MODELLING POLLUTION: OIL SPILLS AND FAECAL CONTAMINATION

M. MATEUS AND R. FERNANDES

1 INTRODUCTION

Human activities in coastal areas degrade biota and affect human health. Pollution caused by oil spills and sewage disposal are among the most obvious examples of this reality. Both have clear detrimental effects, with obvious socio-economic consequences and, over the last decades, have been at the top of the list of estuarine management concerns. Public health risks posed by sewage discharge to sea led the United Nations Group of Experts on the Scientific Aspects of Marine Pollution (GESAMP) to place this threat on the top of its list of concerns, in 1990. While not harming the environment in the same way as oil pollution, sewage impairs human health by the transmission of enteric diseases. Human sewage contains enteric bacteria, pathogens and viruses, and the eggs of intestinal parasites. Contamination of food or drinking and bathing waters may therefore pose a public health hazard. There have been some instances of hepatic and enteric diseases contracted through bathing in contaminated waters (Clark 1992). In most developing countries, discharge of raw sewage in coastal areas and estuaries is still common practice, posing serious threats for the population that makes use of the waters.

Faecal and oil pollution assessment requires descriptive and predictive tools, such as numerical simulation models, that are able to reproduce the dynamics of the systems in study, and simulate the fate of the pollutants under a broad range of scenarios (Bach et al. 1995, Christodoulou et al. 1995, Rodriguez et al. 1995, Garvey et al. 1998, Mahajan et al. 1999, Noutsopoulos et al. 1999). This chapter presents synthetic description of the oil and faecal coliform modules of the MOHID modelling system. They have been applied in the ECOMANAGE study sites to study the influence of the hydrodynamic regime on the fate of these pollutants, their impact on the system, and in some cases, to test different management options.

2 MODELLING FRAMEWORK

Attaining an adequate description of the dynamics of contamination is imperative to define water quality management strategies and to develop realistic contingency plans to deal with potential threats. This is frequently achieved through the use of numerical model simulations. A major advantage of the use of models in pollution studies is that they can be used as a diagnostic tool (identifying and studying actual problems) and as a prognostic tool (testing different scenarios). In addition, numerical tools can be implemented to render forecast capacity to pollution assessments. The numerical tool must be able to achieve basic goals such as (1) an accurate assessment of the dispersion of the pollutant, and (2) a reproduction of the basic processes that affect the state and fate of the pollutant in the environment.

Contrary to oil spills that usually have a tremendous visual impact, feacal pollution can be unnoticed. A striking difference between these two forms of pollution is their residence time in the water; hydrocarbons can last for long periods of time when compared with faecal agents. Faecal bacteria are bioindicators, meaning that their residence time in aquatic systems is comparatively low, usually ranging from less than an hour to a few hours, and occasionally up to some days. However, from a modelling perspective, oil spills and faecal pollution share same basic requirements in respect to the underlying physical mechanisms of transport in water. Hydrodynamic processes govern the dispersion of contaminants in the receiving area. So, by coupling general hydrodynamic processes and pollutant-specific processes, models can determine the plume evolution, enabling the prediction of affected areas and ambient concentrations over time. In summary, models enable the assessment of the magnitude of the pollution.

The effects that transport, ambient conditions, domain geometry and bathymetry, and other variables have on the dynamics of these pollutants in aquatic environments, require that models have the ability to reproduce their contribution to the dynamics of the system. The MOHID numerical platform (more details in the previous chapter) is such a tool because of the wide range of processes it simulates. Within this modelling framework there are independent modules that deal with the dynamics of these pollutants. This chapter deals with these modules, addressing in a brief way the processes they simulate and the baseline modelling philosophy.

3 THE LAGRANGIAN MODULE

Lagrangian transport models are very useful to simulate localized processes with sharp gradients (submarine outfalls, sediment erosion due to dredging works, hydrodynamic calibration, oil dispersion, etc.). The MOHID model uses the concept of lagrangian tracers to assess the spatial-temporal evolution of the contamination plume, determined by tidal regime and local circulation. Tracers are transported by currents calculated by hydrodynamic model and each tracer has the ability to be associated with one or more properties (physical, chemical or biological). This model is a subset of the MOHID modelling system and has been used in other instances also to study pollutant dispersion (Gomez-Gesteira et al. 1999). At the present stage the model is able to simulate oil dispersion, water quality evolution and sediment transport. The lagrangian module interacts with other modules such as the oil dispersion module to simulate oil dispersion and the *Escherichia coli* decay module. Sediment transport can be associated directly to tracers using the concept of settling velocity.

