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FACULTY OF CIVIL AND GEODETIC ENGINEERING
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CONTENTS - VSEBINA

DUŠAN ŽAGAR

**RAZVOJ IN APLIKACIJA TRIDIMENZIONALNEGA
MODELA ZA SIMULACIJO TRANSPORTA IN
PROCESOV PRETVORB ŽIVEGA SREBRA
V MORSKEM OKOLJU**

**DEVELOPMENT AND APPLICATION OF A THREE-
DIMENSIONAL MODEL TO SIMULATE MERCURY
TRANSPORT AND TRANSFORMATION PROCESS
IN THE MARINE ENVIRONMENT**

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UVODNIK

V tokratni številki *Acta hydrotechnica* je objavljen razširjeni povzetek doktorske disertacije dr. Dušana Žagarja, asistenta za mehaniko tekočin na Katedri za mehaniko tekočin z laboratorijem Fakultete za gradbeništvo in geodezijo Univerze v Ljubljani.

Dr. Dušan Žagar je leta 1982 končal Tehniško srednjo šolo – smer gradbeništvo v Celju. Študij je nadaljeval na Univerzi v Ljubljani, na Fakulteti za arhitekturo, gradbeništvo in geodezijo, Oddelku za gradbeništvo, kjer je leta 1989 diplomiral na hidrotehnični smeri. Po opravljeni diplomski se je zaposlil kot projektant v Cestnem podjetju Celje, kjer je uvajal računalniško podprto projektiranje, bil odgovoren za nabavo ustrezne strojne in programske opreme za geodezijo in projektiranje ter dopolnilno izobraževal projektante. Leta 1991 je opravil državni strokovni izpit s področja gradbeništva. Leta 1989 se je vpisal na podiplomski študij gradbeništva - hidrotehnična smer. Leta 1994 je končal magistrski študij z magistrsko nalogo s področja tridimenzionalnega matematičnega modeliranja tokov v Tržaškem zalivu v primeru razlitja nafte.

V času doktorskega študija je bil dr. Žagar kot mladi raziskovalec od 1.12.1995 vključen v raziskovalno delo Katedre za mehaniko tekočin na FGG. V okviru doktorskega študija je sodeloval predvsem pri numeričnem modeliranju hidrodinamike in transporta polutantov ter šest tednov tudi znanstveno deloval na Univerzi Johns Hopkins v Baltimoru v ZDA.

Doktorska disertacija dr. Dušana Žagarja je nastajala v okviru temeljnih in aplikativnih projektov MZT »Izpopolnjevanje in umerjanje modelov za simulacijo procesov v vodnem okolju in ozračju«, »Biogeokemijski cikel in modeliranje živega srebra v Tržaškem zalivu« in »Modeli transporta in disperzije polutantov v površinskih in talnih vodah«.

Glavna naloga disertacije z naslovom »Razvoj in aplikacija tridimenzionalnega modela za simulacijo transporta in procesov pretvorb živega srebra v morskem okolju« je bila opisati problematiko onesnaženja z živim srebrom v morskem okolju in še posebej v Tržaškem zalivu, dopolniti obstoječi tridimenzionalni matematični model z modulom za simulacijo transporta in disperzije raztopljenega in na delce lebdečih plavin vezanega živega srebra v različnih pojavnih oblikah. Tako je bil izdelan nov scenarij za dolgotrajne nestacionarne simulacije, pridobljeni in opisani so bili tudi vhodni podatki takih simulacij. Izpopolnjeni model je bil tudi umerjen in preverjen s primerjavo z analitičnimi rešitvami in meritvami.

Doktorska disertacija predstavlja pomemben prispevek na obravnavanem področju raziskovalnega dela, predvsem je pomembna obdelava problema v treh dimenzijah. Po vsej verjetnosti gre za prvi tridimenzionalni model za simulacijo procesov živega srebra v svetu. Avtor je o svojem delu odmevno poročal na mednarodnem kongresu "Živo srebro kot globalni polutant" v Rio de Janeiru v maju 1999 in svoje izsledke podrobneje objavil v reviji *Science of the Total Environment*. Naj tudi ta objava v *Acta hydrotechnica* pripomore k širitvi najnovejših znanj o živem srebri, ki je v svetu kot toksična snov predmet obširnega raziskovanja.

EDITORIAL

This issue of *Acta hydrotechnica* is publishing an extended summary of a Doctoral Thesis by Dušan Žagar, a teaching assistant in the Chair of Fluid Mechanics, Faculty of Civil and Geodetic Engineering, University of Ljubljana.

Dr. Dušan Žagar completed technical high school (major in civil engineering) in Celje in 1982. After that he studied at the University of Ljubljana, Faculty of Architecture, Civil and Geodetic Engineering, Department of Civil Engineering, where he graduated in 1989 from the Hydraulic Division. After his studies he was employed at the road construction company Cestno podjetje Celje as a designing engineer in charge for CAD, software and hardware in geodetic engineering and design, and for the training of professional engineers. In 1991, he was promoted to the rank of professional civil engineer. In 1989, he enrolled in the Master's Program of the Hydraulic Division. In 1994, he completed his study with a Master's Thesis in the field of a three-dimensional mathematical modelling of the Gulf of Trieste in the case of an oil-spill.

During his doctoral studies, Dr. Žagar was included in the faculty's research team as a junior researcher, and has served in that capacity since December, 1995. He participated in the numerical modelling of hydrodynamics and pollutant transport, and he spent six weeks as a visiting researcher at the Johns Hopkins University in Baltimore, USA.

This Doctoral Thesis by Dušan Žagar was developed within the framework of basic and applied research projects granted by the Ministry of Science and Technology of the Republic of Slovenia, especially the projects : "Improving and Validation of Models for Simulation of Processes in the Water Environment and in the Air", "Biogeochemical Cycle and Modelling of Mercury in the Gulf of Trieste", and "Models of Transport and Pollutant Dispersion in Surface and Ground Waters".

The main aim of the thesis titled "Development and Application of a Three-Dimensional Model to Simulate Mercury Transport and Transformation Process in the Marine Environment" was to describe problems with mercury pollution in the marine environment and especially in the Gulf of Trieste in the Northern Adriatic Sea, and to complete an existing three-dimensional mathematical model with a module for simulation of transport and dispersion of dissolved mercury and mercury bound to suspended load particles in different forms. In this respect, a new scenario for long-term non-steady state simulations has been developed, as well as input data of such simulations acquired and described. The advanced model was calibrated and validated using analytical solutions and measurements.

