University Politehnica of Bucharest

Faculty of Power Engineering

PhD. Thesis Summary

MODELLING in SURFACE WATER QUALITY

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Abstract:

In the present thesis, different mathematical models have been developed to simulate the pollutant dispersion and the water quality along Danube River at Drobeta-Turnu Severin region. These models were based on the fundamental Advection-Dispersion Equation (ADE) for pollutant transport in running waters. The proposed models have a different level of complexity. They are able to simulate releases from point source pollution. The numerical models were solved using the CFD technique (FlexPDE and Fluent codes) to provide valuable information on the flow rate and the pollutant dispersion in the rivers. On the other hand, an attempt has been made to explore the applicability of QUAL2K for simulating the water quality in the Danube River. The main aim was to examine the impact of Danube's tributaries and other waste loads on the river itself. Furthermore, a supported tool for water quality assessment such as multivariate statistical techniques (factor and cluster analyses) and the water quality indices (WQIs) were also used along with the proposed numerical models to identify the major factors affecting the water quality of Danube River and to evaluate the spatial and temporal variations among the sampling stations and monitoring periods. The output results of the simulations along with these water quality assessment tools may provide a comprehensive vision for decision makers to propose strategies for reliable water quality management in the region.

Modelarea calităţii apelor de suprafaţă

În lucrarea de față, au fost dezvoltate diferite modele matematice pentru a simula dispersia poluanților și calitatea apei de-a lungul fluviului Dunărea în regiunea Drobeta-Turnu Severin. Aceste modele au fost bazate pe ecuaţia fundamentală de Advecţie-Dispersie (ADE) pentru transportul poluantului în apele curgătoare. Modelele propuse au un nivel diferit de complexitate. Ele sunt capabile să simuleze eliberări din surse de poluare punctuală. Modelele numerice au fost rezolvate folosind tehnici CFD (FlexPDE și coduri Fluent) pentru a furniza informații valoroase privind dispersia poluanților în râuri și pune în evidență effectual de mal. Pe de altă parte, a fost făcută o încercare de a explora aplicabilitatea QUAL2K pentru simularea calității apei în fluviul Dunărea. Scopul principal a fost de a examina impactul afluenților asupra Dunării și a altor deversări poluante în fluviu. Un instrument acceptat pentru evaluarea calității apei, cum ar fi tehnicile statistice multivariate (analiză cluster şi factorială) și indicii de calitate a apei (WQIs) au fost utilizate împreună cu modelele numerice propuse pentru a identifica factorii majori care afectează calitatea apei fluviului Dunărea și pentru a evalua variațiile spațiale și temporale între stațiile de prelevare și perioadele de monitorizare. Rezultatele simulărilor, împreună cu aceste instrumente de evaluare a calității apei, pot oferi o viziune globală pentru ca organele decizionale să propună strategii pentru managementul fiabil al calității apei în regiune.

Keywords: Pollutant dispersion; Biochemical oxygen demand; Dissolved oxygen; River water quality; Surface water.

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Chapter 1: Introduction

1.2. Problem addressed

Many rivers are deteriorated by anthropogenic impacts and also natural processes. These processes may impair the river use for drinking and other uses. The most common practice that affects rivers is the pollutant discharges. Therefore it is highly required to assess and predict the water quality of rivers and the pollutant dispersion along rivers in order to provide basis for the decision makers. This issue can be addressed using reliable support tools for water quality assessment and modeling. Mathematical modelling and assessment tools of water quality are the most commonly used methods for addressing the pollutant discharges in rivers. These techniques are the main concern of this thesis.

In the present thesis, the Danube River was selected as a case study for the assessment and modeling processes. It has an aggregate length of 2780 km with catchment area of 801500 km^2, with almost 81 million occupants in 19 countries. The importance of the river is given by numerous factors that influence its quality, for example, expanding impacts of human effect, contamination from farming, industries and municipalities which negatively influence the water supply, irrigation, and hydropower generation. Therefore, it is of prime importance to preserve and protect the quality of the river from overabundance contamination and to guarantee its sustainable development.

1.3. Thesis objectives

The main objectives of this thesis are:

- To predict the pollutant dispersion of the Danube River in 2D and 3D modeling using computational fluid dynamics (CFD) tools such as Fluent and FlexPDE.
- To simulate the water quality of the Danube River using 1D steady-state model (QUAL2K) and examine the impact of tributaries and other waste loads on the receiving river,
- To identify the major factors affecting the water quality of Danube River using multivariate statistical techniques,
- To evaluate the spatial and temporal variations among the sampling stations and monitoring periods,
  To assess the water quality in the Danube River using various water quality index models, and to explore the usefulness of these indices in assessing the water quality of Danube River

1.4. Thesis structure

The thesis is organized in 9 chapters; chapter 1 is consisting of an overview, thesis objectives and structure and the framework of the study. Chapter 2 includes general aspects of diffusion and dispersion of pollutant in rivers and pollutant transport phenomena with their modeling means for surface water quality management. Furthermore, brief descriptions of the turbulence flow modeling and reactions kinetics for non-conservative pollutants have also been given in this chapter. Chapter 3 includes a critical review of water quality models in current use. The selection of water quality models in this thesis are based on reviewing 11 popular water quality models. Chapters 4 and 5 include prediction of pollutant dispersion in the Danube River using CFD code. In chapter 4 FlexPDE was used for 2D simulation, whereas, in chapter 5, Fluent has been used to predict the pollutant dispersion in a channel with different flow rate using VOF method and scalar transport. Chapter 6 includes the application of water quality process model (QUAL2K) to simulate the DO and BOD concentration in the Danube River. Chapter 7 includes the assessment of the water quality of Danube River using multivariate statistical analysis such as factor analysis and cluster analysis. The main aim of this chapter is to identify the major factors that affect the water quality of Danube River and to evaluate the spatial and temporal variations. Chapter 8 consist the utilizing of various water quality index models to investigate the usefulness of these indices and to assess the spatial and temporal changes in the Danube River. The last chapter provides the conclusion of the study, the list of my personal scientific contributions and recommendations for future studies. The References are listed at the end along with the Appendices.

1.6. Investigated river stretches and field data

The Danube River is divided into three main parts: the upper Danube course (1060 km), the middle Danube course (725 km) and the lower Danube course (1075 km). The lower Danube course represents Romania’s natural border with Serbia, Bulgaria, Ukraine and the Republic of Moldova. The river flows through regions of distinct morphology. In the lower course, the river is flowing through Baziaş and Gura Văii passing the Iron Gate I (14 km upstream of Drobeta-Turnu Severin city). The Iron Gate I was constructed in 1971 and is considered as the largest dam and reservoir system on the basis of volume, area and hydropower potential among numerous impoundments on the Danube and the tributaries [214]. Drobeta-Turnu Severin is a city in Mehedinți County, Romania, on the left bank of the Danube, beneath the Iron Gates. The city administers three towns: Gura Văii, Dudașu Schelei , and Schela Cladovei (Fig. 1).

This study covers 13 km of the Danube River starting at Gura Văii, 2 km downstream of Iron Gate I, and extends to Drobeta-Turnu Severin city. Two major groups of industries exist in the region: south-west industrial area (upstream of Drobeta-Turnu Severin city), and south-east industrial area (downstream of Drobeta-Turnu Severin city). In addition, agricultural practices from Serbian part use fertilizers and pesticides which are being discharged to the river through surface runoff.

Water quality data were obtained for the year of 2008 in four sampling points, namely Gura Văii (SS1) which is about 2 km downstream of Iron Gate I, Dudașu Schelei (SS2), Schela Cladovei which is located upstream of Drobeta-Turnu Severin (SS3), and downstream of Drobeta-Turnu Severin (SS4) (Fig.1.2). The descriptive statistics of the hydraulic and water quality data are shown in the Table 1.1.

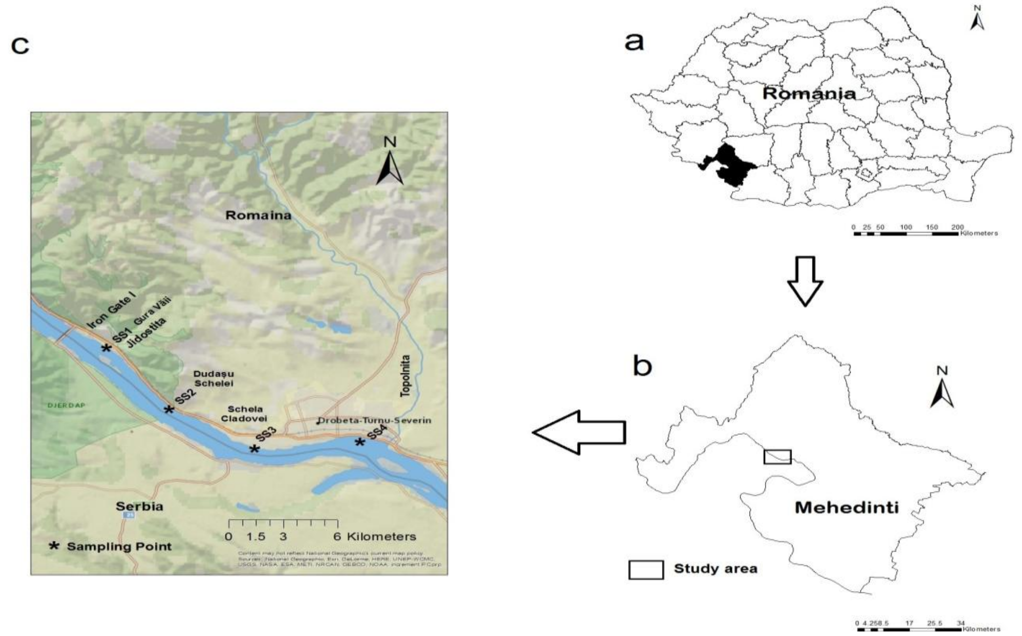


Fig 1.2 Map of the study area: a Romanian Counties, b Mehedinţi County and c Sampling Locations (created through ArcMap GIS)

Table 1.1 Descriptive statistical summary of Danube river water quality and quantity data in four sampling stations during 12 months in the year of 2008, *n* = 48

Parameters	Abbreviation	Unit	Minimum	Maximum	Mean	Std. Deviation
Dissolved Oxygen	DO	mg/L	5.61	12.69	9.12	2.09
Biochemical oxygen demand	BOD	mg/L	1.15	2.37	1.66	0.30
Ammonium	NH_4	mg/L	0.087	0.522	0.19	0.07
Nitrate nitrogen	NO_3	mg/L	0.195	3.614	1.98	0.88
Total phosphorous	TP	mg/L	0.132	1.44	0.43	0.27
Water Temperature	WT	˚C	4	27	15.72	7.27
pH	pH	-	7.1	7.7	7.43	0.15
Discharge	Q	m^3/sec	2650	8760	5642.60	1699.85
Total suspended solids	TSS	mg/L	21	34	26.44	2.93
Cadmium	Cd	µg/L	0.11	0.44	0.28	0.07
Cooper	Cu	µg/L	1.5	4	2.16	0.71
Chromium	Cr	µg/L	1.4	3.5	1.97	0.53
Nickel	Ni	µg/L	1.1	1.8	1.43	0.19
Lead	Pb	µg/L	0.7	1.9	1.37	0.34

Chapter 2: An overview of the pollution transport process in rivers and streams

2.1. Introduction

The literature support (chapter 2) deals with fundamental aspects related to pollutant transport in rivers and streams along with their modelling support, basic equations and theoretical models which have developed previously and related published studies. The non-conservative pollutants along with their reaction kinetics have been presented as this thesis considers these types of pollutants (BOD and DO). Moreover, the types of external sources that affect the river water system have also been described. The last three sections of this chapter present the turbulence modelling approaches along with the Eddy Viscosity Models (EVMs), free surface methods and the turbulent transport of scalars.

Generally, water quality modelling in rivers and streams can be categorized into: hydrodynamic model and water quality process model. Hydrodynamic models are used to simulate the flow and the pollutant dispersion along river with the possibility of considering the chemical/biological transformations. Water quality process models take into account the kinetics reactions of the river in more details. In some rivers, these transformations are very important and should be considered when simulating the non-conservative pollutants. Examples of these reactions: reaeration, settling, respiration, nitrification, denitrification and photosynthesis.

2.2. Pollutant transport in river

2.2.1.2. Turbulent diffusion

In the present thesis, different mathematical models have been developed to simulate the pollutant dispersion and the water quality along Danube River. These models were based on the fundamental Advection-Dispersion Equation (ADE) for pollutant transport in running waters. The basic three- dimensional form of ADE can be written as [183]:

$$\frac{\partial \overline{C}}{\partial t}+\frac{\partial}{\partial x}\left(\overline{u}\,\overline{C}\right)+\frac{\partial}{\partial y}\left(\overline{v}\,\overline{C}\right)+\frac{\partial}{\partial z}\left(\overline{w}\,\overline{C}\right)=\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial \overline{C}}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial \overline{C}}{\partial y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial \overline{C}}{\partial z}\right)+ D_m\left(\frac{\partial^2 \overline{C}}{\partial x^2}+\frac{\partial^2 \overline{C}}{\partial y^2}+\frac{\partial^2 \overline{C}}{\partial z^2}\right)+S(x,y,z,t) \tag{2.7}$$

where

$\overline{C}$ = mean value (in time) of substance concentration (kg/m^3)
t = time (sec)

u, v, w = velocity vector components in direction of x, y, z axis (m/s).

ε_x, ε_y, ε_z = dispersion coefficients on the three axes (m^2/s).

S = sources and sinks due to settling and resuspension

The left side of equation (2.8) is in terms of variation of concentration for the three directions x, y, z. $\frac{\partial}{\partial x}(u\bar{c}) + \frac{\partial}{\partial y}(v\bar{c}) + \frac{\partial}{\partial z}(w\bar{c})$ correspond phenomenon advection terms in the three directions.

Chapter 3: A brief review of rivers and streams water quality models

3.1. Introduction

In this chapter, an attempt has been made to review 11 popular computer water quality models developed by different international agencies in view of different criteria such as basic equations, input and output data, advantages and disadvantages and their applications. The selected computer models are SIMCAT, TOMCAT, QUAL2E/QUAL2EU, QUASAR, QUAL2K/QUAL2Kw, WQRRS, MONERIS, WASP, MIKE-11, AQUATOX and EPD-RIV1. The classifications of water quality modeling were also described. The selected models have already been reviewed individually or coupled with other models in previous studies. However, this review may help modelers by providing a comprehensive review and capabilities of available popular river and stream water quality models.