3.1 Tracer concept

Tracers are characterized by their spatial coordinates, volume and a list of properties, each with a given concentration. The most important property of a tracer is its position in space (*x,y,z*). The tracer can be a water mass, a sediment particle or group of particles, a molecule or group of molecules, or even a phytoplankton cell. The movement of tracers can be influenced by the velocity field from the hydrodynamic module, by the wind from the interface water-air module, by the spreading velocity from oil dispersion module and by random velocity. Both volume and properties concentration of each tracer vary in time in response to different parameters and ambient conditions. For *E. coli*, for example, volume is affected by turbulent mixing while fecal concentration depends on environmental factors like irradiance, temperature and salinity. Tracers belonging to the same origin have the same list of properties and use the same parameters for random walk, *E. coli* decay, etc. Origins can differ in the way they emit tracers. There are three different ways to define origins in space: (1) Point Origins - emits tracers at a given point; (2) Box Origins - emits tracers over a given area; (3) Accident Origins - emit tracers in a circular form around a point. Origins, in turn, emit tracers in two different ways: (i) Continuous - emits tracers during a period of time; (ii) Instantaneous - emits tracers at one instant.

3.2 Tracer Movement

The major factor responsible for particle movement is generally the mean velocity. Spatial coordinates are given by the definition of velocity:

$$\frac{dx_i}{dt} = u_i(x_i, t) \tag{1}$$

where u is the mean velocity and x the particle position. This equation is solved using a simple explicit method:

$$x_i^{t+\Delta t} = x_i^t + \Delta t \cdot u_i^t \tag{2}$$

Higher order accuracy requires the use of an iterative procedure. For most natural flows, the explicit method is sufficiently accurate. Velocity at any point in space is calculated using a linear interpolation between the points of the hydrodynamic model grid. The lagrangian module allows splitting the calculation of the trajectory of the tracers into sub-steps of the hydrodynamic time step.

3.3 Turbulent Diffusion

Turbulent transport is responsible for dispersion. The effect of eddies over particles depends on the ratio between eddies and particle size. Eddies bigger than the particles make them move at random, while eddies smaller than the particles cause entrainment of matter into the particle, increasing its volume and mass according to the environment concentration. Random movement is calculated following the procedure proposed by Allen (1982). The random displacement is calculated using the mixing length and the standard deviation of the turbulent velocity component, as given by the turbulence closure of the hydrodynamic model. Particles retain that velocity during the necessary time to perform the random movement, which is dependent on the local turbulent mixing length. The increase in volume is associated with small-scale turbulence and is reasonable to assume it as isotropic. Under these conditions, small particles keep their initial form and their increase in volume is a function of the volume itself.

4 OIL SPILLS

The prediction and simulation of the trajectory and weathering of oil spills are essential to the development of pollution response and contingency plans, as well as to the evaluation of environmental impact assessments. In order to predict the fate of oil products spilled in coastal zones, the oil weathering model predicts the evolution and behavior of the processes (transport, spreading, evaporation, etc.) and properties (density, viscosity, etc) of the oil products.

Oil density and viscosity, and many different processes such as oil spreading, evaporation, dispersion, sedimentation, dissolution, emulsification and oil beaching have been included in the oil module. Depending on the characteristics of the computational mesh or the magnitude of the spill, the model considers different alternative methods to simulate some of these processes. The oil weathering module (OWM) uses mainly the hydrodynamics and lagrangian transport modules. The hydrodynamic module simulates the velocity field necessary for the lagrangian module to calculate oil trajectories. These oil trajectories are computed assuming that oil can be idealized as a large number of particles that independently move in water.