This thesis represents an important contribution in this respected research field; especially important is the three-dimensional treating of the problem. Very likely, it is the first three-dimensional model for the simulation of mercury processes in the world. The author's presentation at the International Congress on Mercury as a Global Pollutant in Rio de Janeiro in 1999 was met with wide response. The most important conclusions of the thesis were published in the journal *Science of the Total Environment*. We hope that this summary of the thesis published in *Acta hydrotechnica* may help disseminate the latest in mercury research, which is widely under research in the world because of its toxicity.

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**RAZVOJ IN APLIKACIJA TRIDIMENZIONALNEGA MODELA
ZA SIMULACIJO TRANSPORTA IN PROCESOV PRETVORB
ŽIVEGA SREBRA V MORSKEM OKOLJU**

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**DEVELOPMENT AND APPLICATION OF A THREE-DIMENSIONAL
MODEL TO SIMULATE MERCURY TRANSPORT AND
TRANSFORMATION PROCESS IN THE MARINE ENVIRONMENT**

summary of the Doctoral Thesis
Faculty of Civil and Geodetic Engineering, University of Ljubljana
the defence of the Doctoral Thesis was on December 28, 1999

IZVLEČEK

Kot glavni cilj naloge je predstavljena nadgraditev tridimenzionalnega baroklinega matematičnega modela PCFLOW3D, z novima moduloma za račun transporta lebdečih plavin in živega srebra v morskem okolju. Model omogoča račun hidrodinamičnih količin zaradi vpliva vetra, plimovanja ter vtokov in iztokov ob upoštevanju gostotne stratifikacije, račun resuspendiranja sedimenta z dna, račun transporta in disperzije lebdečih plavin ter račun transporta in disperzije živega srebra v raztopljeni obliki in vezanega na delce plavin. Kot verifikacija sedimentacijskega modula je izvedena primerjava z rešitvami analitičnih enačb, meritev v laboratoriju in naravi ter rezultati sorodnega modela.

Zbrani in obdelani so podatki o temperaturnih in slanostnih razmerah ter vetru v Tržaškem zalivu, pretokih, količini lebdečih plavin in temperaturi Soče ter vsebnosti živega srebra v vodi, lebdečih plavinah, sedimentu in pornih vodah. Iz podatkov so izračunane povprečne sezonske vrednosti parametrov, ki skupaj z vložki krajšega trajanja bistveno vplivajo na transport živega srebra in predstavljajo vhodne podatke modela. Na podlagi teh podatkov je narejen scenarij za dolgotrajne simulacije, s katerim nadomestimo modeliranje s povprečnimi letnimi vrednostmi.

Opisana je kalibracija in verifikacija modela PCFLOW3D na treh primerih, pri čemer so uporabljeni podatki meritev in opazovanj iz let 1995, 1996 in 1997. Ugotovljeno je kvalitativno dobro ujemanje rezultatov modela z meritvami, kjer je mogoča kvantitativna primerjava, pa je ujemanje v okviru faktorja dve.

Ključne besede: matematični model, tridimenzionalni model, hidrodinamika, transport sedimentov, lebdeče plavine, resuspenzija, Tržaški zaliv, severni Jadran, živo srebro

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ABSTRACT

An upgrade of the existing three-dimensional baroclinic mathematical model PCFLOW3D is presented. Two new modules were developed to simulate processes in aquatic environment. Resuspension of bottom sediment, transport and dispersion of suspended sediment and transport and dispersion of mercury in its dissolved and particulate form was included in the model. Hydrodynamics due to wind forcing, tidal forcing and river inflow momentum can be simulated, and stratified conditions can be taken into account. A comparison with solutions of analytical equations, laboratory and field measurements, and results of a similar sediment transport model was obtained to verify the sediment transport module.

A large amount of data about temperature and salinity fields in the Gulf of Trieste, wind conditions above the Gulf, Soča River discharges, suspended sediment concentrations and temperatures were collected and interpreted. The described data, together with measurements of the mercury concentrations in the water, suspended sediment, bottom sediment and pore waters in the Soča River and the Gulf of Trieste are used as input for the upgraded PCFLOW3D model. A scenario for long-term simulations on the basis of seasonally averaged parameters and values in a few shorter sequences was developed as a substitution for previous annually averaged simulations.

Measurements and observation data from the years 1995, 1996 and 1997 were applied to calibrate and verify the PCFLOW3D model. A good qualitative agreement of results and measurements was achieved. Whenever a quantitative comparison was possible, an accordance of measured and computed results within a factor of two is reached.

Keywords: mathematical model, three-dimensional model, hydrodynamics, sediment transport, suspended sediment, resuspension, Gulf of Trieste, Northern Adriatic, mercury

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SEZNAM SIMBOLOV - LIST OF SYMBOLS

oznaka <i>symbol</i>	dimenzija <i>dimension</i>	opis <i>pomen</i>	description <i>meaning</i>
a	[m]	referenčna globina	reference level
A_i	[m ²]	površina	surface
C	[kg/m ³]	koncentracija	concentration
C_a	[kg/m ³]	referenčna koncentracija sedimenta (na referenčni globini)	reference concentration of suspended sediment (at the reference level)
C_{ae}	[kg/m ³]	ravnotežna referenčna koncentracija plavin	equilibrium concentration of suspended sediment
D_h	[m ² /s]	horizontalni koeficient turbulentne difuzije	eddy diffusivity coefficient in horizontal direction
D_v	[m ² /s]	vertikalni koeficient turbulentne difuzije	eddy diffusivity coefficient in vertical direction
D_{16}	[m]	premer zrna plavin, od katerega je manjših 16 % zrn	particle diameter of which 16 % of particles are thinner
D_{50}	[m]	srednji premer zrna plavin	mean particle diameter
D_{84}	[m]	premer zrna plavin, od katerega je manjših 84 % zrn	particle diameter of which 84 % of particles are thinner
D_{90}	[m]	premer zrna plavin, od katerega je manjših 90 % zrn	particle diameter of which 90 % of particles are thinner
Fe	[m]	privetrna razdalja	fetch length
f_i	[N/m ³]	prostorninska sila na enoto mase v koordinatni smeri i	volume force per mass unit in coordinate direction i
f_w	[-]	koeficient trenja	friction coefficient
g	[m/s ²]	težnostni pospešek	gravity acceleration
h	[m]	debelina sloja	layer thickness
H	[m]	celotna globina vode od dna do trenutne gladine	total water depth from the bottom to the surface
H_w	[m]	višina vala	wave height
k_{por}	[-]	koeficient poroznosti oziroma zbitosti	porosity
L'	[m]	valovna dolžina	wavelength
n_g	[s/m ^{1/3}]	Manningov koeficient hrapavosti	Manning's coefficient
N_h	[m ² /s]	horizontalni kinematični koeficient turbulentne viskoznosti	eddy viscosity coefficient in horizontal direction
N_v	[m ² /s]	vertikalni kinematični koeficient turbulentne viskoznosti	eddy viscosity coefficient in vertical direction
P	[Pa]	tlak	pressure
Q	[m ³ /s]	pretok	discharge
$Q_{2.5}$	[m ³ /s]	pretok s povratno dobo 2.5 leti	discharge with a recurrence of 2.5 years
s_s	[kg/m ³]	relativna gostota delcev plavin	relative particle density

