MATHEMATICAL MODELS IN WATER SCIENCES

V. B. Zalesny

Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow, Russia

R. Tamsalu

Estonian Marine Institute, Tallinn, Estonia

Keywords: Mathematical model, Climatic system, Data assimilation, Ecosystem, General circulation, Geophysical hydrodynamics, Hydrodynamics, Numerical simulation, Ocean waves, World Ocean

Contents

- 1. Introduction
- 2. Mathematical Models in Hydrodynamics
- 2.1. Incompressible Inviscid Fluid
- 2.2. Compressible Inviscid Fluid
- 2.3. Viscous Incompressible Fluid
- 3. Mathematical Models of Flows in Rivers, Lakes, and Coastal Waters
- 3.1. Rivers
- 3.2. Lakes
- 3.3. Coastal Waters and Estuaries
- 4. Mathematical Models of Circulation in Oceans and Seas
- 4.1. General Circulation of Seas and Oceans
- 4.2. Equations of a General Circulation of Seas and Oceans.
- 4.3. Peculiarities of Large-scale Dynamics of Seas and Oceans
- 4.4. Data Analysis
- 5. Mathematical Models of Water Waves
- 5.1. Tidal waves
- 5.2. Wind waves
- 5.3. Internal waves
- 5.4. Tsunami
- 6 Mathematical Models for Water Resources Management
- 6.1. Modeling of Water Quality and Ecosystems
- 6.2. Structure of Water-Ecosystem Models
- 6.3. Simplified Ecosystem Model
- 6.4. Adjoint Equation Analysis
- 7. Conclusion
- Glossary
- Bibliography

Biographical Sketches

Summary

Mathematical models for description of water motion in the natural water bodies on the Earth are considered. Starting from classic mathematical models of hydrodynamics the

consideration extends over a wide range of the models for different water bodies: rivers, lakes, estuaries, seas, and oceans.

The models considered are related to the new scientific discipline which comes out of classical Hydrodynamics in the last quarter of the 20th century – Geophysical Hydrodynamics. It studies natural water objects and phenomena. The main peculiarities of physical problems and mathematical models of Geophysical Hydrodynamics are rotation, stratification, complex geometry of water bodies, nonlinearity and turbulent character of water flows. Complex physical character of natural objects and processes determines the main mathematical instrument which is mostly used in Geophysical Hydrodynamics – mathematical modeling and numerical analysis.

Models at different levels of physical complexity ranging from conceptual onedimensional model of a selected phenomenon to three-dimensional ones describing a wide spectrum of different scale water motions are presented. Some information about pronounced processes is included and their typical mathematical model equations are discussed. These are river discharge model; models of tidal, surface, internal, and long solitary waves in lakes, seas, and oceans; ocean and sea general circulation model; ecosystem model; etc.

From a mathematical point of view the models discussed are initial – boundary value problems for partial differential equations and system of equations. The governing equations belong to different types of differential equations: hyperbolic, parabolic, and to the non-classical system of equations which contains as evolutionary (prognostic) equations as equations without time derivatives. The following well-known equations are considered: Saint Venant, Korteweg de Vries, Bussinesq, shallow-water, and ocean general circulation primitive equation system.

1. Introduction

Mathematical models in water sciences describe a wide spectrum of processes at different time and space scales which take place in various water bodies on the Earth. The circulation of water in artificial reservoirs in laboratories and engineering (industrial) constructions; currents and waves in rivers, lakes and coastal areas; circulation in the sea and ocean; wave motions are considered here.

Physical processes which are described by mathematical models have a complex character. From a mathematical point of view the peculiarity of the models which are used in water sciences is primarily connected with non-linear phenomena. This makes it difficult, and in most cases impossible, to find their exact solutions and therefore leads to the necessity of using numerical calculations and experiments.

From an engineering and economic point of view, in such studies we should take into account the hardness and high price of measurements and observed data, the heavy expenses spent on protection from natural disasters.