3.4. Discussions

It can be concluded that among the reviewed models, the QUAL2Kw is the most efficient tool for modeling the water quality when considering steady state flow. QUAL2K/QUAL2Kw has several advantages such as free software, can simulates large number of water quality parameters, it has a graphical user interface, user-friendly, existence of complete documentation materials, auto calibration option included and uncertainty analysis tool. Acceding to the review, QUAL2K was chosen for simulation due to its several advantages among other models such as public domain software, simulates large number of water quality parameters, user-friendly, existence of complete documentation materials and uncertainty analysis tool [102]. All of the investigated models are capable of simulating the water quality in river and stream. However, no one model is comprehensive enough and can give the majority of the usefulness required, due to the fact that a particular model has been developed for particular purposes. Different factors should be considered in model selection process such as availability of time, financial support, availability of data and model limitation .etc.

Personal contributions

Chapter 4: Numerical Simulation of the Dispersion of Pollutants in the Danube River

4.1. Introduction

This main aim of this work (chapter 4) is to examine the impact of Jidostita tributary as a waste loading on the receiving river (see Fig. 1.1). The water quality and quantity data of the Danube River in four sampling stations during 12 months in the year of 2008 are shown in Table 1.1 which was depicted as a descriptive statistical summary. FlexPDE solver was chosen for this study which is based on finite element methods. The mesh and geometry of the study is shown in Fig. 4.5.

4.4. Basic equations

The models rely on the fundamental advection–dispersion equation and the parameter considered for dispersion modeling is the Biochemical Oxygen Demand (BOD). Furthermore, Neumann type condition were considered in which $\frac{\partial C}{\partial n}$ = 0. It is considered the first-order decay term for the BOD consumption. The final dispersion equation in these conditions becomes:

$$\frac{\partial \overline{C}}{\partial t}+\frac{\partial}{\partial x}\left(\overline{u}\overline{C}\right)+\frac{\partial}{\partial y}\left(\overline{v}\overline{C}\right)+=\frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial \overline{C}}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial \overline{C}}{\partial y}\right)-k\cdot C \qquad (4.3)$$

4.5. Boundary conditions

The following characteristics were chosen for the simulation of the pollutant dispersion in the Danube River:

- Length of the river = 12 km,
- Average width = 1.3 km,
- Longitudinal dispersion coefficient $\varepsilon_x = 2$,
- Transverse dispersion coefficient $\varepsilon_y = 2$,
- k= 0.1, and
- BOD concentration in the main river was considered as a mean value in the four stations.
- The concentration of BOD in the Jidostita tributary was assumed to be 10 mg/L, since there is no water quality data available for Jidostita tributary.

This study examines three different scenarios of dispersion of BOD along the Danube River by setting different values of river velocities (*u* and *v*). The adopted cases are:

Case 1: u = 3 and v = 0.3 (m/sec).
Case 2: u = 2 and v = 0.2 (m/sec), and
Case 3: u = 1 and v = 0.1 (m/sec).

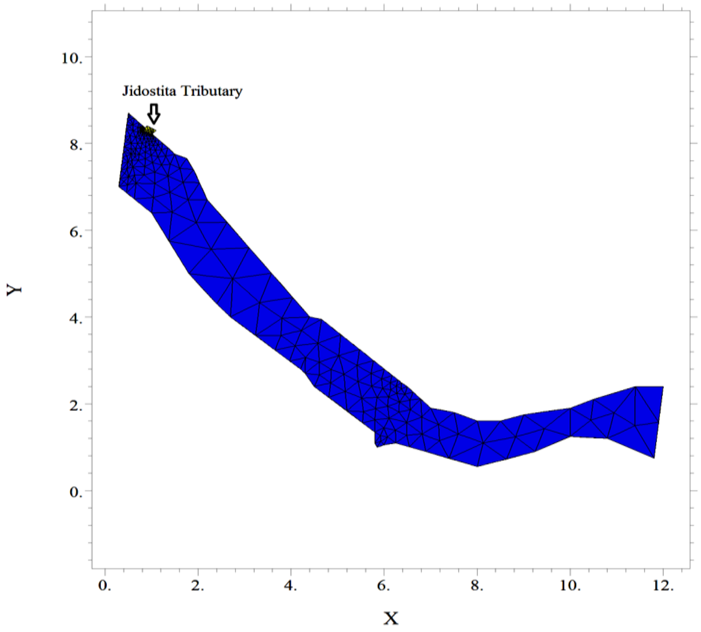


Fig. 4.5 Meshing and the geometry of the study domain (X and Y = distance in km)

4.6. Results and Discussion

In case 1, longitudinal velocity (*u*) and lateral velocity (*v*) were set as 3 m/sec and 0.3 m/sec respectively and the results are shown in Figs. 4.6. In this case, it can be observed that the BOD concentration at Gura Văii (2 km downstream of the Iron Gate 1) in the mid river is about 3.4 mg/L and this value decreased to 0.5 mg/L at Schela Cladovei station. Moreover, the predicted results show good agreement with observed values of BOD in the river with some exceptions as shown in Fig. 4.8. The results were calibrated with minimum, maximum and mean values of observed BOD concentration for 12 months. Only the first three locations were considered for the calibration process in order to examine the errors in the simulation. As shown in Fig. 4.8, the highest errors between the predicted and observed values of BOD were noticed downstream of Schela Cladovei station and extend to Drobeta-Turnu Severin station, however, the results were acceptable.

Moreover, the variations in simulation for BOD concentration along the 13 km were insignificant due to the fact that the pollution load connected to the river from Jidostita tributary has low discharge compared to the flow of the river. Danube River has an average discharge of 5600 m^3/sec [214] and thus this value is very high when compared to the flow rate of Jidostita tributary which make the dilution process is more pronounced.

In case 2, longitudinal velocity (*u*) and lateral velocity (*v*) were set as 2 m/sec and 0.2 m/sec respectively and the results shown in Fig. 4.9. In this case, it can be observed that the BOD concentration at Gura Văii (2 km downstream of the Iron Gate 1) in the mid river is about 3 mg/L and this value decreased to less than 0.5 mg/L at Schela Cladovei station. No significant difference was noticed in comparison with the previous case (case 1)

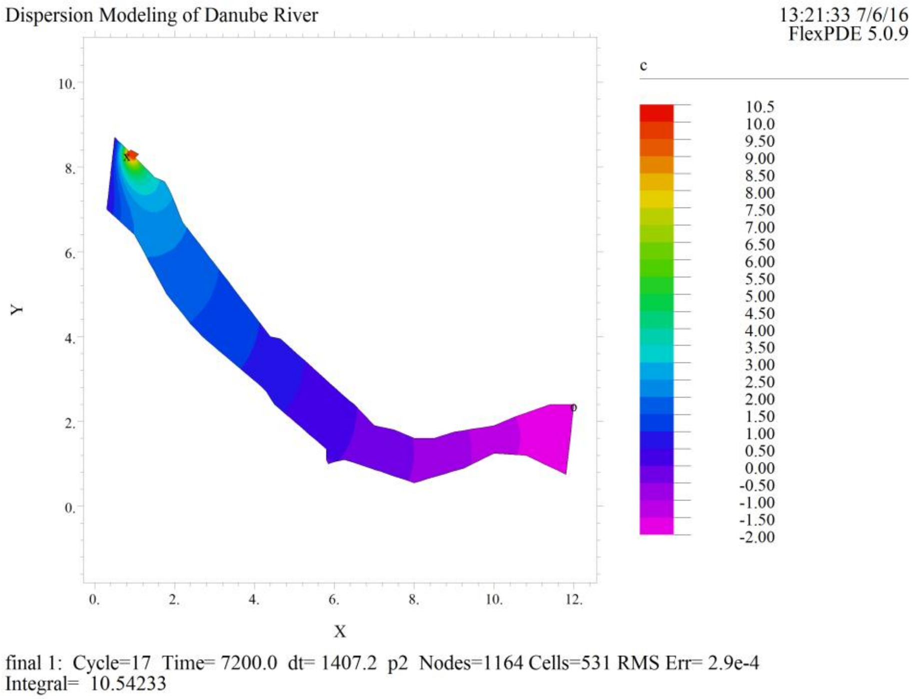


Fig. 4.6 Dispersion of BOD from Jidostita tributary along Danube River, *u*= 3 and *v*= 0.3 (m/s)

In case 3, longitudinal velocity (*u*) and lateral velocity (*v*) were set as 1 m/sec and 0.1 m/sec respectively and the results shown in Fig. 4.12. In this case, it can be observed that the BOD concentration at Gura Văii (2 km downstream of the Iron Gate 1) in the mid river is about 2.5 mg/L and this value decreased to less than 0.5 mg/L at Schela Cladovei station. Therefore, the variation in river velocity can affect the dispersion of BOD along the river, in spite of the simple variation between the three examined cases as shown in Fig. 4.15. It can be concluded that the higher the velocity in the river, the time required for self-purification increased for the river.

Although the water quality of the Danube River in the study region is within the standards (1st quality class) according to SGA Mehedinţi (order of MAPM no. 1146/2002), pollutant transport modeling is considered as a required component in supporting the water quality management options by deciding he prerequisites for meeting the water quality limits, in addition to calculating the effectiveness of actions in limiting the contaminant sources for a designated use, and evaluating risks from accidental releases of contaminants in river ecosystem. The results of the simulated BOD dispersion along the river was quite fit with observed BOD concentration. Thus, FlexPDE solver can be used as a useful tool for predicting pollution dispersion and provide a good basis for future river water quality policy options for limiting the pollutant sources for a designated use.

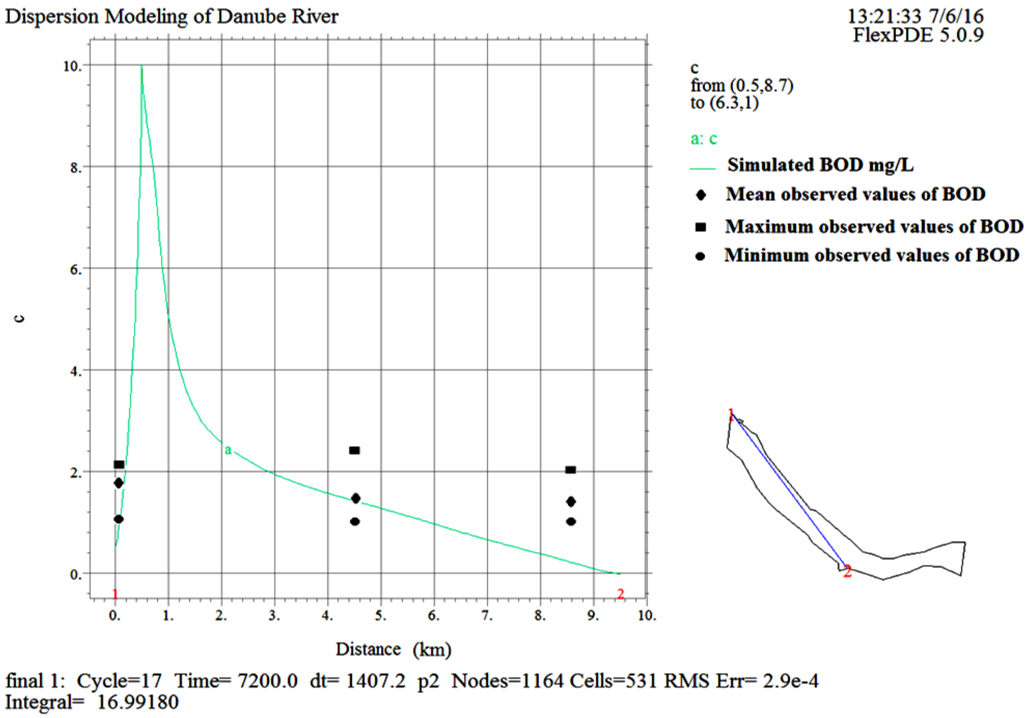


Fig. 4.8 The predicted and observed BOD concentration values along the Danube River, *u*= 3 and *v*= 0.3 (m/s)

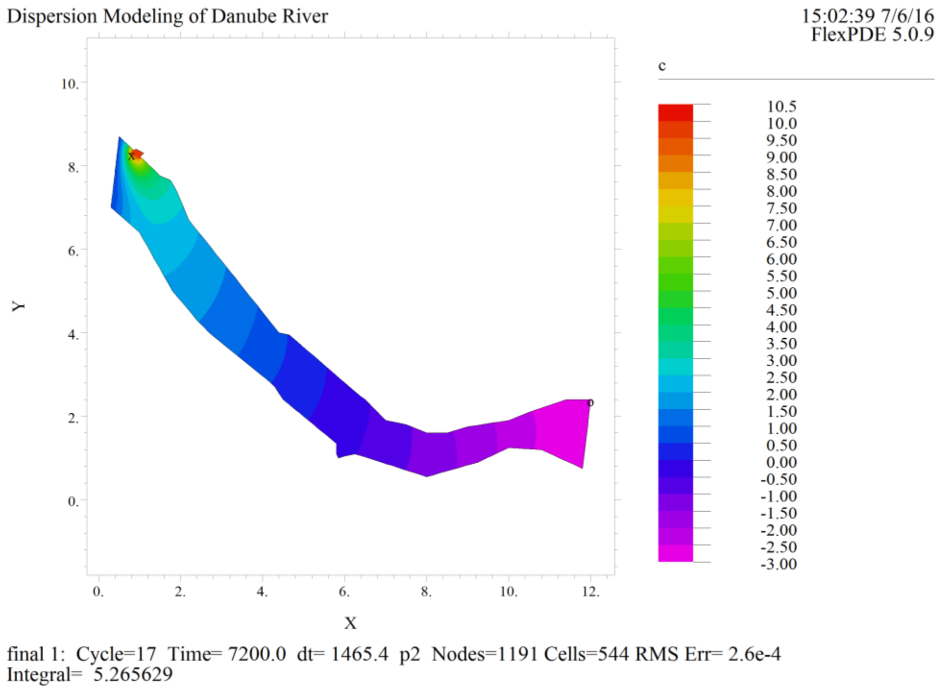


Fig. 4.9 Dispersion of BOD from Jidostita tributary along Danube River, *u*= 2 and *v*= 0.2 (m/s)