S_{Φ}	[-]	izvorni člen skalarja Φ	source term of the scalar Φ
t	[s]	čas	time
T	[-],[°]	transportni parameter, temperatura	transport parameter, temperature
Te	[°]	temperatura	temperature
u, v, w	[m/s]	komponente hitrosti v koordinatnih smereh x, y in z	velocity components in coordinate directions x, y in z
u^*, u_s^*	[m/s]	strižna hitrost ob dnu	bed shear velocity
$u_{*,cr}$	[m/s]	kritična strižna hitrost ob dnu	critical bed shear velocity
$\bar{u}$	[m/s]	po vertikali povprečena hitrost	depth averaged velocity
u_w	[m/s]	hitrost vetra	wind speed
$u_{b,w}$	[m/s]	strižna hitrost ob dnu zaradi valov	bed shear velocity due to waves
$u_{b,c}$	[m/s]	strižna hitrost ob dnu zaradi tokov	bed shear velocity due to currents
$u_{b,cw}$	[m/s]	strižna hitrost ob dnu zaradi tokov in valov	bed shear velocity due to combination of currents and waves
$U_{d,p}$	[m/s]	vršna hitrost vala	wave peak orbital velocity
V_{cell}	[m ³]	volumen celice (kontrolnega volumna)	volume of a cell (control volume)
W_s	[m/s]	hitrost usedanja delcev plavin	settling velocity
x_i	[-]	posamezne koordinatne smeri	individual coordinate directions
z_b	[m]	kota dna	bottom level
Γ_{ϕ}	[-]	laminarna difuzija skalarja Φ	laminar diffusion of scalar Φ
Δt	[s]	časovni korak računa	computational time step
Θ_c	[-]	parameter mobilnosti	parameter of mobility
κ	[-]	von Karmanova konstanta	von Karman's constant
λ	[-]	parameter suspendiranja	suspension parameter
ν	[m ² /s]	kinematični koeficient laminarne viskoznosti	kinematic coefficient of laminar viscosity
ξ	[m]	odmik gladine od referenčne srednje vrednosti	water surface elevation
ρ	[kg/m ³]	gostota	density
ρ_s	[kg/m ³]	gostota delcev plavin	density of suspended sediment particles
ρ_v	[kg/m ³]	gostota vode	water density
τ_b	[N/m ²]	strižna napetost ob dnu	bed shear stress
$\tau_{b,w}$	[N/m ²]	strižne napetosti ob dnu zaradi valov	bed shear stress due to waves
$\tau_{b,c}$	[N/m ²]	strižne napetosti ob dnu zaradi tokov	bed shear stress due to currents
$\tau_{b,cw}$	[N/m ²]	strižne napetosti ob dnu zaradi tokov in valov	bed shear stress due to currents and waves

1. OPIS PROBLEMA

Živo srebro (Hg) se kljub opuščanju okolju neprijaznih tehnologij še vedno uporablja v nekaterih vrstah industrijske proizvodnje, pri posameznih tehnoloških postopkih in pri amalgamiraju zlata. Živosrebrove spojine se sproščajo tudi ob sežiganju fosilnih goriv in odpadkov. Onesnaženje z živim srebrom se v obliki topnih in hlapnih spojin širi po zraku in vodi, zato ima živo srebro značaj globalnega polutanta.

Sredozemlje je še dodatno naravno obremenjeno z živim srebrom, saj se tam na razmeroma majhni površini nahaja večina svetovnih rudnih zalog živega srebra. Tu so največji rudniki živosrebrove rude na svetu, med katere se uvršča tudi rudnik v Idriji, po količini izkopane rude drugi največji na svetu.

Živo srebro se v naravnem okolju nahaja v več oblikah, kot **elementarno (Hg^0)**, **nemetilirano ($HgII$)**, **monometil (MMHg)** in **dimetil živo srebro (DMHg)**. Ob metilirani obliki sta bioakumulativni in zato še posebej nevarni za celotno prehranjevalno verigo.

Meritve v Tržaškem zalivu kažejo močno povišane koncentracije živosrebrovih spojin v vodi, sedimentu in vodnih organizmih. Koncentracije v naravnem zaledju so presežene za red, v sedimentu na dnu zaliva pa za dva reda velikosti in so višje od priporočljivih po WHO. Občasne anoksije v nižjih plasteh zaliva lahko pospešijo proces metilacije Hg, zato je vedno prisotna možnost negativnega vpliva na okoliško prebivalstvo. Znane so zastrupitve večjih skupin ljudi z ribami in s školjkami, ki so vsebovale visoke koncentracije MMHg. V japonskem mestu Minamata je umrlo več kot 140 ljudi, še mnogo več pa jih je ostalo trajno prizadetih. Medicinske raziskave so dokazale vpliv živosrebrovih spojin na človekov centralni živčni sistem, ki se lahko kaže v različnih oblikah od psihomotoričnih motenj, motenj vida, sluha, gibanja pa vse do paralize in smrti. Še pomembnejši pa je vpliv na genetski material, zato se danes posveča velika pozornost že najmanjšim dvigom koncentracij živega srebra v okolju.

1. INTRODUCTION

In spite of the abandonment of environmentally harmful technologies, mercury (Hg) is still used in some industrial branches, technological processes and for amalgamation in gold panning. Mercury is also released by fossil fuel and waste burning. As mercury in its volatile and dissolved compositions is spread through air and water, it can be considered a global pollutant.

The Mediterranean, additionally, is naturally polluted with mercury. Here, within a relatively small area, most of the mercury ore stores and the most important mercury mines in the world can be found. The Idrija mine is the second greatest mercury mine in the world, considering the amount of ore being excavated.

