is automatically taken care of in the hydrodynamic modelling by a Richardson damping technique. The kinematic viscosity can be approximated by:

$$\frac{\nu_m}{\nu} \approx 100^{\frac{c}{600\,g/l}}$$

where ν_m [m^2/s] is the kinematic viscosity of the mixture, and ν [m^2/s] is the kinematic viscosity of the water.

The basis for the mud transport module is the mass conservation equation for mud, which is given by:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_j}\left(c\left(u_j - w_{s,j}\right)\right) = \frac{\partial}{\partial x_j}\left(D_c \frac{\partial c}{\partial x_j}\right) + S_c$$

where $w_{s,j}$ = (0, 0, w_s [mm/s]) is the settling velocity vector, D_c is the dispersion of cohesive sediment, and S_c is a local source (NOT erosion or deposition). The mass conservation equation resembles the conservation equation for temperature and salinity - the only difference is the inclusion of the settling velocity. The major problem in mud transport modelling is the description of the boundary condition at the bed and the description of the settling velocity. The solutions used in the MIKE 3 MT module are outlined in the following.

The settling velocity (w_s) used is related to concentration (hindered settling is taken into account) and to dissipation (the floc sizes depend on the dissipation) as follows:

$$w_s = w_{s0}\left(\frac{c}{c_{s0}}\right)\left(1 - \frac{c}{\frac{5+2n}{n} c_{s0\,\mathrm{MAX}}}\right)^{5+n}\left(1 - \sqrt{\frac{\varepsilon}{\varepsilon_0}}\right)$$

where w_{s0} (~1 mm/s) is a reference settling velocity, c_{s0} (~1 g/l) is a reference sediment concentration, n (~1) is a dimensionless suspended material parameter, c_{s0MAX} (~7 g/l) is the concentration at maximum settling velocity, ε [m^2/s^3] is the dissipation, and ε_0 [m^2/s^3] is the 'floc destruction dissipation', i.e. the dissipation at which the flocs are destroyed. The present formulation relating the settling velocity to the dissipation is used in the entire water column.

The dissipation is taken into account throughout the water column, but only nearest to the bed is the dissipation from short period surface waves also taken into account.

The boundary condition used at the surface is that there is no mud material transport through the surface. The boundary condition at the bed is one of the major problems in mud transport modelling. At the bed we can have either erosion from the bed or deposition to the bed. If erosion (E [g/m^2/s] takes place it is determined by:

$$E = e_0 \sqrt{\rho_b \tau_{ce}} \frac{\tau_b - \tau_{ce}}{\tau_{ce}}, \quad when\ \tau_{bmax} > \tau_{ce}$$

where e_0 (~$5 \cdot 10^{-5}$) is a dimensionless bed material parameter, ρ_b [kg/m^3] is the dry density of the bed surface), τ_{ce} [N/m^2] is the critical shear stress for erosion, and τ_b [N/m^2] is the bed shear stress (index max gives that it is the maximum during a short period surface wave cycle).

If deposition (D [g/m^2/s] of weak and/or strong flocs takes place on the mud bed it is determined by (ignoring possible dispersion of flocs):

$$D = c_b w_s \qquad when\ \tau_{bmax} < \tau_{ce}$$

where c_b [g/l] is the concentration close to the bed and is thus determined from the solution of the mass conservation equation for the cohesive sediment.

The bed is described by multiple layers, where depositing material always enters the first layer.

In MIKE 3 HD, the influence of short surface waves is not considered directly (indirectly through calibrating the bed friction parameter). The short waves are, however, very important when describing the mud transport: time varying shear stress and liquefaction. Typically, the wave period and the wave height are possible to get, whereby the wave length and other information can be determined on the basis of the classical wave theory. Such parameters can be entered into the MT module, which then is able to take surface waves into account.

7 PARTICLE MODULE

MIKE 3 PA is a module for the simulation of transport and fate of dissolved and suspended substances discharged or accidentally spilled in lakes, estuaries, coastal areas or at open sea.

The substance simulated may be a pollutant of any kind, conservative or non-conservative, for example suspended sediment particles, inorganic phosphorus, nitrogen, bacteria or chemicals.

The pollutant is considered as particles being advected with the surrounding water body and dispersed as a result of random processes. To each particle, a corresponding mass is attached. This mass can change during the simulation as a result of decay or deposition.

MIKE 3 PA includes formulations for the effects of decay, light attenuation, exceeding concentrations, cohesive/non-cohesive sediment and constant/time varying sources.

The basic Lagrangian approach involves no other discretisations than those associated with the description of the bathymetry of the model area and the wind, current and water level fields. This concept has several advantages:

- numerical dispersion associated with finite differencing is eliminated
- computer requirements are small

MIKE 3 PA assumes that current velocities and water levels can be prescribed in time and space in a computational grid covering the area of interest. This information may be provided by means of a preceding MIKE 3 HD model simulation or on the basis of a 'library' of flow field.

Application areas for MIKE 3 PA include engineering applications such as studies of:

- sedimentation problems
- planning and design of outfalls
- risk analyses and accidental spillage of hazardous substances
- environmental impact assessment
- monitoring of outfalls
- monitoring of dredging works

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