Water properties and atmospheric conditions are introduced in the lagrangian module and used by the oil module to determine oil processes and properties. Except for the spreading and oil-beaching, all weathering processes and properties are assumed to be uniform for all tracers, like water properties and atmospheric conditions. These are assumed to be equal to the environmental conditions at the accident's origin. Oil temperature is assumed equal to water temperature, neglecting solar radiation or any other energy transfer process that may influence oil temperature. In its current setup MOHID OWM is not a 3D application. It simulates the amount of oil that leaves the water surface (by different processes like evaporation, or dispersion in water), without simulating the evolution at the subsurface and variations in the water column.

4.1 Modelled processes

Only a description of the modelled processes is presented here, since detailed information on the governing equations and model parameterization is available in the form of a User's Manual for download at the MOHID's model website (`http://www.mohid.com`).

4.1.1 Spreading

For an instant spill accident, the initial area of spilled oil is calculated according to Fay's formulation (Fay 1969). Two different algorithms are available to estimate oil spreading. One of the algorithms determines random velocities assuming a uniform distribution inside a range (in directions *x* and *y*), proportional to diffusion coefficients, which are calculated assuming that lagrangian tracers spreading is equivalent to Fay's formulas solution (Fay 1969). The only phase simulated in spreading is the gravity-viscous phase, from solutions proposed by Fay.

The other algorithm proposed for oil spreading is based in thickness differences inside the oil slick, presuming that the existence of a thickness gradient generates a ”spreading force” in the direction of minor thickness. Therefore, a tracer will move from the computational cell with larger oil thickness to the thinner one. This formulation uses a coefficient to approach the solution to the Fay solution, in order to make results sensible to some factors, like different oil densities, originating different behaviors. In the oil module, velocities are calculated in the faces of cells where oil is present, in directions *x* and *y*. Subsequently, in the lagrangian module tracer velocities are interpolated based on cell faces velocities and tracer position. If the average oil thickness becomes too thin (less than a value between 0.1 and 0.01 mm, depending of product viscosity), oil spreading is stopped.

4.1.2 Density and viscosity

Oil density is estimated considering the density of the emulsion at ambient temperature, the density of fresh oil at a reference temperature and the water temperature. The oil's initial density is obtained from the algorithm proposed by the American Petroleum Institute (API). Only oil products with lower density than water are modelled, because higher density products will sink. In the model the oil viscosity is controlled by three major factors: temperature, evaporation and emulsification.

4.1.3 Evaporation and emulsification

In MOHID the oil evaporation process can be estimated by two different methods: an analytical method, also known as the evaporative exposure method (Stiver and Mackay 1984), and by a more recent methodology proposed by Fingas (1998), where the relevant factors are time and temperature. Square root equations can also be used in some refined oils and in short term simulations (1-2 days). The emulsification process consists in the incorporation of water in oil, usually starts after a certain amount of oil has evaporated. An emulsification constant is used, which means the percentage of oil evaporated before emulsification starts. By default, this constant is 0%. When emulsification starts, incorporation of water in oil can be simulated by two different algorithms: the widely used equation of Mackay et al. (1980) and the Rasmussen equation (Rasmussen 1985).

4.1.4 Dispersion

This is the process where oil droplets entrain the water column. Two different methods are available to predict this weathering process, based on the formulations proposed by Delvigne and Sweeney (1998), and Mackay et al. (1980). The latter method is a simplified algorithm developed for vertical dispersion as a function of squared wind velocity, for conditions where turbulent energy is difficult to determine.

4.1.5 Dissolution

Dissolution is quantified through the Cohen method, considering the analytical solution for the solubility of typical oil proposed by Huang and Monastero (1982).

4.1.6 Sedimentation

Although the process of oil sedimentation is relatively difficult to estimate, the MOHID model uses a formulation developed by Science Applications International (Payne et al. 1987) for this purpose. Only droplets greater than 70 microns and smaller than 200 microns are considered for sedimentation. Bigger droplets are less likely to stick to sediment particulate matter, and those smaller than 70 microns are already estimated in the dispersion process.

4.1.7 Oil-Beaching

When oil reaches a coastal zone, it might become beached. This model estimates the amount of beached oil when the model user predefines a beaching probability (or different beaching probabilities for different coastal zones).