Several forms of mercury are present in the natural environment: **native (Hg^0)**, **non-methylated ($HgII$)**, **mono-methylated (MMHg)** and **di-methylated (DMHg)**. Both methylated forms are bioaccumulative, and, as such, they represent a particular risk for the whole food chain.

Recent measurements in the Gulf of Trieste have shown greatly increased mercury concentrations in the water, sediment and some marine organisms. The concentrations in the water and the biota were as much as an order of magnitude higher, and concentrations in the bottom sediment, even as much as two orders higher than the corresponding natural background values. The WHO recommended concentrations were also exceeded. Occasional anoxia at the bottom of the Gulf may increase the methylation of mercury; thus, a potential impact on the humans living near the Gulf is present. The intoxication of people by eating fish and seashells containing high concentrations of MMHg are known from the past. In the city of Minamata, in Japan, more than 140 people died, and many more were affected permanently. Medical research has proved the impact of mercury on the central nervous system of human beings. It can be represented in various other ways, such as psychomotoric disturbances, disturbance of sight, hearing or motion, paralysis and death. The impact on genetic material is even more important; therefore, great attention has recently been paid, to even the smallest MMHg concentration increase in the environment.



Slika 1.1. Tržaški zaliv z zaledjem.
 Figure 1.1. The Gulf of Trieste and the mainland area considered.

Raziskave dokazujejo, da je glavni vir onesnaženja Tržaškega zaliva z živim srebrom zdaj že opuščeni rudnik živega srebra v Idriji. Posledica večstoletnega izkoriščanja so visoke koncentracije anorganskega živega srebra v okolici rudnika zaradi odlaganja jalovine in žgalniških ostankov, pa tudi visoke vsebnosti živega srebra v sedimentu in plavinah Idrijce

Recent studies have shown that the former Idrija Mercury Mine is the main source of mercury pollution for the Gulf of Trieste. In about 500 years of ore mining, concentrations of inorganic mercury near the mine, itself, have significantly increased due to tailing depositions and smelting remains. Moreover, the suspended and bottom sediment of both the Idrija and the Soča rivers is highly

in Soče, obe reki pa to živo srebro v raztopljeni ter partikularni (vezani na delce plavin) obliki odnašata v Tržaški zaliv. Kljub temu, da rudnik že deset let ne obratuje več, se koncentracije živega srebra v rečnih plavinah, vodi in sedimentu na dnu Tržaškega zaliva niso bistveno znižale (Horvat et al, 1999).

Meritve koncentracij živega srebra v zraku, zemljini, vodi in lebdečih plavinah v Idrijci in Soči ter vodi, lebdečih plavinah, sedimentu ob dnu, pornih vodah in organizmih v Tržaškem zalivu so zaradi nizkih koncentracij v vodi (nekaj ng/l, MMHg pa nekaj pg/l) zahtevne in drage. Za poznavanje procesov povezanih z živim srebrom se poleg meritev uporabljajo tudi matematični modeli. Znani so modeli transporta po zraku, modeli kemijskih in biokemijskih procesov v zemljini, zraku in vodnem okolju (Henry et al, 1995) ter njihove kombinacije. Narejenih je tudi nekaj modelov prehranjevalne verige (Harris, 1991; Harris et al, 1994). Ti modeli so večinoma nič- ali enodimenzionalni in tako manj primerni za račun v večjih jezerih in morju, kjer je transport polutantov odvisen predvsem od hidrodinamičnih parametrov.

Leta 1996 je bil na FGG izdelan dvodimenzionalni (2D) matematični model STATRIM za simulacijo transporta in pretvorb živega srebra v Tržaškem zalivu, eden prvih večdimenzionalnih modelov živega srebra v svetovnem merilu. V model so bile vgrajene enačbe metilacije, demetilacije, sedimentacije, redukcije in vnosa iz atmosfere. Živo srebro je bilo razdeljeno na celokupno in metilirano in obravnavano v treh različnih oblikah: raztopljeni, partikularni in planktonski (vezani na plankton). Podrobnosti o modelu in rezultate simulacij je opisal Širca (1996).

Rezultati izvedenih simulacij so bili spodbudni, kljub poenostavitvam v modelu in razmeroma majhnemu številu meritev za kalibracijo in verifikacijo modela je bilo doseženo ujemanje rezultatov modela in meritev v okviru istega velikostnega razreda, z dodatno kalibracijo modela (Širca in Rajar, 1997b) pa celo ujemanje s faktorjem 3.

contaminated with mercury, which in its dissolved and particulate (adsorbed to suspended particles) form is carried away to the Gulf of Trieste. Even 10 years after the closure of the Idrija Mine, mercury concentrations in river sediments, water and sediment at the bottom of the Gulf do not show a significant decrease (Horvat et al, 1999).

Measurements of mercury concentrations in the air, soil, water and the suspended sediments of both rivers, the Idrijca and Soča, as well as in the bottom sediment, water and biota of the Gulf of Trieste are difficult to perform, as they require specially trained analysts and special equipment, and expensive, due to the extremely low concentrations in the water (a few ng/l, MMHg a few pg/l). Besides measurements, mathematical modelling is also used to perceive mercury transport and transformation processes. Several air transport models, models of chemical and biochemical processes in the soil, air and water (Henry et al, 1995), as well as their combinations, are known, and even a few food chain models have been developed (Harris, 1991; Harris et al, 1994). All these are mostly zero- or one-dimensional models, less accurate for simulations in larger lakes or coastal sea, where transport of pollutants depends mostly on hydrodynamics.

In 1996, the two-dimensional (2D) mathematical model STATRIM was developed to simulate the transport and transformation of mercury compounds in the Gulf of Trieste. It was one of the first multi-dimensional mercury models in the world. Equations of methylation, demethylation, sedimentation, reduction and atmospheric input were included in the model. The transport and transformation of total and methylated mercury in three different forms (dissolved, particulate and plankton-bound) were simulated with the model. A detailed description of the model can be found in (Širca, 1996).