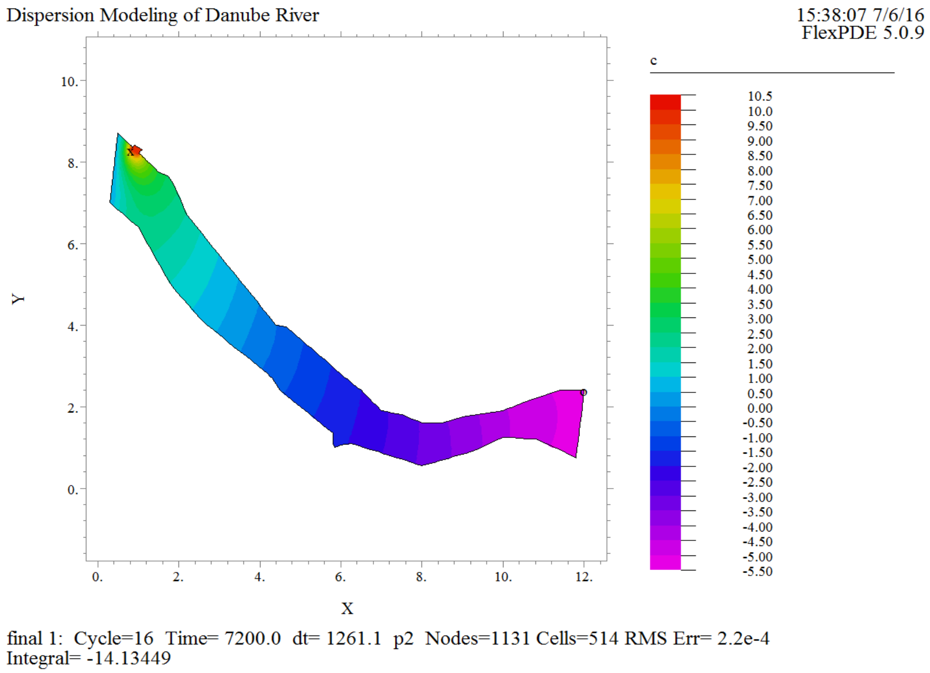


Fig. 4.12 Dispersion of BOD from Jidostita tributary along Danube River, *u*= 1 and *v*= 0.1 (m/s)

4.7. Conclusions

Three different scenarios were presented to explore the effect of velocity variation on the dispersion behavior and to examine the effect of the pollution load from Jidostita tributary on the Danube River. The results demonstrated that the relationship between simulated results by FlexPDE was in agreement with the observed data. In cases 1, 2 and 3, the BOD concentration at Gura Văii in the mid river was about 3.5, 3, 2.5 mg/L respectively, and these values decreased to equal or less than 0.5 mg/L at Schela Cladovei station. In conclusion, the variation in river velocity can affect the dispersion of BOD along the river, in spite of the simple variation between the three examined cases.

Furthermore, the results revealed that, the higher the velocity in the river, the time required for self-purification increased. Moreover, the variations in simulation for BOD concentration along the 13 km distance were insignificant due to the fact that the pollution load connected to the river from Jidostita tributary has low discharge compared to the flow of the river. In spite of some error between simulated dispersion of BOD along the river and observed values of BOD, the numerical simulation results show a good agreement with observed data.

The water quality of the Danube River in the study region in terms of BOD is within the standards (1st quality class) according to SGA Mehedinţi. Further studies may be required to predict and simulate other parameters responsible for deterioration of the river water quality considering the other sources of pollution in the region.

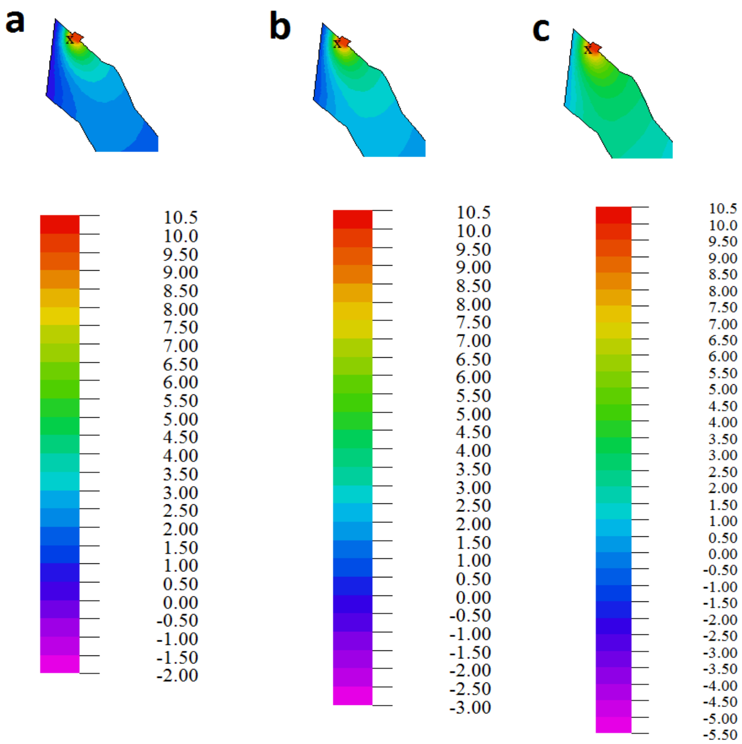


Fig. 4.15 BOD dispersion from Jidostita tributary along the study region of Danube River for the three examined cases, a = case 1, b = case 2, c = case3

Chapter 5: Numerical simulation of the pollutant dispersion from the Arges river into the Danube river using CFD technique (Original Contributions)

5.1. Introduction

In chapter 5, the pollutant dispersion from the Arges river into the Danube river has been investigated using two-dimensional and three dimensional numerical models [103]. A curve-shaped open channel flow with a side discharge has been considered for modelling process. Numerical computations were carried out using Fluent, which is based on the finite volume approach. Both the volume of fluid (VOF) and user defined scalar (UDS) methods were used in this study. VOF method was used to allow the free-surface to deform freely with the underlying turbulence. The study comprised the effect of flow rate and diffusivity coefficient on the dispersion behavior for different scenarios.

Different values of flow rate and diffusivity coefficient were examined to explore the impact of diffusivity and flow rate on the dispersion behavior of the pollutant using volume of fluid (VOF) method and scalar transport. Biochemical oxygen demand (BOD) was selected as a pollutant in the present work. This study may serve as a basis for understanding the influence of the flow rate and diffusivity coefficient on the concentration of the pollutant from the polluted tributary (Arges) on the Danube river.

5.3. Field Data

In order to explore the effect of side discharges and velocities on the dispersion behavior of the pollutant from Arges River as a tributary on the Danube River, three different scenarios were considered and each scenario has three different values of diffusivity coefficients. The Danube River has discharges values ranging between (4000 – 10000) m^3/sec and Arges River between (50 – 90) m^3/sec (Table 5.1). Consequently, three cases were presented in which three different values of flow rate in the Danube River and a fixed value in Arges River were assumed in each case. The BOD concentrations were set as fixed values in all cases and it was 5 mg/L as a maximum in the Danube River and 40 mg/L in the Arges River. All the values that have been adopted in this study were collected from different previous technical sources and studies [11, 169].

Table 5.1 The three adopted scenarios of this study.

Adopted Scenarios		Danube River Discharges (m^3/sec)	Arges River Discharges (m^3/sec)	Diffusivity coefficient (m^2/sec)
Case 1	**a**	4000	90	5
	b	4000	90	10
	c	4000	90	15
Case 2	**a**	7000	90	5
	b	7000	90	10
	c	7000	90	15
Case 3	**a**	9000	90	5
	b	9000	90	10
	c	9000	90	15

5.4. Two-dimensional modeling of pollutant dispersion

5.4.1. Assumptions

The geometry used in this study is shown in Fig. 5.1. Gambit was used for mesh generation. In order to calibrate the simulated results, it was considered that the main open channel flow is representing the Danube River at the lower course and the side discharge is represented as a tributary of the Danube (Arges River). Curve-shaped open channel flow was considered to provide valuable information on the pollutant dispersion behavior. Different sets of flow rate with different diffusivity value [195] were adopted to explore the dispersion of pollutant behavior during different flow conditions along the river. Biochemical oxygen demand (BOD) was considered as a pollutant and the aim is to produce different scenarios of the BOD dispersion along the river on the basis of the discharges. Both Multiphase free surface flow (volume of fluid) and user defined scalar (UDS) were used in this study. For volume of fluid (VOF), Euler-Euler multiphase models were used. Furthermore, this study assumed that the BOD is in a liquid form and mixed throughout the system as a scalar.

In the present study, the air and water are set as primary phase and secondary phase respectively. The tracking of the interface between these two phases is done with the solution of the continuity equation for the water phase. The "standard κ-ε model" was used for turbulence modelling. The transport equation for an arbitrary, "user-defined scalar" (UDS) is solved similarly to the transport equation for a scalar.

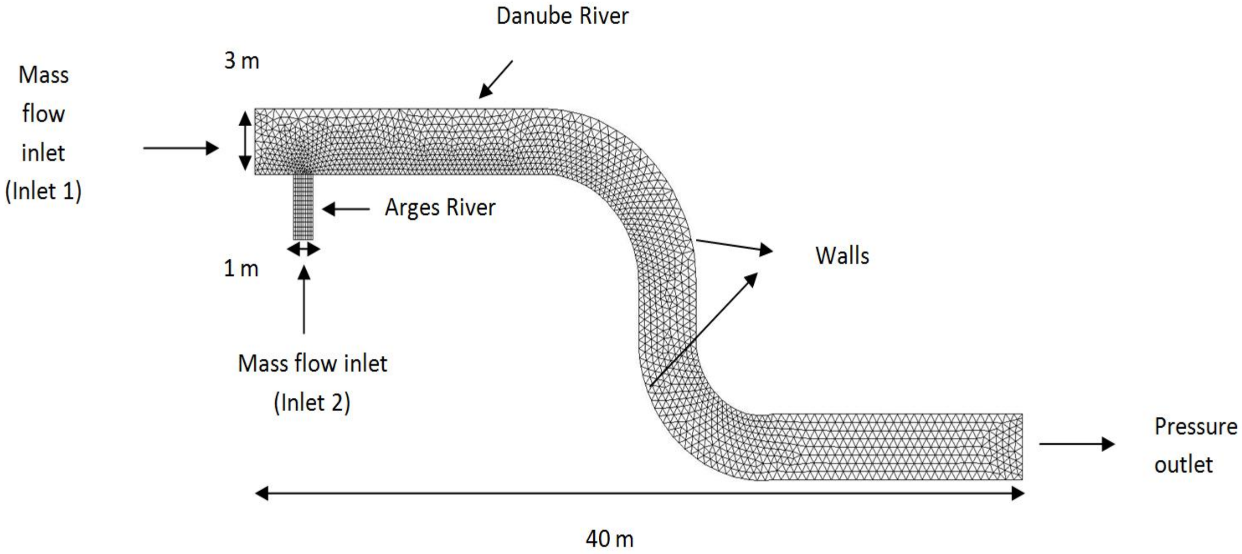


Fig. 5.1 and 5.2 Geometry and boundary condition of the study (combined Figure)

5.4.3. Boundary condition

Different boundary conditions were set until appropriate conditions at domain boundaries were identified. In the present case, the boundary conditions were set as follow (see Fig. 5.2):

- inlet 1 and inlet 2 of the channel: mass flow inlet
- outlet of the channel: pressure outlet
- no-slip boundary condition was chosen (i.e. velocity = 0 at the solid boundaries)
- walls and bed were presumed to be rough

The number of nodes was 1770 of the channel geometry and this mesh was found to provide required spatial resolution for studied channel. The solution has been converged when the variation between successive iterations is less than 10^{-6} for all variables.

5.4.4. Numerical methods

The numerical methods used in this chapter are:

- The segregated solution method was used to solve discretized equations, along with the initial and boundary conditions. The main idea of this method is that the governing equations being solved sequentially (segregated from one another).
- In order to discretize the solution, the first order upwind scheme was used which is one of the simplest and most stable discretization scheme.
- The "PISO" algorithms were considered to calculate the "pressure–velocity coupling". This approach is more reliable than "SIMPLE" and "SIMPLEC", especially for unsteady-state calculations. The main advantage of PISO approach is that it has additional corrections: "neighbor correction" and "skewness correction" which can satisfy the momentum balance after the pressure-correction equation is solved.

5.4.5. Results and Discussions

In case 1, the Q $inlet_1$ was set as 4000 m^3/s and Q $inlet_2$ = 90 m^3/sec and three values of diffusivity coefficient were considered, i.e. diffusivity coefficient for case 1a = 5 m^2/sec, case 1b = 10 m^2/sec case 1-c = 15 m^2/sec. Velocity contour along the channel for Case 1 is shown in Fig. 5.3. It can be seen that when the flow rate of Danube River is minimum, the maximum velocity in the river about 1.9 m/sec. The results of dispersion of BOD along the channel for case 1a, case 1b and case 1c are shown in Figs. 5.4, 5.5 and 5.6. It is clear that the pollutant dispersion behavior from the side discharge (Arges River) on the Danube River is tending to be different and dependent to the diffusivity coefficient.

In case 1-a, and when flow rate is lower and diffusivity = 5 m^2/sec, it can be seen that the BOD dispersed from the side discharge (Arges River) downstream which causing decreases in its concentration due to dilution process. Lower BOD concentration was observed at 30 km longitudinal distance which is less than 5 mg/L. Furthermore, it was observed that with the increase in value of diffusivity (case 1-b and 1-c), the transverse dispersion of BOD increases.

The self-purification process is one of the most important indicators for the river health. The capacity for the self-purification of the Danube River may act as one of the indicators in regulating the discharge standards [217]. It can be seen that this process is highly affecting the BOD concentration in this case.

In case 2, the Q $inlet_1$ was set as 7000 m^3/s and Q $inlet_2$ = 90 m^3/sec and three values of diffusivity coefficient were considered, i.e. diffusivity coefficient for case 2-a = 5 m^2/sec, case 2-b = 10 m^2/sec case 2c = 15 m^2/sec. Velocity contour along the channel for Case 2 is shown in Fig. 5.7. In this case, maximum velocity observed in the Danube River was 3.3 m/sec. The results of dispersion of BOD along the channel for case 2a, case 2b and case 2c are shown in Figs. 5.8, 5.9 and 5.10. The concentration of BOD was dispersed at long distance in this case in which the BOD concentration returns to its origin concentration of 5 mg/L i.e. before the discharge from Arges River at about 38 km distance which is more than the distance of case 1. Therefore, self-purification process becomes slower than the self-purification process of case 1. As same for case 1, it is clear that with the increase in value of diffusivity (case 2b and 2c), the transverse dispersion of BOD increases.