5 FAECAL CONTAMINATION

The reduction of faecal contaminant loads in the water is achieved by a combination of three main factors: initial dilution, dispersion and bacterial decay. Dynamic models usually take into consideration the physical processes of dilution and dispersion but frequently ignore the influence of abiotic effects on bacteria mortality by assuming a fixed mortality rate. Under certain conditions, this limitation hinders the results. For the specific case of the decline in faecal indicator bacteria, several studies have shown a particularly relevant role of abiotic factors like temperature, salinity and irradiance (Pereira and Alcantara 1993, Sarikaya and Saatci 1995, Serrano et al. 1998). A more realistic assessment of temporal and spatial faecal contamination can be achieved by using a feacal decay model with a dynamic T90 as a function of instant solar radiation, water temperature and salinity. Faecal dispersion can be simulated using both the lagrangian and the eulerian transport schemes.

5.1 Faecal decay model

TC and FC groups have similar decay rates (Marais 1974) and have been commonly used as indicators to assess water quality state. The die-off rate of this class of organisms is represented by a first-order equation (Chick's Law for disinfection), which states that the rate of loss is proportional to the concentration:

$$\frac{\partial N}{\partial t} = -kN \tag{3}$$

where N is the initial bacterial concentration in the effluent and k, the first-order decay rate (day^{-1}) or die-off coefficient, usually described in the form of a sum of individual parameters:

$$k = k_b + k_i + k_s + k_p \tag{4}$$

where k_b is the base mortality - a function of temperature and salinity - k_i is the death rate due to solar radiation, k_s is the net loss/gain due to settling/resuspension, and k_p is the mortality rate induced by predation. In the MOHID framework the fecal mortality model accounts for the impacts of temperature, salinity and ambient light in the decay of fecal indicators. It is derived from in situ and laboratory studies of mortality rates of *E. coli* made in the Cantabrian Sea (Canteras et al. 1995). The contribution of settling/suspension and grazing were not considered. As such, the simultaneous combination of all factors considered is expressed as:

$$k = 2.533 \times 1.04^{(T-20)} \times 1.012^{S} + 0.113 i_z \tag{5}$$

where S and T are the surrounding water salinity and temperature (°C), respectively, and i_z is the irradiance (watt m^{-2}) at depth z (m). Irradiance levels in the water environment are estimated by the hydrodynamic model where the light extinction is already parameterized and the irradiance is known for each vertical layer (depth integrated). This implies that for 2D-horizontal settings a mean value is calculated from irradiance levels at surface, considering the light attenuation effect of water molecules over the height of the water column. Bacterial decay is usually expressed as T90, the time in which 90% of population is no longer detectable, meaning 1 log reduction in number of pathogens. Assuming a first-order loss, the 90% mortality time is obtained by:

$$T_{90} = 2.303 k^{-1} \tag{6}$$

Together with FC concentrations, the model also outputs T90 values since these can be used to explain the underlying dynamics of the contamination patterns. This is particularly useful is systems with a high spatial and temporal changes in ambient conditions.

5.2 The influence of abiotic parameters

Fixed T90 values are still widely used in modelling studies to assess the impact of bacterial inputs in water bodies (Kashefipour et al. 2002). However, when this methodology is applied to areas with strong daily fluctuations of irradiance, usually associated with tidal movements ressuspending sediments and blocking light, it may fail to consider the major influence of light in bacterial decay. The explicit modelling of abiotic effects on FC decay, on the other hand, accounts for the variation in ambient conditions. The wide range of T90 values over a daily cycle is obvious when we consider a typical diel period in late spring and summer at mid latitudes. It has been pointed that impact studies of FC contamination usually consider T90 values lower than the values measured in culture experiments (Guillaud et al. 1997). This assumption can compromise the quality of model predictions, limiting the role of models has predictive tools. This is further aggravated because static values are used from the entire simulation period.