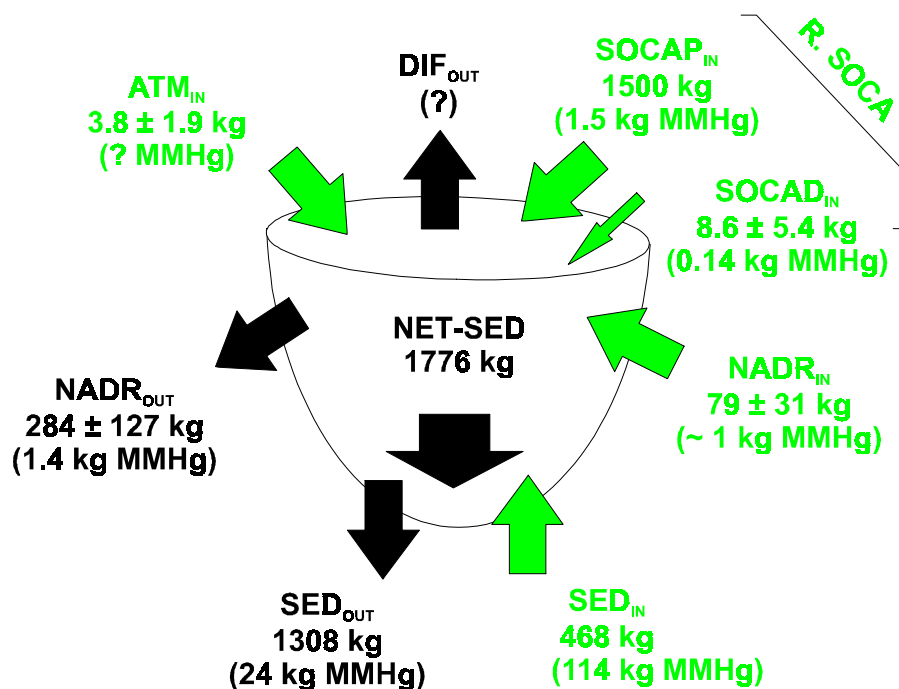
Results of the modelling were encouraging. Despite simplifications in the model and a relatively low amount of measurements for calibration and verification of the model, an agreement with measurements within an order of magnitude was reached. After an additional calibration of the model (Širca and Rajar, 1997b), an agreement within a factor of 3 was reached.

2D model je skupaj z meritvami dal tudi odgovore na nekatera ključna vprašanja v zvezi z nadaljnjim modeliranjem:

1. Glavni vir celokupnega živega srebra v Tržaškem zalivu je reka Soča.
2. Večji del MMHg nastane v zalivu samem, s Sočo pritečejo zanemarljivo majhne količine.
3. Večina živega srebra doteka v zaliv v partikularni obliki, zato je izdelava kakovostnega sedimentacijskega modela prednostna naloga nadaljnjega modeliranja.
4. Katere meritve so potrebne za nadaljevanje modeliranja ter kdaj in kako jih izvajati?

The 2D model, together with measurements, has given answers to some very important questions about further modelling:

1. The Soča River is the main source of inorganic mercury in the Gulf of Trieste.
2. Most of the MMHg is formed in the Gulf itself; only a negligible amount flows into the Gulf by means of the Soča River.
3. Most of the mercury is transported in particulate form; therefore, development and application of a reliable sediment transport model is the priority task of further modelling.
4. Knowing which measurements are needed, and how and when to collect samples is necessary to get the input data for further modelling.



Legenda/Legend:

ATM _{IN}	vnos iz atmosfere	atmospheric deposition
DIF _{OUT}	difuzija	evasion
SOCAP _{IN}	dotok s Sočo – partikularno Hg	the River Soča inflow – particulate Hg
SOCAD _{IN}	dotok s Sočo – raztopljeno Hg	the River Soča inflow – dissolved Hg
NADR _{IN}	dotok iz Severnega Jadrana	inflow from the Northern Adriatic
NADR _{OUT}	iztok v Severni Jadran	outflow to the Northern Adriatic
NET-SED	usedanje	downward flux
SED _{IN}	resuspendiranje	resuspension
SED _{OUT}	neto odlaganje	burial

Slika 1.2. Masna bilanca živega srebra v Tržaškem zalivu (Širca et al, 1999b).
Figure 1.2. Mercury mass balance for the Gulf of Trieste (Širca et al, 1999b).

Rezultat modeliranja in meritev je bila tudi bilanca živega srebra v zalivu (Širca, 1999b), ki kaže, da kljub prenehanju delovanja rudnika v Idriji s Sočo v zaliv še vedno doteka več kot 1500 kg živega srebra letno, od tega pa se okoli 1300 kg živega srebra v zalivu tudi odloži. Iz bilance (slika 1.2) je razvidno tudi razmerje med raztopljenim in na delce vezanim živim srebrom ter razmerje med celokupnim in metiliranim živim srebrom.

2D model pa ima kljub izpopolnitvam nekatere pomanjkljivosti, saj z njim ni mogoče simulirati porazdelitve parametrov po globini. Hkrati so bile simulacije omejene na stacionarno stanje, s povprečnimi letnimi vrednostmi vseh parametrov kot vhodnimi podatki. Prav tako z modelom ni bilo mogoče simulirati enkratnih ekstremnih dogodkov, npr. visokovodnega vala Soče novembra 1997, s katerim je v zaliv prispelo okrog 4700 kg živega srebra v le nekaj dneh, kar je bistveno več od letnega povprečja (Širca et al, 1999b). K pomanjkljivostim 2D simulacij lahko štejemo še preredko numerično mrežo ob ustju Soče, zaradi česar je bilo ujemanje rezultatov prav na tem območju najslabše.

Kot rešitev naštetih pomanjkljivosti se ponuja uporaba nestacionarnega tridimenzionalnega (3D) modela. Osnovna modula takšnega modela, hidrodinamični in transportno-disperzijski modul, sta bila že izdelana, zato je bil za 3D simulacije izpopolnjen nelinearni 3D baroklini hidrodinamični in transportni model PCFLOW3D (Četina, 1992), ki je bil doslej že večkrat uporabljen za matematično modeliranje hidrodinamike in transporta polutantov v morskem okolju (Rajar in Četina, 1997; Rajar et al, 1995; 1997).

Glavni cilji predstavljene naloge so bili torej :

1. Nadgradnja matematičnega modela PCFLOW3D s 3D sedimentacijskim modulom z vgrajenim upoštevanjem resuspendiranja materiala z dna.
2. Izpopolnitve matematičnega modela, ki bi omogočale čim bolj točne simulacije transporta in disperzije živega srebra v raztopljeni in na delce vezani obliki.
3. Kalibracija in verifikacija izpopolnjenega

An annually mercury mass balance for the Gulf (Figure 1.2) was established from both the measurements and results of model simulations (Širca, 1999b). Despite the fact that the mercury mine in Idrija was closed 10 years ago, the Soča River still carries more than 1500 kg of mercury into the Gulf and about 1300 kg of mercury settles to the bottom of the Gulf annually. Proportional rates between dissolved and particulate, as well as between total and methylated mercury, are also evident from the mass balance.