Historically, development of water sciences is connected first of all with the development of hydrodynamics, one of the oldest of sciences. Hydrodynamics is concerned with the laws of fluid motion and physical objects which have fluid property.

Fluidity is an ability to deform under the influence of weak external forces. Fluidity is also typical for a gas; that is why a gas is often regarded as a fluid. The main difference between a gas and fluid (liquid) is that they have diverse degrees of compressibility. Fluids as water, for instance, are slightly compressible. Their ability to form a free surface is connected with this property, slight compressibility if the fluid is contained in some reservoir.

For the description of water movement in hydrodynamics mathematical models on the basis of general laws of mechanics, particularly the conservation law for momentum, mass, and energy are used. In addition to these three conservation laws, models require a state equation relating several of the components in the other equations, and sometimes additional equations, for example salinity equation for sea water. They are combined with some conditions and parameters which characterize the specific properties of water environment: fluidity, incompressibility, turbulence, etc.

Applying the general laws of mechanics and using supplementary physical dependencies and parameters the problem of studying water motion is reduced to some systems of differential or intego-differential equations. As the described movement is restricted by some boundaries such as lateral walls, bottom, and free surface, great attention is paid to the formulation of boundary conditions while constructing mathematical models. Boundary conditions are formulated on solid motionless and moving parts of the contour lines, liquid and free boundaries. The system of equations and boundary conditions includes also a description of the influence of the external forces, for example the influence of wind at the sea surface. Initial conditions are added to the systems which characterize the state variables at initial moment, for instance, motionlessness.

After the formulation of a mathematical model as a system of equations with initial and boundary conditions, the question about its solution or qualitative study of the solution's behavior arises. Historically, hydrodynamics was developed under the influence of mathematics. It used mathematical methods of the theory of differential and integral equations; the theory of complex variables and special functions; statistical methods; the theory of potential, etc. On the other hand, it too had an influence on mathematics itself. Many parts of mathematics were initiated and developed while solving hydrodynamical problems.

With the development of theoretical methods and gain of practical experience, nonlinear models arose in hydrodynamics and special parameterizations of turbulent processes are taken into account. This results in considerable complexity of mathematical models and it also excludes in most cases the possibility of their exact solution. Particularly, it becomes distinctive for geophysical hydrodynamics, a young science which comes out of classical hydrodynamics in the last quarter of the 20th century.

Geophysical hydrodynamics studies geophysical hydrodynamical objects and phenomena. These are turbulent flows on the rotating Earth, stratified by density. The main peculiarities of physical problems and mathematical models of the geophysical hydrodynamics, which is connected with water sciences are rotation, stratification, complex geometry of the water bodies, and turbulent character of water flow. Because of the complex mathematical and physical character, the position and solving of problems in geophysical hydrodynamics are connected and determined by the development of approximate methods. The main method of them is the method of numerical modeling. Further progress in the solution of problems of hydrodynamics and geophysical hydrodynamics is linked with fast development of computers at the end of the 20th century and with methods of computational mathematics.

On a level with the methods of mathematics, computational mathematics and numerical modeling, it should be mentioned that there is a continuous coupling of hydrodynamics and geophysical hydrodynamics, with physical experiments and possible natural observations. On the one hand, it brings these scientific fields closer to physics and on the other hand it stimulates the search of new mathematical approaches and methods. As an impressive example here we see that the methods of optimal control, statistical methods, data assimilation and data processing methods are more and more widely used.

2. Mathematical Models in Hydrodynamics

Extensive use of mathematical simulation methods became a distinctive feature of modern researches in hydrodynamics. Science and practice put forward in hydrodynamics such problems whose full investigation in most cases can be made only approximately, numerically or with the help of physical or natural experiments. Most hydrodynamical processes and phenomena are so complex that it is difficult to make their universal theory and it may be done very seldom. We mean the theory which would be adequate in all space-time domains. Here mathematical simulation, numerical experiment and observational data analysis can help the theory.