REFERENCES

Allen C M (1982) Numerical-Simulation of Contaminant Dispersion in Estuary Flows. Proceedings of the Royal Society of London Series a-Mathematical Physical and Engineering Sciences 381: 179-194

Bach H K, Orhon D, Jensen O K, Hansen I S (1995) Environmental-Model Studies for the Istanbul Master-Plan .2. Water-Quality and Eutrophication. Water Science and Technology 32: 149-158

Canteras J C, Juanes J A, Perez L, Koev K N (1995) Modeling the Coliforms Inactivation Rates in the Cantabrian-Sea (Bay-of-Biscay) from in-Situ and Laboratory Determinations of T-90. Water Science and Technology 32: 37-44

Christodoulou G C, Ioakeim I, Ioannou K (1995) Modeling of pollution from the wastewater discharge of the city of Limassol. Water Science and Technology 32: 197-204

Clark R B (1992) Marine Pollution. Clarendon Press, Oxford. 172p.

Delvigne G A L, Sweeney C E (1998) Natural Dispersion of Oil. Oil & Chemical Pollution 4: 281-310

Fay J A (1969) The spread of oil slicks on a calm sea. In: (eds) Oil on the Sea. Plenum Press, New York, pp 53-63

Fingas M. 1998. The evaporation of oil spills: development and implementation of new prediction methodology. In: Marine Environmental Modelling Seminar ’98. Lillehammer, Norway.

Garvey E, Tobiason J E, Hayes M, Wolfram E, Reckhow D A, Male J W (1998) Coliform transport in a pristine reservoir: Modeling and field studies. Water Science and Technology 37: 137-144

Gomez-Gesteira M, Montero P, Prego R, Taboada J J, Leitao P, Ruiz-Villarreal M, Neves R, Perez-Villar V (1999) A two-dimensional particle tracking model for pollution dispersion in A Coruna and Vigo Rias (NW Spain). Oceanologica Acta 22: 167-177

Guillaud J F, Derrien A, Gourmelon M, Pommepuy M (1997) T90 as a tool for engineers: Interest and limits. Water Science and Technology 35: 277-281

Huang J C, Monastero F C (1982). Review of the state-of-the-art of oil spill simulation models - Final Report. American Petroleum Institute.

Kashefipour S M, Lin B, Harris E, Falconer R A (2002) Hydro-environmental modelling for bathing water compliance of an estuarine basin. Water Research 36: 1854-1868

Mackay D, Buistt I A, Mascarenhas R, Paterson S (1980). Oil spill processes and models., Environment Canada Manuscript Report No. EE-8, Ottawa, Ontario.

Mahajan A U, Chalapatirao C V, Gadkari S K (1999) Mathematical modeling - A tool for coastal water quality management. Water Science and Technology 40: 151-157

Marais G R (1974) Fecal Bacterial Kinetics in Stabilization Ponds. Journal of the Environmental Engineering Division-Asce 100: 119-139

Noutsopoulos C, Gavalaki E, Andreadakis A (1999) Evaluation of the impact from the discharge of treated sewage on the south-east Saronicos Gulf through mathematical water quality modelling. Water Science and Technology 39: 63-70

Payne J R, Kirstein B E, Clayton J R, Clary C, Redding R, McNabb D, Farmer G (1987). Integration of Suspended Particulate Matter and Oil Transportation Study. Final Report, Report to Minerals Management Service, MMS 87-0083

Pereira M G, Alcantara F (1993) Culturability of *Escherichia-Coli* and Streptococcus-Faecalis in Batch Culture and in-Situ in Estuarine Water (Portugal). Water Research 27: 1351-1360

Rasmussen D. 1985. Oil Spill Modelling - A tool for cleanup operations. In: Oil Spill Conference, American Petroleum Institute. pp243-249

Rodriguez A, SanchezArcilla A, Redondo J M, Bahia E, Sierra J P (1995) Pollutant dispersion in the nearshore region: Modelling and measurements. Water Science and Technology 32: 169-178

Sarikaya H Z, Saatci A M (1995) Bacterial Die-Away Rates in Red-Sea Waters. Water Science and Technology 32: 45-52

Serrano E, Moreno B, Solaun M, Aurrekoetxea J J, Ibarluzea J (1998) The influence of environmental factors on microbiological indicators of coastal water pollution. Water Science and Technology 38: 195-199

Stiver W, Mackay D (1984) Evaporation Rate of Spills of Hydrocarbons and Petroleum Mixtures. Environmental Science & Technology 18: 834-840