In spite of upgrading, the 2D model still had a few limitations; vertical distribution of parameters can not be simulated with such a model. Besides, only steady-state simulations with annually averaged input parameters were performed. The simulation of sudden extreme events was not possible with the model; for example, the Soča River flood wave in November, 1997. At that time, about 4700 kg of mercury was carried into the Gulf in a few days, which is far over the annually averaged amount (Širca et al, 1999b). Another deficiency of 2D simulations was the too coarse numerical grid around the Soča River mouth, where agreement between the measurements and the results of the simulations was worse.

As a solution, the application of a non-steady-state three-dimensional (3D) model is being proposed. Both basic modules of such a model: the hydrodynamic and transport-dispersion module, have already been developed; therefore, the 3D non-linear baroclinic hydrodynamic and transport model PCFLOW3D (Četina, 1992) was upgraded. The model has already been verified and applied in several practical hydrodynamic and pollutant transport problems in the marine environment (Rajar and Četina, 1997; Rajar et al, 1995; 1997).

Main goals of the present work were:

1. To upgrade the PCFLOW3D model with a sediment transport module. Resuspension of sediment from the bottom must be included in the new module.
2. To improve the model in such a way as to simulate the transport and dispersion of mercury in both dissolved and particulate forms as accurately as possible.
3. To calibrate and verify the upgraded model with simulations of some characteristic

modela s pomočjo simulacij nekaterih značilnih pojavov, za katere so bili na voljo rezultati meritev in opazovanj.

V predloženem delu so opisane teoretične osnove, na katerih temelji model PCFLOW3D, teoretične osnove, kalibracija in verifikacija sedimentacijskega modula in modula za transport živega srebra ter simulacije, izvedene z novim, izpopolnjenim modelom.

2. OSNOVNI MATEMATIČNI MODEL

PCFLOW3D je baroklini matematični model, sestavljen iz hidrodinamičnega in transportno-disperzijskega modula. Model je bil že večkrat podrobno opisan v literaturi, verificiran in preizkušen pri reševanju praktičnih primerov (Četina, 1992; Rajar in Četina 1997, Rajar et al, 1997).

2.1 HIDRODINAMIČNI MODUL

Enačbe, ki jih rešujemo s hidrodinamičnim modulom, so:

- kontinuitetna enačba

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (2.1)$$

- dinamična enačba

$$\frac{\partial U_i}{\partial t} + \frac{\partial U_i U_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} + f_i \quad (2.2)$$

- advekcijsko-disperzijska enačba za temperaturo, slanost in/ali poljuben aktiven polutant

$$\frac{\partial \Phi}{\partial t} + \frac{\partial U_i \Phi}{\partial x_i} = \Gamma_\Phi \frac{\partial^2 \Phi}{\partial x_i \partial x_i} + S_\Phi \quad (2.3)$$

- enačba stanja

$$\rho = \rho(T, s, C) \quad (2.4)$$

phenomena for which measurements and observation data were available.

In the present work, the theoretical background of the basic PCFLOW3D model, as well as the new sediment transport module, is described. Calibration and verification of the sediment transport module, mercury transport module and modelling with the new, upgraded model is presented.

2. BASIC MODEL PCFLOW3D

The baroclinic mathematical model PCFLOW3D consists of a hydrodynamic and a transport-dispersion module. A detailed description of the model, which has already been verified and applied to different practical problems, can be found in literature (Četina, 1992; Rajar and Četina 1997; Rajar et al, 1997).

2.1 HYDRODYNAMIC MODULE

Basic equations of the hydrodynamic module are:

- Mass conservation equation

- Momentum equation

- Advection-dispersion equation for temperature, salinity and/or other conservative pollutant

- Equation of state

Oznake v enačbah pomenijo: U_i ($i=1, 2, 3$) so trenutne hitrosti v posameznih koordinatnih smereh, P - trenutni tlak, x_i - posamezne koordinatne smeri, t - čas, ν - kinematični koeficient laminarne viskoznosti, ρ - gostota, f_i - prostorninska sila na enoto mase v koordinatni smeri i , Φ - trenutna vrednost skalarja (koncentracije C , temperature T , slanosti s ipd.), S_Φ - izvorni člen skalarja Φ , Γ_Φ - laminarna difuzija skalarja Φ .

Enačbe (2.1) do (2.3) povprečimo po času in jih integriramo znotraj posameznih slojev debeline h ter upoštevamo hidrostatično porazdelitev tlakov, nato pa iz njih z upoštevanjem ustreznih robnih pogojev (Četina, 1992) izračunamo hidrodinamične količine (hitrosti, tlake, potek gladin in gostoto ter porazdelitev slanosti in temperature), ki so podlaga za račun transporta in koncentracij poljubnega polutanta. Z upoštevanjem neenakomerne porazdelitve gostote zaradi spremenljive temperature in slanosti je mogoče z modelom upoštevati tudi stratificirane razmere na obravnavanem območju.

Za rešitev enačb je potrebno še poznavanje horizontalnih in vertikalnih koeficientov turbulentne viskoznosti in difuzije, ki jih izračunamo z modelom turbulence. V horizontalni ravnini upoštevamo princip konstantne viskoznosti in difuzije, v vertikalni pa model z eno transportno enačbo (za transport kinetične energije k), ki ga opisujeta Koutitas in O'Connor (1989). V modelu je upoštevana parabolčna porazdelitev vertikalnega koeficienta turbulentne viskoznosti in difuzije.

Enačbe rešujemo z numerično metodo končnih razlik, imenovano metoda kontrolnih volumnov, kjer definicijsko območje po vertikali razdelimo na posamezne sloje, v horizontalni smeri pa na mrežo celic. Metodo in njene rešitve opisujeta Patankar (1980) in Četina (1992).

Pri reševanju je pomembna pravilna izbira števila in debeline slojev, da z njimi čimbolj

Symbols in the equations mean: U_i ($i=1, 2, 3$) momentary velocities in coordinate directions, P - momentary pressure, x_i - coordinate directions, t - time, ν - kinematic coefficient of the laminar viscosity, ρ - density, f_i - volume force per mass unit in coordinate direction i , Φ - value of the scalar (concentration C , temperature T , salinity s etc.), S_Φ - source term of the scalar Φ , Γ_Φ - laminar diffusion of the scalar Φ .