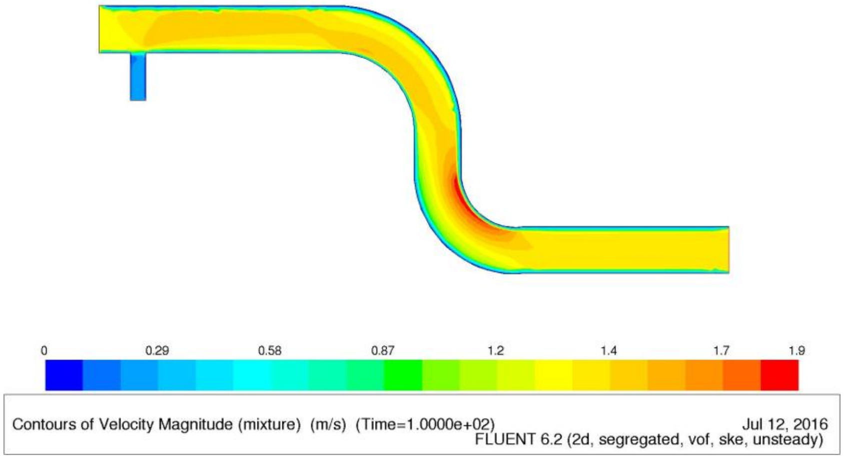
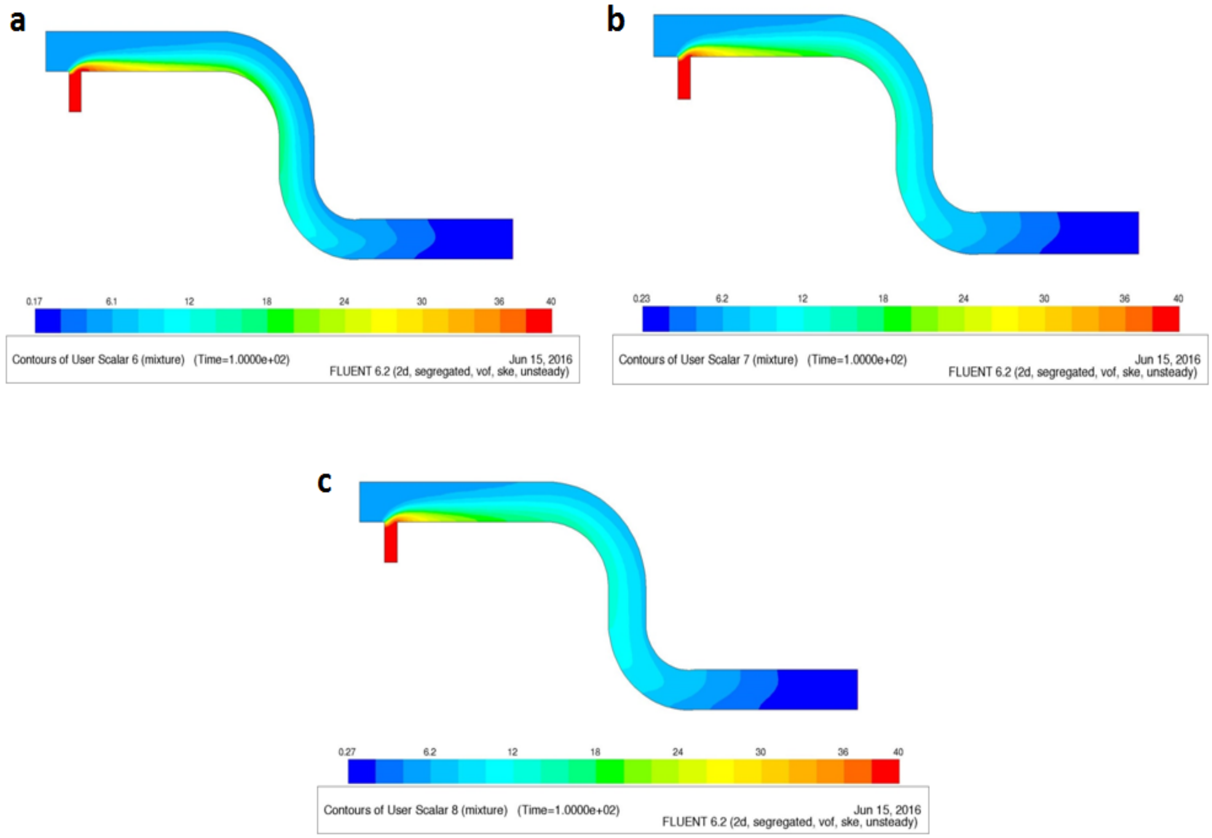


Fig. 5.3 Velocity contour along the channel for Case 1



Figs. 5.4, 5.5 and 5.6 Dispersion of BOD along the channel, a- case 1a, b- case 1b, c- case 1c (combined Figures)

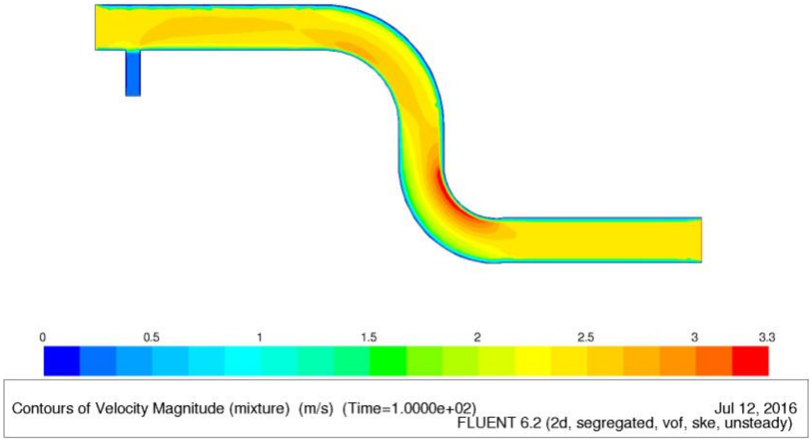
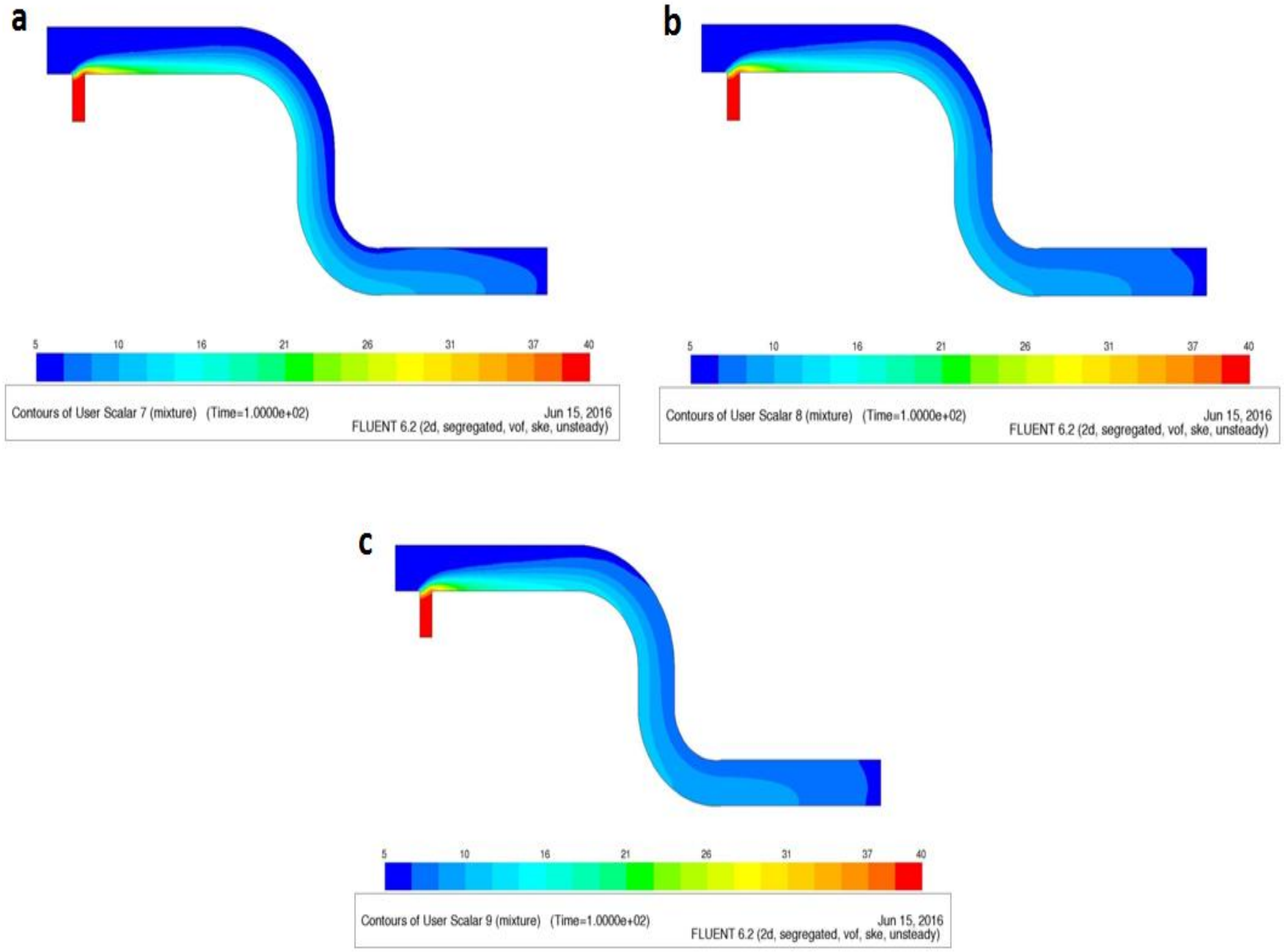


Fig. 5.7. Velocity contour along the channel for Case 2



Figs. 5.8, 5.9 and 5.10 Dispersion of BOD along the channel, a- case 1a, b- case 1b, c- case 1c (combined Figures)

In case 3, the Q $inlet_1$ was set as 9000 m^3/s and Q $inlet_2$ = 90 m^3/sec and three values of diffusivity coefficient were considered, i.e. diffusivity coefficient for case 3a = 5 m^2/sec, case 3b = 10 m^2/sec case 3c = 15 m^2/sec. Velocity contour along the channel for Case 3 is shown in Fig. 5.11. In this case, the observed velocity in the Danube River tends to be more than 4 m/sec. The results BOD dispersion along the channel for case 3a, case 3b and case 3c are shown in Figs. 5.12, 5.13 and 5.14.

In this case, the concentration of BOD has been dispersed at the longest distance when compared to the two previous cases (1 and 2). BOD concentration does not return to its origin concentration of 5 mg/L. Less downstream BOD concentration was observed to be more than 5 mg/L in all the geometry of the study. Thus, self-purification process becomes slower than the self-purification process of the previous cases (1 and 2).

Moreover, transverse dispersion of BOD in this case, even with the variation of diffusivity coefficients (case 3-a, 3-b and 3-c), is very slow due to the high discharge in the Danube river (9000 m^3/sec).

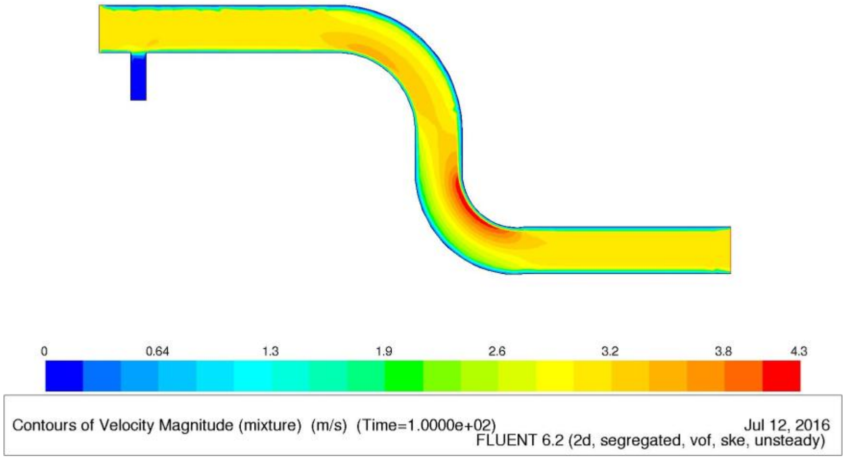


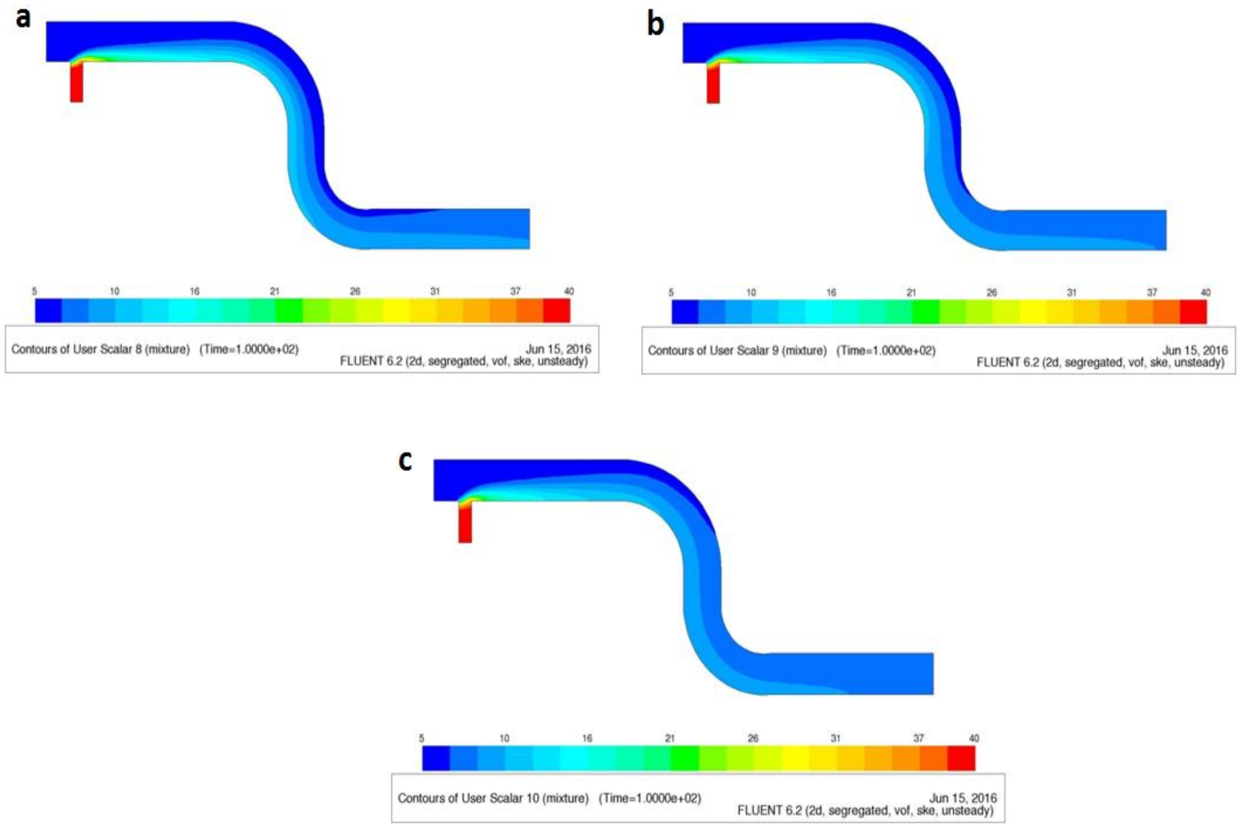
Fig. 5.11 Velocity contour along the channel for Case 3

Generally, the dilution process of BOD concentration is quite clear due to the high flow rate in the main channel, which makes the concentration of BOD is reduced downstream in the channel. Moreover, the BOD concentration is dispersed more closely along the bank of the channel when the flow rate in the main channel is high (Case 3), i.e. the highest the flow rate in the main channel (inlet 1), the dispersion behavior tends to be along the bank of the channel. The three scenarios that have been considered are related to actual situations from the Danube River in order to understand the concept of scalar transport through multiphase flow (air-water).