Using experiments and observational – experimental data analysis it is necessary to understand the key factors which control the process over the some time- space subdomain. By selecting these factors, and leaving the less important ones in the given space-time subdomain, we can create a mathematical model of the process. Such a model could be regarded as a conceptual one, describing the main hydrodynamic process taking into account just the selected factors. Sometimes, by simplifying the geometry of the currents and sketching the process, as much as possible, one can reduce the model to a system of differential equations that admit an analytical study. Then considering secondary, finer, but still essential factors, in order to get a more detailed description of the real physical process, one may successively enrich the model.

2.1. Incompressible Inviscid Fluid

When studying the water motions, the water compressibility may be often ignored. Free inviscid fluid motion is expressed by Euler's equations

$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U}, \nabla)\mathbf{U} = -\frac{1}{\rho}\mathbf{grad}P + \mathbf{F},\tag{1}$$

$$\operatorname{div} \mathbf{U} = \mathbf{0}.$$
 (2)

The first equation comes from Newton's second law of motion. This is one of the main equations of hydrodynamics and was originally established by Euler in 1755. It contains the moving particles' acceleration on its left-hand side and on the right-hand side the forces acting on them: pressure gradient and forcing (\mathbf{F}). The second equation is the continuity equation. It is a mathematical form of the incompressibility condition.

The fluid is regarded as a continuum. It means that any small size element of a water volume including fluid parcels, is considered so big that still it contains a great number of molecules. The function in (1) - (2): U -fluid parcel velocity, P - pressure, ρ -density, and **F** - forcing, are functions of coordinates "x, y, z" and time "t". The velocity U(x, y, z, t) with its components u(x, y, z, t), v(x, y, z, t), w(x, y, z, t) is defined at all the space points (x, y, z) and at the time point t. The velocity is related exactly to the points of the motionless space, not to the particles of the moving fluid. The same concerns P and ρ .

Initial and boundary conditions.

The motion, described by Equations (1) – (2), is considered over the period $t \in (t_0, t_1]$ in a certain domain D with boundary ∂D . In this connection Equations (1) - (2) require additional initial and boundary conditions.

The initial conditions are reduced to setting a velocity vector U at initial moment t_0

$$\mathbf{U} = \mathbf{U}_{\mathbf{0}}$$
 at $t = t_0$, everywhere in D (3)

The motion depends on the boundary conditions at ∂D for all $t \in (t_0, t_1]$. In most problems the boundary ∂D is divided into four parts: a solid motionless boundary ∂D_1 (coastline of a lake or ocean); free surface boundary ∂D_2 (sea surface); solid moving boundary ∂D_3 (side of a floating ship) and liquid boundary ∂D_4 (conventional surface separating, for example, the ocean from littoral waters). On each part of the boundary ∂D one has to set certain conditions for the velocity vector **U**.

At the solid motionless boundary ∂D_1 the kinematic (no-normal-flow) condition is usually set as:

$$U_{n} = 0$$
 or $(U, n) = 0$. (4)

At the upper free surface boundary ∂D_2 , satisfying $z = \zeta(x, y, t)$, the following conditions are set:

$$\frac{\partial \zeta}{\partial t} + (\mathbf{U}, \operatorname{grad} \zeta) = w \tag{5}$$
$$P = P_a,$$

where P_a is the atmospheric pressure. The unknown function $\zeta(x, y, t)$ satisfies a certain initial condition.

At the solid moving boundary ∂D_3 which is described by equation

G(x, y, z, t) = 0,

the following condition is set

$$\frac{\partial G}{\partial t} + (\mathbf{U}, \operatorname{grad} G) = 0.$$

The open liquid motionless boundary ∂D_4 requires certain velocity vector components or its function set. It should be noted that the position of boundary conditions at the open boundary is a delicate question because the Equations (1) – (2) are close to being hyperbolic.

(6)

Note.

Along with Euler's equations (1) - (2) other forms are known. There are equations in Lagrange's variables and in Gromeka – Lamb's form. Equations in Lagrange's variables: a_i, t where $a_i (i = 1, 2, 3)$ are Cartesian coordinates were also suggested by Euler, simultaneously with Equations (1) - (2).