Afterwards, equations (2.1) to (2.3) are averaged within time and integrated within a single layer. The hydrostatic approximation is used for the distribution of pressure in the vertical direction. From these equations, together with the equations of boundary conditions described in (Četina, 1992), hydrodynamic parameters (velocities, pressure, free surface elevations, density, temperature and salinity distribution) are calculated. These values are further used to calculate the transport and concentrations of any pollutant. Taking into account the non-uniform density distribution due to variable temperature and salinity, it is also possible to simulate stratified conditions within the computational domain.

Eddy viscosity and eddy diffusivity coefficients in both horizontal and vertical directions are needed to solve the equations. Constant eddy viscosity and diffusivity is supposed in a horizontal plain, while a one equation turbulence model (equation of turbulence kinetic energy k) is used in the vertical plain. The turbulence model is described in (Koutitas and O'Connor, 1980). Parabolic distribution of the vertical viscosity and diffusivity coefficient is used in the model.

A finite difference numerical method called *finite volume method* is used to solve the equations. In the horizontal plain, the computational domain is divided into cells by an orthogonal grid, and in the vertical direction, layers of uniform thickness are formed. The method, itself, and its solutions, are described in (Patankar, 1980; Četina, 1992).

The decision about the number and thickness of layers in the vertical direction is of great importance. The detailed geometric description of the computational domain, as

točno opišemo geometrijo definicijskega območja, ker je od izbire debeline slojev odvisna točnost računa robnih pogojev na gladini in ob dnu, še posebej pa, ker je zaradi stabilnosti numerične metode časovni korak računa omejen.

2.2 TRANSPORTNO-DISPERZIJSKI MODUL

Osnova modula je adveksijsko-disperzijska (AD) enačba, izpeljana iz enačbe (2.3), zapisana za koncentracijo poljubnega nekonvativnega polutanta C . Izvorno/ponorni člen SRC , ki je odvisen od polutanta oz. procesov, ki jih želimo opisati, pri konservativnih polutantih odpade.

$$\begin{aligned} \frac{\partial (hC)}{\partial t} + \frac{\partial (huC)}{\partial x} + \frac{\partial (hvC)}{\partial y} + \frac{\partial (hwC)}{\partial z} = \frac{\partial}{\partial x} \left(hD_h \frac{\partial C}{\partial x} \right) + \\ + \frac{\partial}{\partial y} \left(hD_h \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(hD_v \frac{\partial C}{\partial z} \right) + SRC \end{aligned} \quad (2.5)$$

V enačbi pomenijo u , v in w – komponente hitrosti v posameznih koordinatnih smereh, D_h in D_v – horizontalni in vertikalni koeficient turbulentne difuzije.

V osnovnem modelu PCFLOW3D sta bili vgrajeni dve AD enačbi, namenjeni predvsem računu temperature in slanosti. Z njima je mogoče simulirati tudi transport poljubnega polutanta, kadar enačbi nista uporabljani za račun porazdelitve temperature in slanosti oz. pri simulaciji ne upoštevamo vpliva spremenljive gostote na hidrodinamične količine.

Enačbo rešujemo po *metodi kontrolnih volumnov* (MKV) (Patankar, 1980, Četina, 1992), ali po *metodi sledenja delcev* (MSD) (Širca, 1992). V splošnem je pri hidrodinamičnih problemih bolj primerna prva metoda, pri širjenju polutantov v vodnem okolju pa metoda sledenja delcev zagotavlja elegantnejšo rešitev enačbe in boljše fizikalno predstavo problema.

well as the accuracy of the boundary condition calculations at the bottom and at the free surface depends on the proper thickness of the layers. Most importantly, layer thickness impacts the computational time step which is limited due to the stability of the numeric method.

2.2 TRANSPORT-DISPERSION MODULE

An advection-dispersion (AD) equation that is derived from equation (2.3), written for the concentration of any non-conservative pollutant C , is the governing equation of the module. The source/sink term SRC , which is not taken into account with the conservative pollutants, depends on the sort of pollutant and processes being simulated.

In the equation u , v and w denote components of the velocity vector in the coordinate directions; D_h and D_v are horizontal and vertical eddy diffusivity coefficients.

Two AD equations were included in the basic PCFLOW3D model, mainly to simulate temperature and salinity distribution. When temperature and salinity distribution was not calculated and the influence of variable density to the hydrodynamic parameters was not accounted for, both AD equations can also be used to simulate the transport of any conservative pollutant.

The *finite volume method* (FVM) (Patankar, 1980, Četina, 1992) or the *particle tracking method* (PTM) (Širca, 1992) is used to solve the equation. The first is more appropriate with the hydrodynamic problems, while, with the pollutant dispersion in the marine environment, the second provides a more elegant solution of the governing equation and a physically better description of the problem.

As each method has its benefits and deficiencies, the decision about which method

Vsaka od metod ima svoje prednosti in pomanjkljivosti, zato je izbira odvisna od konkretnega problema, ki ga rešujemo. Pri simulacijah transporta živega srebra se je MSD zaradi močno nestacionarnih procesov in ploskovnih izvorov polutanta izkazala za manj primerno od MKV in pri kalibraciji in verifikaciji modela ni bila uporabljena.

3. DOPOLNITVE MODELA PCFLOW3D

3.1 MODUL ZA TRANSPORT LEBDEČIH PLAVIN

Po dosedanjih raziskavah (Širca, 1996; Covelli et al, 1999a; Covelli et al, 1999b; Horvat et al, 1998; Horvat et al, 1999) je večina živega srebra v Tržaškem zalivu vezanega na delce lebdečih plavin in sedimenta na dnu zaliva. Modeliranje transporta in procesov pretvorb živega srebra torej zahteva točno poznavanje koncentracij lebdečih plavin v vodnem stolpcu, tem zahtevam pa ustreza le 3D sedimentacijski model z upoštevanjem resuspendiranja.

3.1.1 Osnovna enačba

Osnovno enačbo za transport in disperzijo lebdečih plavin v posameznem sloju debeline h zapišemo v obliki:

$$\begin{aligned} \frac{\partial (hC)}{\partial t} + \frac{\partial}{\partial x}(huC) + \frac{\partial}{\partial y}(hvC) + \frac{\partial}{\partial z}[(w - W_s)hC] = \frac{\partial}{\partial x}\left(hD_h \frac{\partial C}{\partial x}\right) + \\ + \frac{\partial}{\partial y}\left(hD_h \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(hD_v \frac{\partial C}{\partial z}\right) \end{aligned} \quad (3.1)$$

V enačbi pomeni C koncentracijo lebdečih plavin, W_s pa hitrost usedanja delcev plavin (sedimentacijsko hitrost). Ostale oznake v enačbi so analogne oznakam v enačbi (2.5). Za rešitev enačbe torej poleg hitrostnega polja, ki je rezultat hidrodinamičnega modula, potrebujemo še porazdelitev hitrosti usedanja

to use depends on the type of problem being solved. With the mercury transport simulations, PTM was found to be less appropriate than the FVM due to the highly non-steady state of the processes and the surface pollutant sources. Therefore, the FVM has been used for calibration and verification of the upgraded model.