Comparison and agreement between the numerical simulation results and experimental data of BOD along the river which have been observed in the literature show some error between the results in cases 1, 2 and 3. However, the agreement between the prediction and the field observation is acceptable and the present model is reliable for the predictions the impact of Arges River as tributary on the Danube River, i.e. the computational fluid dynamics (CFD) can be used as an effective tool for predicting the pollutant transport phenomena in open channel flow with a side discharge flow.

5.5. Three-dimensional modeling of pollutant dispersion

BOD concentration in z-direction decreases if the flow rate in the river is relatively high and thus, self-purification process is being slowed. BOD reduction in the river is due to high dilution rates. BOD concentration along Danube River in a plot direction (1, 0) has been shown in Fig 5.15. The results revealed that, the higher the flow rate, the more time was required for self-purification for the Danube River.



Figs. 5.12, 5.13 and 5.14 Dispersion of BOD along the channel, a- case 1a, b- case 1b, c- case 1c (combined Figures)

5.6. Conclusions

The findings of this study may provide a proper basis for water quality management in Danube River. Moreover, this study may serve as a basis for understanding the effect of the flow rate on the concentration of pollutant from the polluted tributary on the river. It was found that the BOD concentration is dispersed more closely along the bank of the channel when the flow rate in the main channel is high (Case 3), i.e. the highest the flow rate in the main channel (inlet 1), the more the dispersion behavior tend to be along the bank of the channel. BOD concentration returns to its origin concentration of 5 mg/L (before the discharge point from Arges River) at about 30 km distance for case 1, and at about 38 km distance for case 2. Whereas, in case 3, the concentration of BOD has been dispersed at longest distance than the two previous cases (1 and 2). BOD concentration does not return to its origin concentration of 5 mg/L. Less downstream BOD concentration was observed to be more than 5 mg/L in all the geometry of the study. Moreover, Flow rate can highly affect the self-purification process which becomes slower at high flow rate.

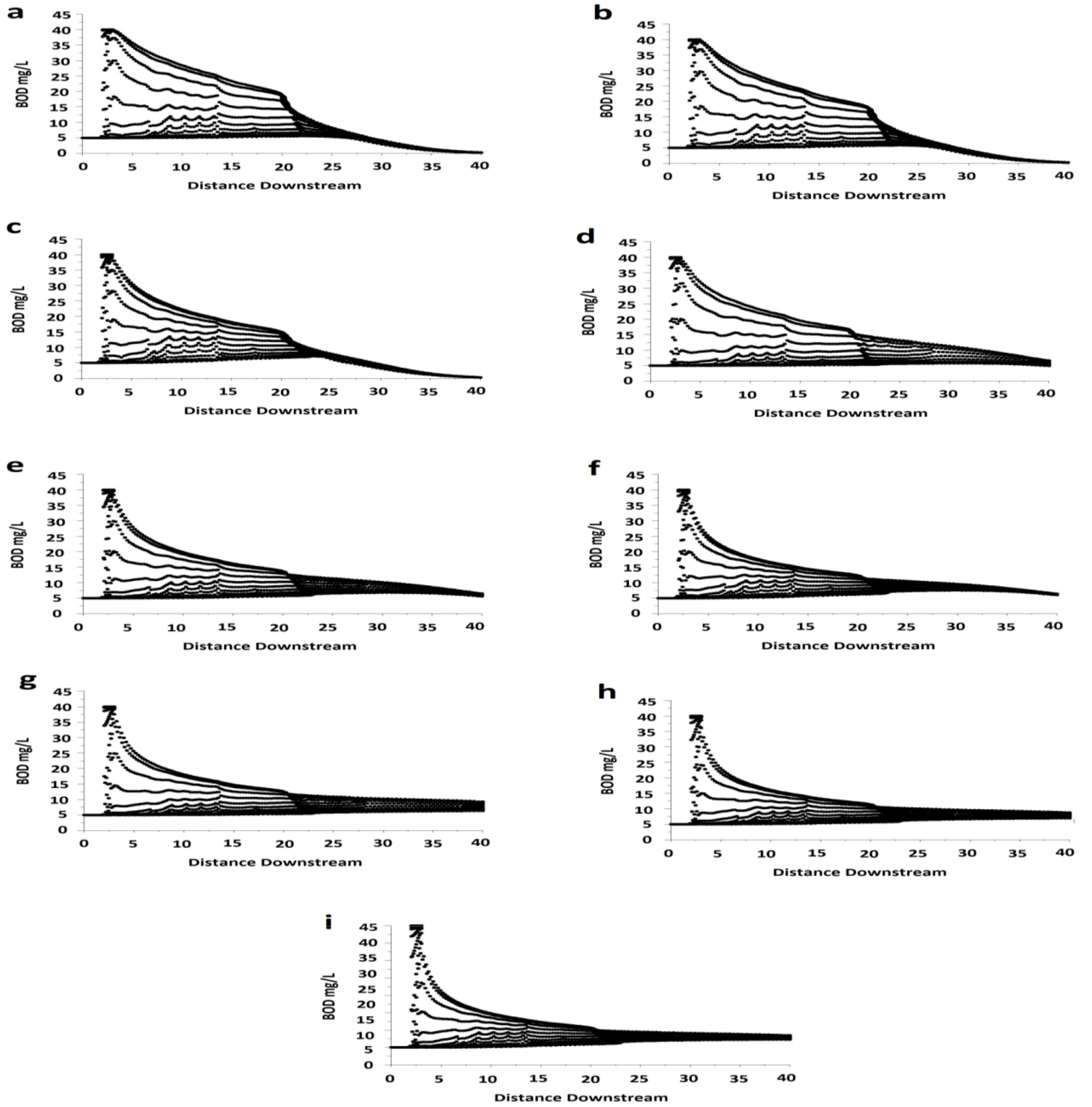


Fig. 5.15 BOD concentration along Danube River in a plot direction (1, 0, 0), a- case 1-a, b- case 1-b, c- case 1-c, d- case 2-a, e- case 2-b, f- case 2-c, g- case 3-a, h- case 3-b, i- case 3-c (My Figure contribution)

Chapter 6: Application of QUAL2K for simulation the water quality in the Danube River

6.1. Introduction

In chapter 6, a public domain model (QUAL2K) was chosen for simulation the water quality in the Danube river as it widely tested in the literature, and has complete documentation materials. The model provides uncertainty analysis tools in its process and it has some features such as public domain software, user-friendly, frequent upgrades [102, 195]. The selection of this model was based on a brief review of 11 water quality models presented in chapter 3.

6.4. Model Input

The input data required by QUAL2K are: discharge value and concentrations for headwater, discharges values of point source pollution and abstractions, reach segment lengths, hydraulic geometry and meteorological data [38]. Water quantity and quality data for headwater are available from obtained dataset in four sampling points in the study area. The hydraulic parameters such as river geometry have been obtained from technical reports. The meteorological data were obtained from Romanian National Meteorological Administration.

Water quality data were obtained for the year of 2008 in four sampling points, namely Gura Văii (SS1) which is about 2 km downstream of Iron Gate I, Dudașu Schelei (SS2), Schela Cladovei which is located upstream of Drobeta-Turnu Severin (SS3), and downstream of Drobeta-Turnu Severin (SS4). Water quality and quantity datasets for April (spring) and September (autumn), 2008, were used for model calibration and verification respectively. Whereas, datasets for February and June (2008) were used for predicting the water quality in winter and summer seasons.

The total length of the study region (13 km) was divided into 4 reaches, further subdivided into 17 segments ranging between 0.43 – 1.24 km. Fig. 6.1 shows the river discretization along with the locations of point and non-point sources pollution. Two tributaries exist in the study area and are not modeled explicitly, but they are considered as point sources. Discharges of non-point sources pollution loads in the study area were assumed to be 1 m^3/sec as maximum. A trapezoidal cross-section channel was considered for modeling with a channel slope of 0.001 and a bottom width 210 m. Manning roughness coefficient was assumed as 0.035, since the Danube River is a natural stream channel, clean and straight [45].

In QUAL2K, the model simulates the ultimate CBOD (CBODu) instead of 5 day CBOD ($CBOD_5$) and therefore, the observed $CBOD_5$ was converted to (CBODu) using the following relationship [100]:

$$CBOD_u = \frac{CBOD_5}{1-e^{-5k}} \quad (6.24)$$

where, k is the CBOD decomposition in the bottle, 1/day. The polluted water and wastewater contaminated with organic carbon has a k values in the range 0.05–0.3 1/day. The value of k was calculated as 0.13 1/day, assuming the CBODu/$CBOD_5$ ratio as 2.05.

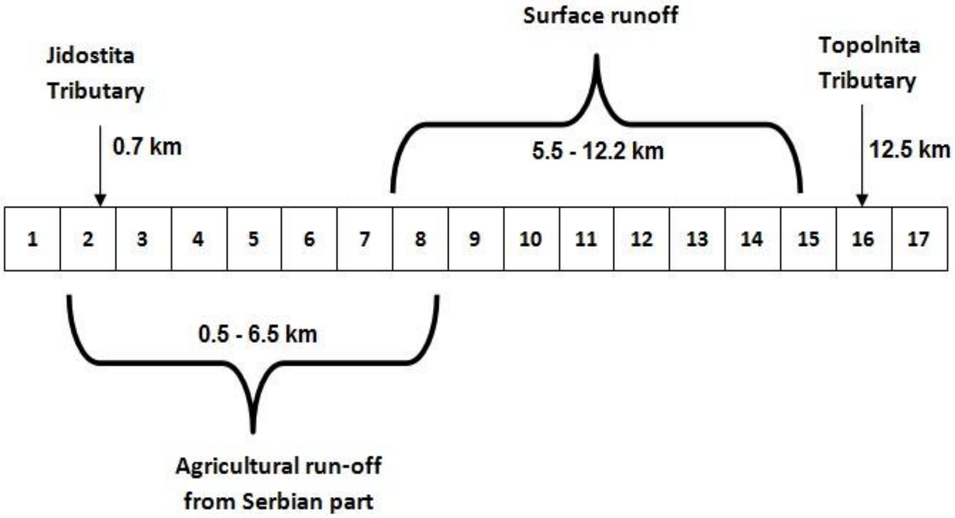


Fig. 6.1 Segmentation of Danube River with location of pollution sources

The model rates were obtained from various technical sources: the default values presented by the QUAL2K user manual [38], the Environmental Protection Agency, and literature from QUAL2E and QUAL2E-UNCAS. The stoichiometry parameters such as carbon (gC), nitrogen (gN), phosphorus (gP), dry weight (gD) and chlorophyll (gA) were specified according to the default values given in the QUAL2K user manual as 40, 7.1, 1, 100 and 1, respectively. The slow CBOD hydrolysis rate and fast CBOD oxidation rate were calibrated as 1.53 and 3.56 respectively. Churchill et al. [47] formula was chosen to estimate the reaeration rate for Danube River, since this formula was developed for large rivers with mean depths ranging from 0.65–3.48 m and mean velocities ranging from 0.56–1.52 m/s [49]. The input data of headwater parameters were temperature, flow, pH, DO, BOD, NH_4-Nitrogen, NO_3-Nitrogen, organic phosphorus and inorganic phosphorus. Alkalinity was assumed as 100 mg/L of $CaCO_3$ (default value for QUAL2Kw) and inorganic suspended solids, conductivity, detritus, phytoplankton and pathogen were left blank as they not available.

6.6. Results and Discussions

The model was calibrated using data from April, 2008 (spring season). The calculation step for the model was set at 0.015 hour, to increase the model stability. In order to maximize the goodness of model fit between the simulated results and observed data, the model was run iteratively until the model coefficients were adjusted and a reasonable agreement were achieved. Furthermore, the model was validated using data from September, 2008 (autumn season) without changing the calibrated system parameters in order to test the ability of the calibrated model. Then, the model was used to simulate water quality conditions during the summer (June, 2008) and winter seasons (February, 2008).

QUAL2K model was calibrated and validated for two different seasons: spring (April 2008) and autumn (September 2008). The model calibrated and validated results for the water quality data at the four sampling sites are shown in Fig. 6.2 and Fig. 6.3, respectively. Both the calibration and validation results were in agreement with the observed values, with some exceptions. The relative error is used for estimating the errors in simulation. The relative error of calibrated and validated results between the simulated and observed values for flow rate, BODu, DO and pH are shown in Table 6.2. The model calibration and validation results showed that the concentrations of DO were above the limits of 4 mg/L in the study region [119]. Moreover, the variations in simulation for BODu and DO concentration along the 13 km distance were insignificant due to the fact that the pollution load connected to the river from the two tributaries (Jidostita and Topolniţa) have low discharge compared to the flow of the river.