The partial differential equations (1) - (2) have a common character. Adding supplementary conditions might generate some applications and special cases. The most commonly used conditions are the following.

Potential motion.

If the fluid is under potential forcing field, then

$\mathbf{F} = \mathbf{grad}A$,

where A is the potential particularly, in the gravity field which acts along the downward vertical axis z:

A = gz.

For potential motion, the theorem about circulation of the velocity vector Γ along arbitrary closed liquid contours l is applied:

$$\frac{d\Gamma}{dt} = \frac{d}{dt} \int_{l} (\mathbf{U}, d\mathbf{x}) = 0.$$
(7)

The circulation of velocity vector along a closed contour during motion remains constant. Hence, if at the initial moment the fluid was at rest $(\mathbf{U} = 0)$, then circulation along an arbitrary contour is identically equal to zero for all time moments. Hence, owing to the Stokes's theorem we have:

$$\int_{l} (\mathbf{U}, d\mathbf{x}) = \int_{\Sigma} (rot \, \mathbf{U}, \mathbf{U}) d\Sigma$$
(8)

(where Σ is a surface having the contour l). Because Σ is an arbitrary surface, for all times, it follows that

 $rot \mathbf{U} = 0.$

(9)

The function rot**U** is called vorticity. It determines the angular velocity of the rotating fluid volume. In this way Equation (9) denotes absence of the rotation. If motion is considered in a simply-connected domain, then (9) is a necessary and sufficient condition of the potentiality of the velocity field. In this case there is a scalar function $\varphi(\mathbf{x},t)$ - velocity potential

$$\mathbf{U} = \operatorname{grad}\varphi.\tag{10}$$

Owing to the continuity equation the potential of the velocity φ is a harmonic function satisfying Laplace equation

$$\Delta \varphi \equiv \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0.$$
(11)

Besides, from the momentum equation it follows that

$$\operatorname{grad}(\frac{\partial\varphi}{\partial t} + \frac{u^2 + v^2 + w^2}{2} + \frac{P}{\rho} - A) = 0$$
(12)

and Cauchy-Lagrange equation is valid

$$\left(\frac{\partial\varphi}{\partial t} + \frac{u^2 + v^2 + w^2}{2} + \frac{P}{\rho} - A\right) = \Phi,$$
(13)

where $\Phi = \Phi(t)$ is an arbitrary function of time.

Steady motion

One can construct a further simplification of the model assuming that the motion is in equilibrium, i.e. a velocity field does not depend on time. In this case the mathematical model is described by the equations:

$$\Delta \varphi = 0, \qquad \qquad \mathbf{U} = \operatorname{grad} \varphi,$$

$$\frac{u^2 + v^2 + w^2}{2} + \frac{P}{\rho} - A = \text{const}.$$
 (14)

Equation (14) is called the equation of Bernoulli.

2.2. Compressible Inviscid Fluid

The compressibility of a fluid is essential when we consider its motion at high velocities which are comparable with the speed of sound in the fluid. In this case density variation becomes important. Density can not be considered as known constant quantity and it should be considered as an unknown function. The problem becomes more complex and absolutely new effects and phenomena appear which do not exist for incompressible fluid. Equations describing the motion of compressible inviscid fluid are of the kind:

$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U}, \nabla) \mathbf{U} = -\frac{1}{\rho} \mathbf{grad} P + \mathbf{F}, \tag{15}$$

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{U}) = 0, \tag{16}$$

$$\frac{ds}{dt} = \frac{\partial s}{\partial t} + (\mathbf{U}, \nabla) s = 0, \tag{17}$$

$$P = P(\rho, s). \tag{18}$$

Thermodynamic equation (17) expresses the absence of heat exchange between water parcels. The entropy *s* of every parcel is constant. Equation (18) which connects the unknown functions s, ρ with pressure is called the equation of state. It comes from the general laws of thermodynamics. A definite form of dependency is determined by the properties of medium. The model equations for compressible inviscid fluid (15) – (18) are used, as a rule, for describing gas motion. For water system they are not applied in their original form. On the one hand they are interesting for us as a theoretical development of the model and on the other one as they are similar to the shallow-water equations. A well-known system of the shallow-water equations which describe plane motion have the form:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = g \frac{\partial \zeta}{\partial x},\tag{19}$$

$$\frac{\partial \upsilon}{\partial t} + u \frac{\partial \upsilon}{\partial x} + \upsilon \frac{\partial \upsilon}{\partial y} = g \frac{\partial \zeta}{\partial y},\tag{20}$$