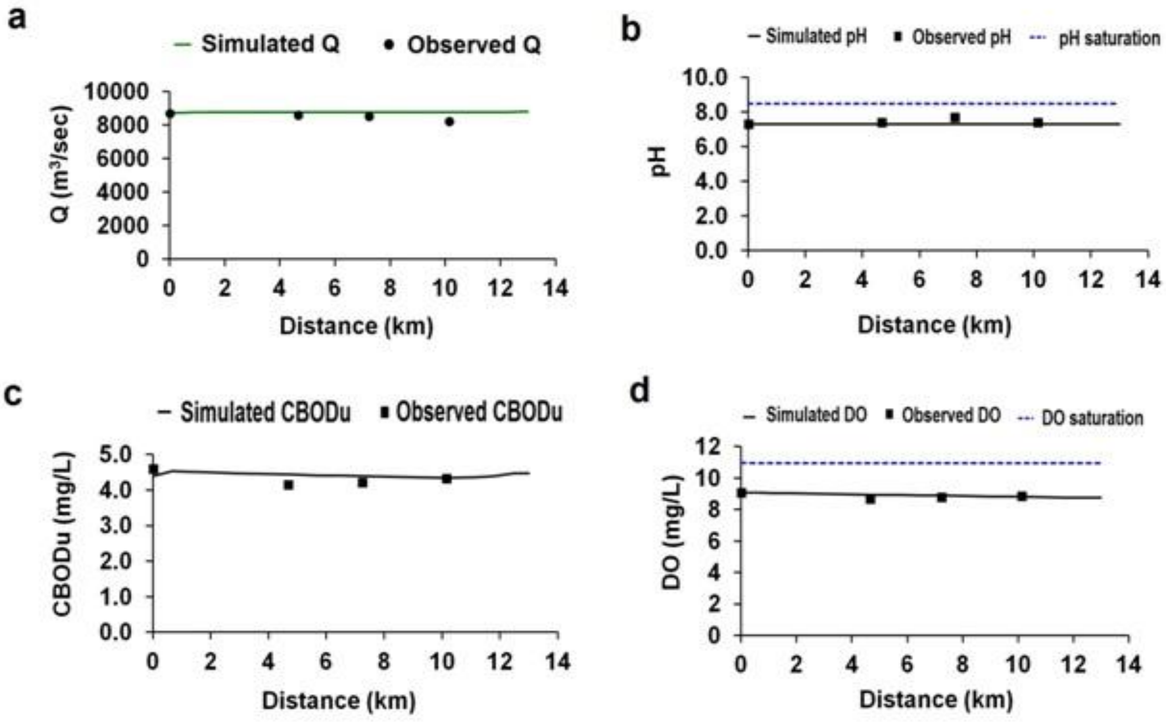


Fig. 6.2 Calibrated results in autumn season for Danube River: a flow rate, b pH, c ultimate CBOD, d dissolved oxygen (DO), (September 2008).

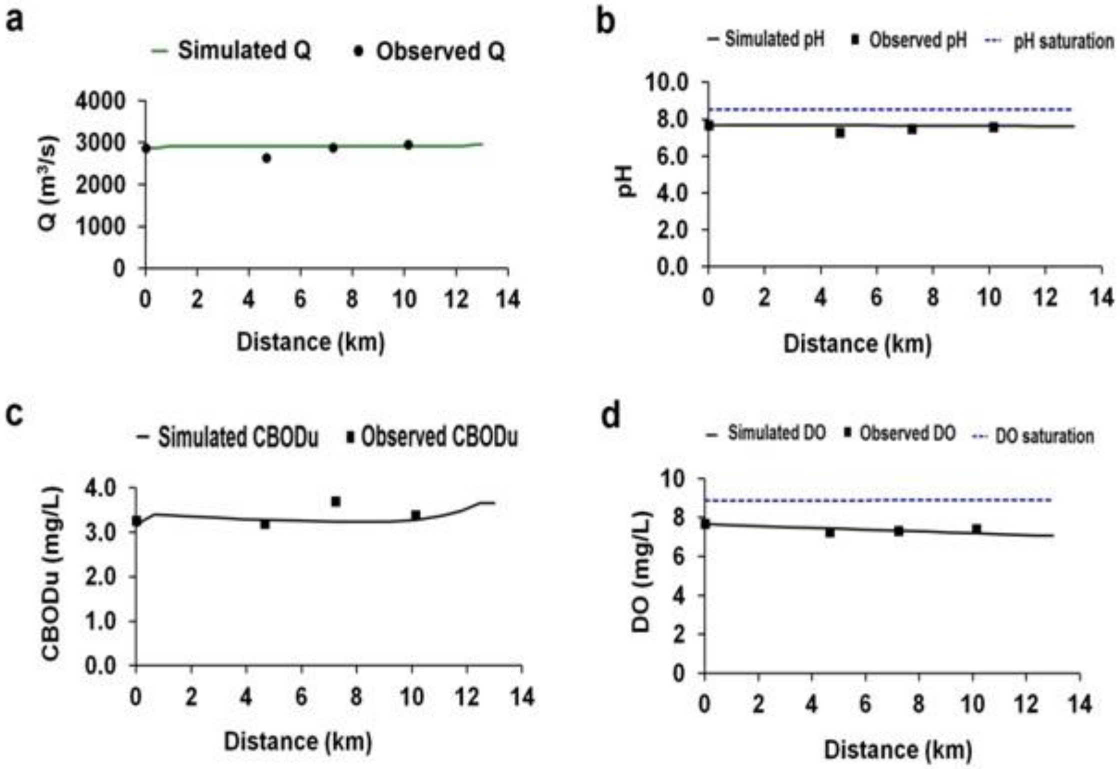


Fig. 6.3 Validated results in spring season for Danube River: a flow rate, b pH, c ultimate CBOD, d dissolved oxygen (DO), (April 2008)

Table 6.2 Relative Error (%) of calibrated and validated results between the simulated and observed values for water quality of Danube River, approximate values

Calibrated Results	**% Relative Error**			
Parameters	**SS1**	**SS2**	**SS3**	**SS4**
Q	0	1.5	2.5	6
BODu	4	6.5	3.5	0.5
DO	0	2.5	0.5	0.5
pH	0	1.5	5	1.5
Validated Results	**% Relative Error**			
Parameters	**SS1**	**SS2**	**SS3**	**SS4**
Q	0	10	1	1.5
BODu	4	2	12.5	2
DO	0	2	0.5	3
pH	0	5	2	1.5

Generally, the results revealed that the BODu concentrations in the four seasons were below 5 mg/L and DO concentrations above 7 mg/L which reflect a good quality of the river in Drobeta-Turnu Severin during the year. pH values were ranging between

7.29 - 7.7 in the study area for all seasons. Furthermore, it was observed that the flow (Q) was not varying along the 13 km of river. Although QUAL2K is a steady state model, the simulated results for flow satisfied the literature. The model was also used to predict the BODu and DO of the river in different scenarios as a proactive management. Four different scenarios were examined; Case 1: low flow period (1000 m^3/s), Case 2: high flow period (Q = 10000 m^3/s), Case 3: low flow period (Q = 1000 m^3/s) with BOD = 70 mg/L and DO = 0 mg/L for point sources, and Case 4: high flow period (10000 m^3/s) with BOD = 70 mg/L and DO = 0 mg/L for point sources. The water quality modelling results in four different scenarios for BOD and DO is shown in Fig. 6.6.

The dissolved oxygen concentrations along the river in all cases were within the minimum dissolved oxygen standard of 4 mg/L, which reflect a good health for the river in this region. As for the CBODu, it can be noticed that the highest concentration for the simulated CBODu in cases 1, 2, 3 and 4 were 5, 3, 8, 3.5 mg/L respectively. The highest values were noticed close to Drobeta-Turnu Severin in which Topolniţa tributary was the major source influencing the water quality of the river in the study region. Moreover, the discharge (Q) is the main factor influencing the variation of CBOD concentration rather than DO in the Danube River.

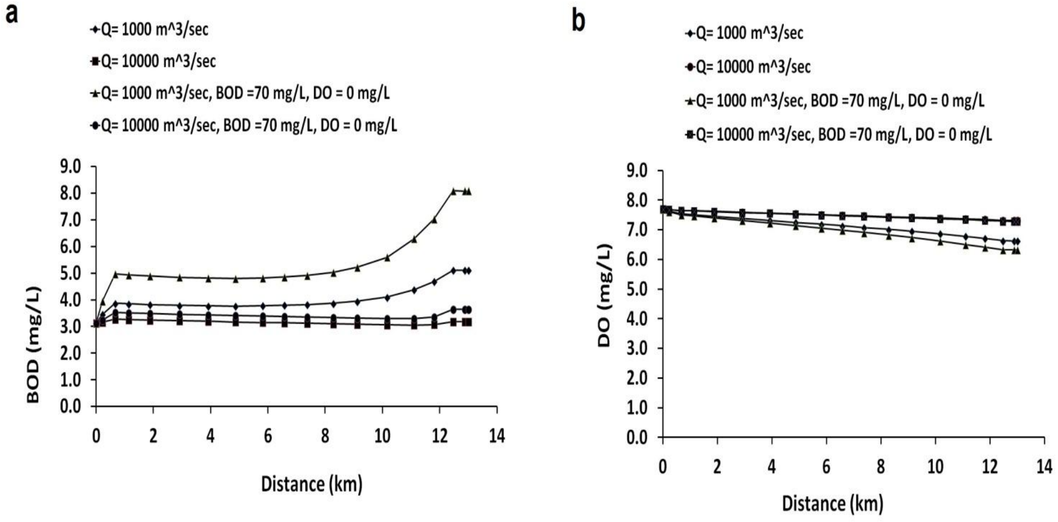


Fig. 6.6 Water quality simulation of Danube River in different scenarios: a BODu, b DO (My Figure contribution)

6.7. Conclusions

The simulated results showed good fit with the observed values with some exceptions. CBODu and DO showed some differences between simulated and measured data sets at some points, however, the results could be acceptable. The results showed that the DO was within the minimum dissolved oxygen standard of 4 mg/L, which reflects a good health for the river in the study area. Simulation results for

CBODu in all seasons were below 5 mg/L. Furthermore, the discharges have a significant effect in the water quality of Danube River and the Topolniţa tributary was the major source influencing the water quality of the river in the study region. In spite of some limitation, it can be conclude that QUAL2K can be used as a suitable tool for simulating the water quality in a large river.

Chapter 7: Application of multivariate statistical techniques in the assessment of the water quality of Danube River

7.1. Introduction

In chapter 7, the main aim was to apply the multivariate statistical techniques such as factor and cluster analyses to identify the major factors affecting on water quality of Danube River in Drobeta-Turnu Severin city and to get information about the spatial and temporal variations among the sampling sites and monitoring periods.

7.3. Data treatment and multivariate analysis

The normality distribution of each variable was checked using the Shapiro–Wilk (W) test prior to using multivariate statistical methods [99] since the factor and cluster analyses require water quality variables to fit to the normal distribution. The Shapiro–Wilk (W) test demonstrated that the variables: BOD, pH, Q, TSS, Cd, Ni and Pb were normally distributed, whereas DO, TP, NH4, NO3, WT, Cu and Cr were not normally distributed. Consequently, the original data of non-normal distribution variables were transformed in the form $x' = \log_{10}(x)$. After log-transformation and according to the Shapiro–Wilk (W) test, only DO and TP were normalized and thus, other variables: NH_4, NO_3, WT, Cu and Cr were excluded. Thereafter, in order to avoid misclassification due to the wide variations in data dimensionality, the original data of variables: BOD, pH, Q, TSS, Cd, Ni, Pb and the log-transformed variables: DO and TP were also standardized by setting the mean equal to 0 and the variance equal to one.

Factor analysis (FA) was applied to identify the most important variables influencing the water quality of the Danube River. FA were conducted via three stages, (i) generating the correlation matrix for all variables, (ii) extracting the initial set of factors using principal component analysis (PCA) method, and (iii) rotating the extracted factors by Varimax rotation. Factor analysis was performed using principal component analysis method on the normalized data sets and varimax rotation was made on the factor loading matrix to infer the principal parameters. Eigenvalues of 1.0 or greater are considered significant and eigenvalues less than 1 have been eliminated [101]. The Scree plot was used to identify the retained factors in order to comprehend the underlying data structure.

Cluster analysis (CA) was also utilized to evaluate the spatial and temporal variations among the sampling sites and monitoring periods. In this paper, hierarchical agglomerative clustering was made using Ward's method of linkage, and squares Euclidean distance method was used for determining similarity distance, and the results of CA illustrated by a dendrogram. All the statistical computations were performed using Microsoft Office – Excel 2007 spreadsheet and SPSS 18 for Windows.

7.4.1. Factor analysis (FA)

Factor loadings with values of >0.75, 0.75–0.50 and 0.50–0.30 were classified as strong, moderate and weak, respectively. As shown in the scree plot (Fig. 7.15), it can be noticed that 3 major factors have eigenvalues greater than one and explain 64.369% of the total variance in each water quality datasets.

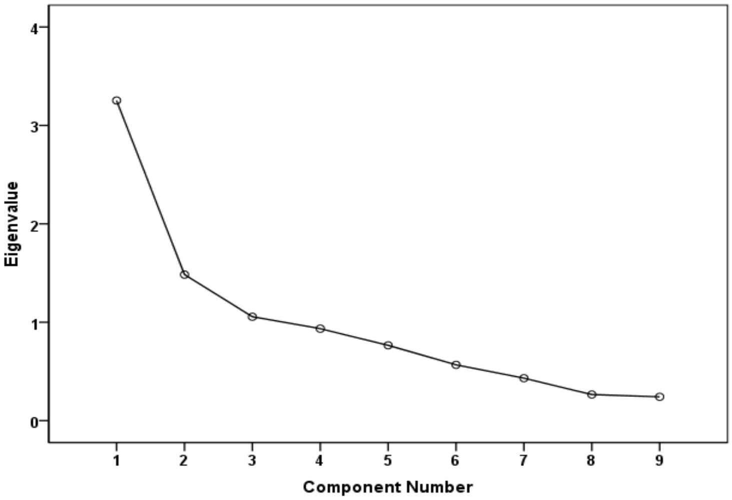


Fig. 7.15 Scree plot for the water quality dataset

Table 7.2 shows the output results of factor analysis (FA). Factor 1 explained 26.11% of the total variance and has strong positive correlation with TSS, negative moderate correlation with Q and BOD, and positive moderate correlation with Cd and Pb. The high loading factor of TSS is likely due to the high discharge of the river. Despite that the geology-related factors such as Na, K, Ca and Mg were not considered in this study, it is clear that the high loading factor of TSS and the negative moderate correlation with Q indicate the hydro-geochemical variables. The negative sign of discharge in this factor may indicate that the dilution processes of dissolved minerals increase with discharge. The other variables loading represent the contribution of organic pollution from domestic wastewater and non-point source pollution.

The second factor (Factor 2) explained 26.10% of the total variance which has strong positive correlation with TP, strong negative correlation with DO and moderate positive correlation with Cd, Ni and Pb. This factor represents the impacts from industrial effluent and agricultural practice from agriculture area. A group of industries are located upstream and downstram of the Drobeta-Turnu Severin city and the agricultural practices from the Serbian part that use fertilizers and pesticides which are being discharged to the river through surface runoff. The third factor (Factor 3) is contributed by pH which explains 12.16% of the total variance. It can be observed that Factor 3 regulates the dissolution of cations and anions in which this factor reflects the acidity–alkalinity scale in river water.

Table 7.2 Rotated factor loading matrix and total variance explained (Varimax rotation)

Parameters	**Factor 1**	**Factor 2**	**Factor 3**
DO	0.088	-0.821**	-0.140
BOD	-0.657*	-0.173	0.019
pH	0.006	0.014	0.960**
Q	-0.572*	0.348	-0.103
TP	0.129	0.748**	-0.013
TSS	0.806**	0.063	-0.085
Cd	0.612*	0.573*	-0.166
Ni	0.251	0.575*	-0.326
Pb	0.693*	0.549*	0.011
Eigenvalue	2.350	2.349	1.094
% Total variance	26.11	26.10	12.16
Cumulative % variance	26.11	52.21	64.37

*Indicate moderate correlation with the factor loading; and **Indicate strong correlation with the factor loading.

7.4.2. Cluster analysis (CA)

As for cluster analysis, classification of sampling site and monitoring periods was performed using of cluster analysis on z-standardized dataset. The output result of cluster analysis was shown as a dendrogram in which it provides a useful graphical tool determining the number of clusters which describe underlying process that lead to spatial and temporal variation.

For spatial similarity and site grouping, all the four sampling stations of the Danube river were grouped into two significant clusters and the spatial cluster analysis is shown in Fig. 7.16. Group A consisted of SS1 and SS2 and group B consisted of SS3 and SS4. Group A (SS1 and SS2) corresponds to relatively less polluted stations. In group A, sites are situated upstream of Drobeta-Turnu Severin city. These sites get contamination from nonpoint sources, i.e., especially from agricultural practices. Group

B (SS3 and SS4) corresponds to relatively moderate polluted stations in comparison with Group A. In group B, stations are located in the industrial area of Drobeta-Turnu Severin city. These stations may receive pollution from point and nonpoint sources, i.e., domestic and industrial effluent, and surface runoff from the city.

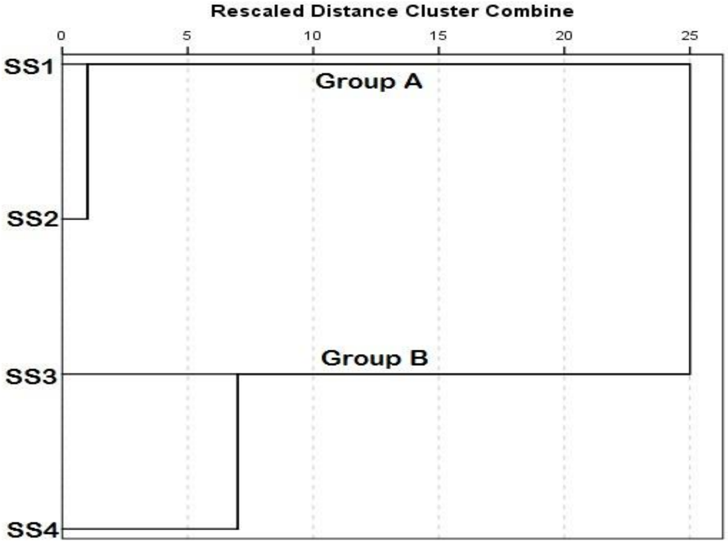


Fig. 7.16 Dendrogram showing spatial clustering of monitoring sites

For temporal cluster analysis, the output result has been shown in Fig. 7.17 as a dendrogram, grouping the 12 months into two major Groups (A and B). Group A included only two months (April and July). Group B comprised two significantly different subgroups (Group B1 and B2) which agglomerated remaining months. Group B1 included January, February, March, May, June, August, October, and December, whereas, Group B2 included September and November. However, if 12 months had been empirically divided into spring (March to May), summer (June to August), autumn (September to November), and winter (December to February), a mistake in grouping could have been made. The temporal variation in the Danube river water quality was not strictly determined by local climate (spring, summer, autumn, winter).

Furthermore, it was observed that the discharge is the main factor influencing temporal variation among other parameters in the Danube River. The discharge fluctuation in the region may affect the water quality in the river. Kurunc et al., [130] studied the effect of seasonal discharge fluctuation on the water quality variables in Yeşilırmak River. They stated that there is a negative relationship between discharge and some water quality variables. Teodoru and Wehrli, [214] has reported a time series flow rate at Drobeta–Turnu Severin station from 1960 to 1988 and the average outflow at the Iron Gate dams for the year 2001 (Fig. 7.18). Obviously, it can be noticed that the discharge values were roughly in the range 4000 – 8000 m^3/sec. Moreover, the discharge values in this study ranging from 2650 – 8760 m^3/sec with a mean value 5643

m^3/sec. Therefore, the water quality of the river in this region is highly affected by the discharge.

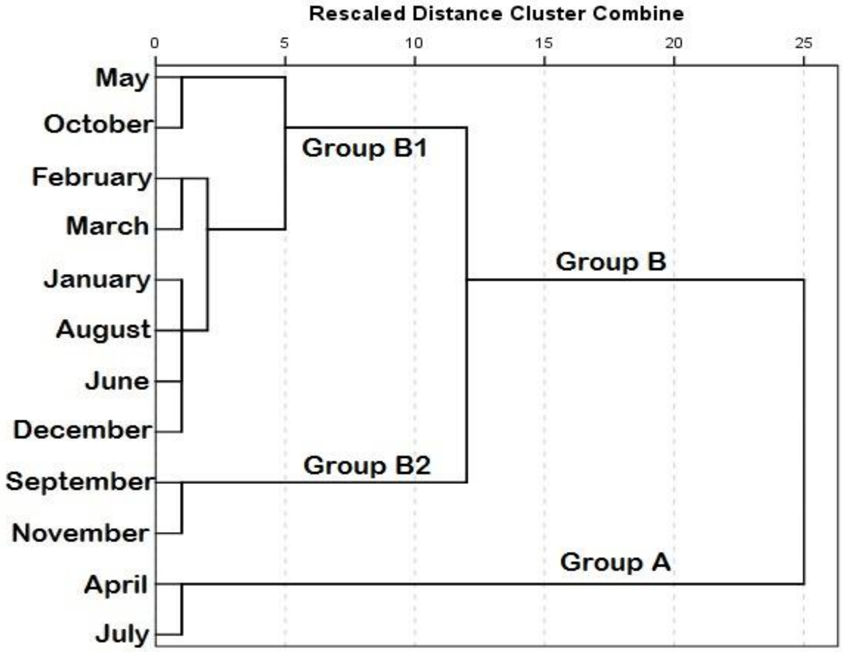


Fig. 7.17 Dendrogram showing spatial clustering of monitoring periods

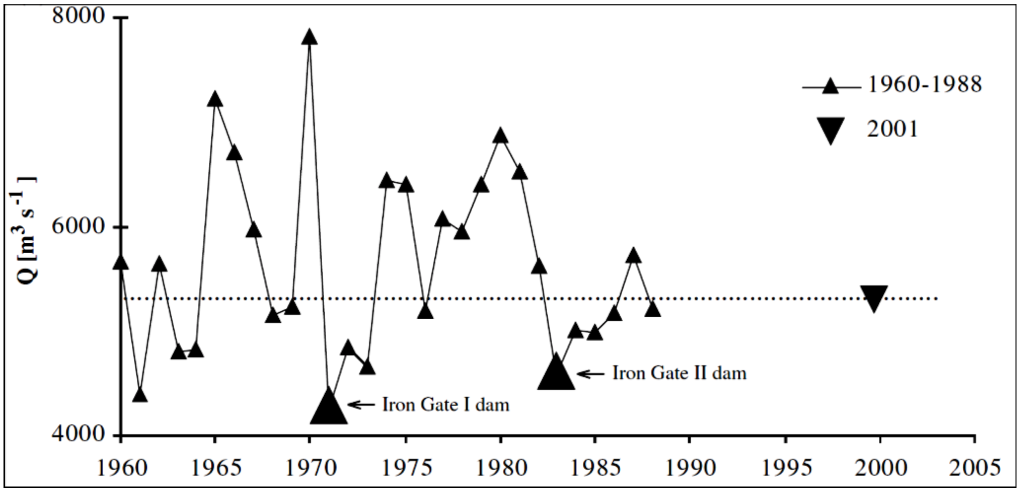


Fig. 7.18 Time series flow rate at Drobeta–Turnu Severin station from 1960 to 1988 and the average outflow at the Iron Gate dams for the year 2001 [214]

7.5. Conclusions

In conclusion, the main factors/sources influencing the quality of the river are the hydro-geochemical variables, organic pollution from domestic wastewater, industrial discharge and non point source pollution such as agriculture activities from agricultural areas and surface runoff.

Spatial CA grouped the four sampling sites on the river into two statistically significant clusters. First (SS1 and SS2) corresponds to relatively less polluted sites whereas, the second (SS3 and SS4) corresponds to relatively moderate polluted sites. It was concluded that the study area is highly affected by pollution load from domestic and industrial discharges in comparison with pollution load from the agriculture area. Temporal CA grouped the 12 months into two major groups. The results demonstrate that the temporal variation in the Danube river water quality was not strictly determined by local climate (spring, summer, autumn, winter). It was observed that the discharge (Q) is the main factor influencing temporal variation among other parameters in the Danube River. Therefore, multivariate methods are believed to be an effective tool for proper management of water resources and providing a good explanation to understand complex dataset of surface water quality.

Chapter 8: Water quality assessment of the Danube River using WQI models

8.1. Introduction

In chapter 8, six different water quality index models have been applied to explore the usefulness of these indices in assessing the water quality of Danube River, to identify the effectiveness of the selected water quality index models through a comprehensive comparison, and to get information on the temporal and spatial variations of water quality in a simple and easy manner. The selected water quality index models are Canadian Council of Ministers of the Environment Water Quality Index (CCME-WQI) [33], Oregon Water Quality Index (OWQI) [53], Aquatic Toxicity Index (ATI) [233], Universal Water Quality Index (UWQI) [27], Overall Index of Pollution (OIP) [188] and BWQI [16].

The water quality index (WQI) can be defined as the aggregation of observed values of water quality parameters to obtain a single number that represents the overall description of the quality of water (i.e. gathering a large amount of water quality data into single number). Usually, the WQI has a scale from 0 to 100, the highest value representing better water quality and lowest value indicates poorest water quality. Moreover, it can be used to express the quality of water for different uses such as drinking, irrigation and industrial.

8.5. Water Quality Index Models

8.5.1. Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI)

The CCME-WQI index has been employed by various countries all over the world to assess water quality. The main advantage of this index is that a large number of variables can be included in the calculation steps of CCME-WQI. Therefore, in this study, all the 13 water quality parameters were considered. It has a totally different approach among others in which it comprised three factors for calculating the final index.

8.5.2. The modified Oregon Water Quality Index (OWQI)

OWQI integrates the measurement of eight parameters to produce the overall water quality, namely DO, BOD, pH, temperature, NH_3 + NO_3, TP, TS and fecal coliform. OWQI uses the non-linear sub-indices to transform the measurement of water quality parameters. The OWQI does not examine the quality of water for specific uses; rather it reflects the water quality for general recreational use. In this study, the modified OWQI were used.

8.5.3. Aquatic Toxicity Index (ATI)

ATI takes into account the toxic effects of different physical, chemical and toxic metals on aquatic life, especially fish. The water quality variables included in ATI are pH, DO, turbidity, NH_4, TDS, F^-, K, PO_4, Zn, Mn, Cr, Cu, Pb, and Ni. This index uses non-linear sub-indices to transform the measurement of water quality variables into a value between 0 and 100.

8.5.4. Universal Water Quality Index (UWQI)

UWQI assess the quality of surface water for drinking water abstraction. It includes 12 water quality parameters to calculate the final index (viz. pH, DO, NO_3, BOD, As, F^-, TP, Hg, Se, Cyanide, Cd, and total coliform). Mathematical equations were formulated for each parameter in order to determine the sub-index value. Furthermore, a weight assigned to each parameter according to its importance ranged from 1 – 4.

8.5.5. Overall Index of Pollution (OIP)

OIP was developed to assess the surface water quality. OIP took into consideration standards from various national and international agencies such as Central Pollution Control Board (CPCB), the European Community (EC), WHO and others. The water quality variables included in OIP index are color, pH, turbidity, DO, BOD, hardness, TDS, total coliforms, Cl^-, NO_3, SO_4, As, and F^-. It uses the segmented non-linear sub-indices for most of variables to transform the measurement of water quality variables into a unit less value ranged from 1 to 16. The index scale of OIP is differing from all other water quality indices used in this study.

8.5.6. Bascaron WQI (BWQI)

BWQI has been widely used over the world. The major advantage of BWQI is that a large number of water quality variables can be included in calculating the final index after assigning the normalization factors as well as their weights. However, only 22 water quality variables were found that already have been normalized and weighted in various reported studies. In this study, eight water quality parameters were included for the evaluation process, namely temperature, pH, DO, BOD, NH_4, NO_3, TP, and TSS. Comparison between the results of the selected indices is also presented in this study.

Table 8.2 shows the water quality parameters that have been used in each selected index model.

Table 8.2 The water quality parameters that used in each selected WQI model.

Parameters	**CCME WQI**	**OWQI**	**ATI**	**UWQI**	**OIP**	**BWQI**
DO	×	×	×	×	×	×
BOD	×	×		×	×	×
NH_4	×		×			×
NO_3	×	×		×	×	×
TP	×	×		×		×
WT	×	×				×
pH	×	×	×	×	×	×
TSS	×					×
Cd	×			×		
Cu	×		×			
Cr	×		×			
Ni	×		×			
Pb	×		×			

8.6. Results and Discussions

The results of CCME WQI are shown in Fig. 24. The European Community (EC) standards for drinking water abstraction were used for CCME WQI calculation and presented in Table 8.4. EC standards proposed guidelines for surface water used as raw water for drinking water based on three types: simple physical treatment and disinfection (A1), normal full physical and chemical treatment with disinfection (A2) and intensive physical and chemical treatment with disinfection (A3). Water quality standards values were presented as Guide Level (GL) value and Maximum Allowable Concentration (MAC) value for 38 parameters. In this study, guide level values were considered for all variables except for Cr and Pb. In addition, total phosphorus and Ni were not included in EC standards and therefore, water quality standards from National Administration of Romanian Waters were used. In CCME WQI, all the variables were taken into account for the evaluation process. The water quality classification scheme for sampling stations was found to be fair in SS1, SS3 and SS4, whereas marginal in SS2. The most important variables that affect the water quality were NH_4, TP, WT and TSS.