- -
- -
- -

TO ACCESS ALL THE **65 PAGES** OF THIS CHAPTER, Visit: <u>http://www.eolss.net/Eolss-sampleAllChapter.aspx</u>

Bibliography

A.E.Gill, 1974, *Atmosphere – ocean dynamics. –* Academic Press, New York. [This is a well known book that presents fundamental aspects of atmospheric and ocean dynamics].

G.J.Komen, L. Cavaleri, M. Donelan, K. Hasselman and P.A.E.M. Janssen, 1994, *Dynamics and modelling of ocean waves.* – Cambridge University Press, Cambridge, 523 p. [The book presents fundamental and applied aspects of ocean waves modeling, including the use of satellite observations in wave models].

Lavrentiev M.A., Shabat B.V., 1973, *Problems of hydrodynamics and their mathematical models.* – Moscow, Nauka, 416 p. [This is a book that presents and discussed some mathematical problems of hydrodynamics].

Landau L.D., Lifshitz E.M., 1959, *Fluid mechanics, vol 6 of Course of theoretical physics.* – London, Pergamon Press. [This classic textbook presents the background for theoretical hydrodynamics].

Marchuk G.I., 1992, *Adjoint equations and analysis of complicated system*. Nauka, Moscow. [This book presents essential aspects and approaches for complex system analysis on the base of adjoint equations].

Marchuk G.I., Dymnikov V.P., Zalesny V.B., 1987, *Mathematical models in geophysical fluid dynamics and numerical methods of their realization.* – Leningrad Gigrometeoizdat, 296 p. [The book presents and discusses methods of mathematical modeling and numerical analysis of atmospheric and oceanic general circulation].

Martin J.L., McCutcheon S.C., 1999, *Hydrodynamics and transport for water quality modeling*, Lewis Publishers, Boca Raton, London, New York, Washington D.C., 794 pp. [This is a handbook that presents a wide information about physics, modeling, and numerical technique for water flows in rivers, lakes, estuaries, etc.].

Biographical Sketches

Zalesny Vladimir B. Professor, Institute of Numerical Mathematics, Moscow, Russia, was born on 12.08.1946. and graduated from the Department of Mechanics and Mathematics of the Novosibirsk State University. He is the author of 4 books and more than 90 scientific publications in the field of mathematical modeling in Geophysical Hydrodynamics and Oceanology. His interests are in the development of numerical models of the large-scale marine dynamics, simulation of ocean general circulation and its interaction with atmospheric processes. During more than 20 years he has been teaching students at the Moscow Institute of Physics and Technology on the subject of Computational Physics.

Tamsalu Rein, Professor, Estonian Marine Institute, Tallinn, Estonia, was born on 27.03.1940 and graduated from the Department of Natural Science of Tartu University. Then he left for St. Petersburg, where he studied Physics under Professors V. Timonov and B. Kagan. In 1968 he went to Novisibirsk, Academic City, and became a scientific collaborator for Academician G. Marchuk. In 1972 he returned to Estonia and established the marine system modeling team. In the 1980's Tamsalu together with P. Malkki started a long development process through Estonian-Finnish cooperation in marine hydrodynamic-ecosystem modeling. During 1992-1999 he worked at the Finnish Institute of Marine Research. He is a

specialist in the field of numerical simulation of the tidal motion, water dynamics and ecosystem modeling. He is the author of 3 books and more than 80 scientific publications.

			302	5
	<			
	\sim	AL,		
N'AL	<u>S</u>			
SA				