Table 8.4 the EC standards for surface water quality used for drinking water abstraction (directive 76/464/EEC)

Variables	**Units**	**Guide Level**
DO	mg/L	>70%
BOD	mg/L	<3
NH_4	mg/L	0.05
NO_3	mg/L	25
Total P	mg/L	0.1[a]
WT	°C	22
pH	pH units	6.5-8.5
TSS	mg/L	25
Cd	µg/L	1
Cu	µg/L	20
Cr	µg/L	50[b]
Ni	µg/L	50[a]
Pb	µg/L	50 [b]

[a] National Administration of Romanian Waters [b] maximum allowable concentration

The water quality categorization of OWQI for all sampling sites was found as very poor. The result of this index is shown in Fig. 8.6. The major parameters that affect the water quality are NO_3 and TP. The result of ATI is shown in Fig. 8.6. ATI was used to assess the health of aquatic life, especially fish, in the river. The classification scale of the water quality for all sampling sites suggests that the river is of suitable quality for all fish life. In universal water quality index (UWQI), six parameters were used. The result of ATI this index is shown in Fig. 8.6. The water quality categorization for all sampling sites was found as good. Excellent water quality was observed in the month of January for all sampling stations. Total P was the prominent parameter in this index. OIP has a scale ranged from 0 to 16; this scale has been converted to a scale ranged from 0 to 100 for comparison purposes. The categorization of water quality in all stations was found as acceptable (see Fig. 8.6). It was observed that all the variables used in this model have the same degree of significance on water quality. The last index used in this study is the Bascaron WQI (BWQI). The categorization of water quality in all stations was found as good (see Fig. 8.6). The most important parameters that affect adversely on water quality are NH_4 and WT. Moreover, the temporal variation in all sampling sites was insignificant.

The selected water quality index models have different approaches in the implementation process. It was observed that CCME-WQI has a totally different approach and distinct characteristics among others. CCME-WQI has the ability to take into account all the water quality variables, in addition to its flexibility of selecting the water quality standards and comparatively tolerant in case of missing data. Moreover, it can be applied to assess the water quality for different uses and it does not utilize sub-index to transform the measurement of water quality into a unit less number. It comprised three factors for the evaluation process (scope, frequency, and amplitude). However, this index is not free of flaws, such as considering all the water quality variables have the same degree of importance, and it can be applied only when there are available guidelines on water quality parameters.

The other water quality index models rely on sub-indices values in the calculation process with different aggregation methods. In OWQI, non-linear sub-index is used and unweighted harmonic square mean function for aggregation. OWQI evaluates the general recreational use of water like fishing and swimming. The results of this index indicate that the water quality is very poor in all sampling station, despite the low values of BOD and high values of DO in the river. NO_3 and TP were the major factor affecting the water quality in this model and however, NO_3 was within the standards limit (Table 8.4). Therefore, OWQI was not applicable in assessing the water quality of Danube River (study region), which resulted in biased index.

ATI accounts for some heavy metals parameters to evaluate the fish life of the river. The results revealed that the river quality is suitable for all fish life in all sampling stations. ATI is using the unweighted additive function for aggregation process. ATI model was somewhat acceptable in spite of an eclipsing problem for the NH_4 value which exceeded the limits.

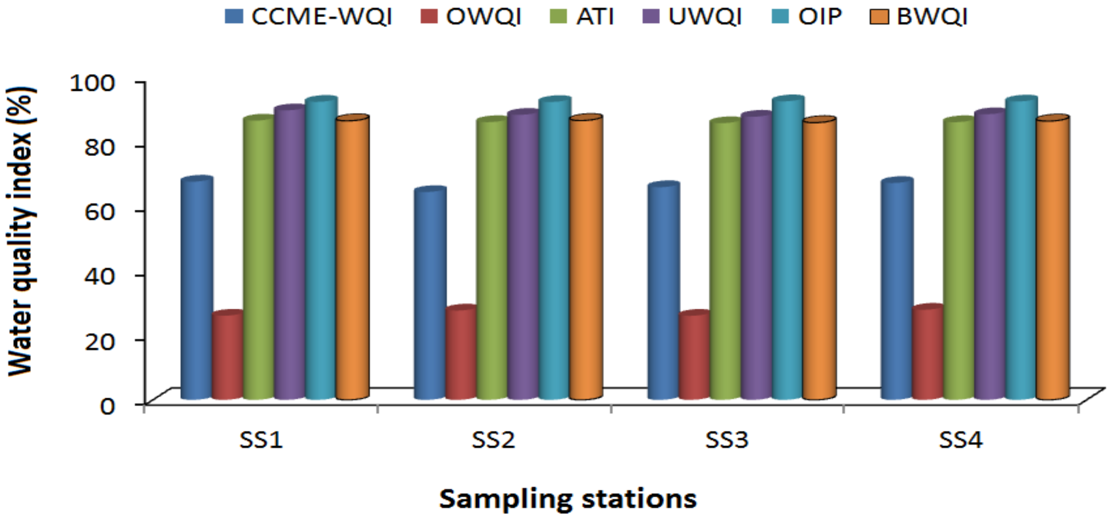


Fig. 8.6 WQI values of different water quality indices in four sampling stations

UWQI is developed to assess the surface water quality for drinking water abstraction. It uses the weighted sum function for aggregation process and segmented linear sub-index. This model gives a weighting factor for each variable which makes it differ from others (i.e. the water quality variables do not have the same degree of importance). The results showed that the river water quality is good with a value of more than 87 in all stations (Fig. 8.6) in spite of very low sub-index values for TP. The weighed sum function has eclipsed the effect of TP.

In OIP, only four water quality parameters were considered for calculating the final index. This model has a different scale among others and the results revealed that the river water quality is acceptable. The comparison process would be unfair because the model takes into account 13 water quality variables versus four parameters considered in this study. However, this model does not account for phosphorus compounds.

The BWQI is used to assess the water quality for general uses. It uses weighted sum function for aggregation process and segmented linear sub-index (step type). This model assigns relative weight for each water quality variable. The results demonstrate that the river water quality is good. The major issue in this index is that the given relative weight for each variable may be varied due to the multiple perspectives of the experts. A comparison between the different water quality index models used in this study is presented in Table 8.10.

Table 8.10 Comparison between the different water quality indices used in this study

WQI models	**Sub-indices for the most variables**	**Aggregation methods**	**Water uses**	**Number of variables**
CCME-WQI	Formula	Harmonic Square sum function	Various water uses	L[a]
OWQI	Non-linear	Unweighted harmonic square mean function	General recreational use	8
ATI	Non-linear	Unweighted additive aggregation function	Health of aquatic ecosystems	14
UWQI	Segmented linear	Weighted sum function	Drinking water abstraction	12
OIP	Segmented non-linear	Unweighted arithmetic mean function	Surface water quality	13
BWQI	Segmented linear (step)	Weighted sum function	General uses	22[b]

[a] Large numbers of variables can be included in the calculation of CCME-WQI but not less than four variables

[b] The available water quality variables that already have been normalized and weighted in various reported studies.

Based on the above discussion and the outcomes depicted in Fig. 8.6, it can be concluded that the CCME-WQI has provided realistic results in comparison to the raw data of the Danube River. The results of CCME-WQI were fair in three stations (SS1, SS3 and SS4) and marginal in one station (SS2). Fair category indicates that “the water quality is frequently threatened or impaired; conditions often depart from natural or desirable levels”. Marginal category indicates that “the water quality is almost always threatened or impaired; conditions usually depart from natural or desirable levels”. CCME-WQI has given the best results among other models. The results of the other models (OWQI, ATI, UWQI, OIP, and BWQI) did not introduce representative outcomes of the raw data of the river.

8.7. Conclusions

The conclusions drawn of this chapter are: (i) the selected index models express the quality of water for different uses such general uses, drinking water abstraction, the health of aquatic life etc. CCME-WQI is the only model that can be applied to assess the water quality for different uses. (ii) the water quality of the Danube River in four sampling stations ranged from marginal to fair for CCME-WQI, very poor for OWQI, suitable for all fish life for ATI, good for UWQI, acceptable for OIP and good for BWQI. (iii) among selected index models, CCME-WQI has a totally different approach. It uses a formula and does not include sub-indices for the implementation process. It comprised three factors for the evaluation process (scope, frequency, and amplitude). Moreover, all the water quality variables have been used in the calculation of CCME-WQI. This model gave more reasonable results in comparison to other models. (iv) the results of the other models (OWQI, ATI, UWQI, OIP, and BWQI) did not introduce representative outcomes of the raw data of the river. (v) no significant changes were observed for temporal variation in the Danube river water quality.

Chapter 9: Conclusions, personal contributions and future research directions

9.1. Overall conclusions

This thesis comprised the use of surface water quality modeling to simulate the dispersion behavior of the biochemical oxygen demand (BOD). The Danube River at Drobeta Turnu–Severin city stretch was chosen as a case study and different modeling approaches have been applied to simulate the water quality in the river. Advection-dispersion equation (ADE) in 1D, 2D and 3D was used for simulation, since it allows the prediction of pollutant behavior at various distances downstream of the point source pollution. ADE is widely employed to build models for pollutant transport, and it has proved to be suitable for a large number of cases. CFD codes such as FlexPDE and FLUENT have been used to simulate the BOD dispersion in the river and its tributaries.

Moreover, some water quality assessment tools such as multivariate statistical techniques and water quality indices were also employed to produce a comprehensive understanding of the river water quality status in the study region. The overall conclusions drawn of this thesis are as follows:

1. FlexPDE solver was capable of simulating the dispersion of BOD from Jidostita tributary in 2D form. The results demonstrated that the simulated BOD was in agreement with the observed data. Furthermore, BOD dispersion from Jidostita tributary is highly affected by the river velocity. The major difficulty was to identify the longitudinal and transverse dispersion coefficients as obtained from previous technical reports.
2. FLUENT was used to predict the BOD dispersion of a curve-shaped open channel flow with a side discharge using 2D and 3D numerical model. A real open channel flow was considered for the calibration of the model, in which the values adopted demonstrate the actual values in the Danube River and its tributary (Arges river). In spite of some error between simulated dispersion of BOD along the channel and observed water quality data, the numerical simulation results show a good agreement with observed data in the literature.
3. The RANS method tends to give a good estimation for Reynolds stress model or the flow turbulence intensity. It required relatively low computational costs in comparison to other models such as DNS and LES models.
4. Furthermore, RANS involves four Boussinesq eddy viscosity turbulence models. The two-equation model (standard k–ε turbulence model) has provided a good representation for simulating the flow in an open channel. In spite of its limitations, it is still very popular and can be used to give suitable results within engineering accuracy when applied to appropriate cases.
5. The volume of fluid (VOF) and user defined scalar (UDS) methods provided appropriate results when they were used to compute the free surface flow in open channel flow and pollutant transport respectively.
6. The coefficients of the mixing length are highly dependent on the geometrical characteristics, hydraulic and flow regime of the river.
7. One-dimensional model (QUAL2K) that was applied for simulating the BOD, DO, Q and pH in the Danube River at Drobeta Turnu–Severin city was able to predict the water quality in different seasons and scenarios. The results showed that the DO and BOD were within the limits, which reflect a good health for the river in the study area. It can be concluded that QUAL2K can be used as a suitable tool for simulating the water quality in a large river.
8. The Topolniţa tributary was the major source influencing the water quality of the river in the study region.
9. The main sources influencing the quality of the Danube river in the study area are the hydro-geochemical variables, organic pollution from domestic

wastewater, industrial discharge and non point source pollution such as agricultural activities from agricultural area and surface runoff.

10. The study area is highly affected by pollution load from domestic and industrial discharges in comparison with pollution load from the agricultural area.
11. The temporal variation in the Danube river water quality was not strictly determined by local climate (spring, summer, autumn, winter).
12. The discharge (Q) is the main factor influencing temporal variation among other parameters in the Danube River.
13. CCME-WQI can be applied to assess the water quality in Danube River as it can express the results more closely. However, other selected index models may be applicable to other water bodies.

9.2. Personal contributions

1. Review of 11 popular computer water quality models developed by different international agencies based on a set of criteria such as basic equations, input and output data, model capability, model limitations and its application to provide a comprehensive summary and capabilities of available models in current use.
2. Developing methods for modeling and simulation the dispersion of pollutant suitable for engineers, students and researchers which they need to know about the dispersion behavior in a river or stream.
3. Development of a 2D numerical model to predict the dispersion of pollutant (BOD) in the Danube River at Drobeta Turnu–Severin stretch using FlexPDE and evaluating the impact of Jidostita tributary as a waste loads on the receiving river.
4. Development of a numerical model to simulate the BOD dispersion (2D and 3D) in a curve-shaped open channel flow with a side discharge with different values of flow rate and diffusivity coefficient using volume of fluid (VOF) method and scalar transport to examine the effect of the flow rate and diffusivity coefficient on the concentration of pollutant from the polluted tributary on the river.
5. Application of QUAL2K model (1D steady-state) for simulating the water quality (i.e. pH, DO and BOD) in the Danube River and to compare the results with our original model.
6. Examine the impact of tributaries and other waste loads in the study area such as Jidostita and Topolniţa on the receiving river and predict the BOD and DO of the river in different scenarios as a proactive management.
7. Explore the applicability of a one-dimensional, steady-state model for simulating the water quality in large (i.e. deep and wide) river.
8. Application of multivariate statistical techniques to identify the major factors affecting the water quality of Danube River at Drobeta-Turnu Severin city using Factor Analysis.

9. Provide a comprehensive understanding about the spatial and temporal variations among the sampling sites and monitoring periods using cluster analysis.
10. Application of six different water quality index models to explore the usefulness of these indices in assessing the water quality of Danube River.
11. Identify the effectiveness of the selected water quality index models through a comprehensive comparison.
12. Utilization of WQIs to get information on the temporal and spatial variations of water quality in a simple and easy way.

9.3. Future research directions

1. This study was limited to assess only 13 physico-chemical parameters of the water quality. Future studies may take into account the biological water quality parameters and their influence on human health.
2. The simulation process may be extended to include the nutrients in the river as this study considered only the simulation of the organic pollution (BOD and DO).
3. GIS techniques may be introduced in the assessment and modeling of the Danube river. GIS can be used as support tool for simulating the water quality in the river.

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