3. UPGRADE OF THE PCFLOW3D MODEL

3.1 SUSPENDED SEDIMENT MODULE

Recent studies (Širca, 1996; Covelli et al, 1999a; Covelli et al, 1999b; Horvat et al, 1998; Horvat et al, 1999) have shown that mercury in the Gulf of Trieste is mostly bound to suspended and bottom sediment particles. Therefore, modelling of mercury transport and transformation processes requires exact values of suspended sediment concentrations along the depth, which can only be provided by using a 3D sediment transport module with an included calculation of resuspension.

3.1.1 Governing equation

The governing equation for the simulation of the transport and dispersion of suspended sediment in each layer (where h represents the layer's thickness) can be written as:

In the equation, C denotes suspended sediment concentration and W_s is settling velocity. Other symbols are analogue to the symbols used in equation (2.5). Besides velocity field, which is a result of the hydrodynamic module, distribution of settling velocity and boundary condition equations are needed to solve the equation.

delcev in enačbe robnih pogojev.

Vertikalni koeficient turbulentne difuzije v sedimentacijskem modulu je lahko enak koeficientu, izračunanemu z modelom turbulence, lahko pa uporabimo parabolično-konstantno porazdelitev, ki sta jo predlagala Lin in Falconer (1996) in daje bolj realen opis koncentracij lebdečih plavin po vodnem stolpcu in je opisana z enačbama:

$$D_v = 4 \cdot \frac{z}{H} \cdot \left(1 - \frac{z}{H}\right) \cdot (D_v)_{\max} \quad \rightarrow \quad \frac{z}{H} \leq 0.5 \quad (3.2)$$

$$D_v = (D_v)_{\max} = 0.25 \cdot \kappa \cdot u_* \cdot H \quad \rightarrow \quad \frac{z}{H} \geq 0.5 \quad (3.3)$$

V enačbah pomeni z - oddaljenost od dna, H je globina vode, κ von Karmanova konstanta in u_* strižna hitrost.

3.1.2 Hitrost usedanja delcev

Hitrost usedanja W_s določimo s pomočjo empiričnih enačb (van Rijn, 1984; van Rijn, 1986; van Rijn 1993), potrebujemo pa podatke o zrnivosti plavin (premere zrna D_{16} , D_{50} , D_{84} in D_{90}), gostoto delcev plavin ρ_s in gostoto vode ρ_v , hitrostno polje in kinematično viskoznost vode ν_k .

Za določitev hitrosti usedanja veljajo naslednje empirične enačbe (van Rijn, 1993):

$$W_{so} = \frac{1}{18} \cdot \frac{(s_s - 1) \cdot g \cdot D_s}{\nu_k} \quad \rightarrow \quad D_s \leq 100 \mu\text{m} \quad (3.4)$$

$$W_{so} = 10 \frac{\nu_k}{D_s} \left\{ \left[1 + \frac{0.01 \cdot (s_s - 1) \cdot g \cdot D_s^3}{\nu_k^2} \right]^{0.5} - 1 \right\} \quad \rightarrow \quad 100 \mu\text{m} \leq D_s \leq 1000 \mu\text{m} \quad (3.5)$$

$$W_{so} = 1.1 \cdot [(s_s - 1) \cdot g \cdot D_s]^{0.5} \quad \rightarrow \quad D_s \geq 1000 \mu\text{m} \quad (3.6)$$

V enačbah pomeni s_s razmerje med gostoto plavin in vode, D_s pa je reprezentativni premer zrna, ki je odvisen od lastnosti plavin in hitrosti toka. Enačbe za določitev posameznih parametrov in postopek reševanja podrobo opisujejo van Rijn (1993) in Žagar et al. (1997).

The same vertical eddy diffusivity coefficient as calculated with the turbulence model can be also used in the sediment transport module. However, a parabolic-constant distribution of the diffusivity coefficient proposed by Lin and Falconer (1996), which gives a more realistic description of suspended sediment concentrations along the depth, can also be used. The latest distribution is described by the following equations:

In the equations, z means distance from the bottom, H is water depth, κ is von Karman's constant and u_* is the bed-shear velocity.

3.1.2 Settling velocity

Empirical equations proposed by van Rijn (van Rijn, 1984; van Rijn, 1986; van Rijn 1993) are used to calculate the settling velocity. Granulometric parameters of sediment are needed (particle diameters D_{16} , D_{50} , D_{84} and D_{90}), as well as sediment density ρ_s , water density ρ_v , velocity field and the kinematic viscosity of water ν_k .

The following empirical relations are used to determine the settling velocity (van Rijn, 1993):

In the equations, s_s is the proportional rate between the sediment and water density; D_s is the representative particle diameter which depends on water velocity and sediment properties. A detailed description of the equations and methods of calculation of the parameters can be found in (van Rijn, 1993;

Hitrost usedanja delcev se s povečevanjem koncentracije plavin v vodi zmanjšuje. V modelu je uporabljena najustreznejša (van Rijn, 1993) empirična enačba za zmanjšanje hitrosti usedanja. Ta daje po vsem razponu koncentracij rezultate, ki se najbolj ujemajo z meritvami:

$$W_s = (1 - 2.15 \cdot C) \cdot (1 - 0.75 \cdot C^{0.33}) \cdot W_{so} \quad (3.7)$$

V enačbi pomeni W_{so} prvotno hitrost usedanja plavin, C pa koncentracijo lebdečih plavin.

3.1.3 Robni pogoji

Za rešitev enačbe (3.1) morajo biti znane še koncentracije plavin na robovih definicijskega območja. Enačbi robnih pogojev na odprtem robu in ob obali sta enaki kot pri osnovnem modelu PCFLOW3D, kjer sta tudi opisani (Četina, 1992).

Na prosti gladini je neto pretok v vertikalni smeri enak nič, koncentracije plavin v površinskem sloju pa iterativno določimo iz enačbe:

$$\left[W_s \cdot C + D_v \cdot \frac{\partial C}{\partial z} \right]_{\zeta} = 0, \quad (3.8)$$

pri čemer indeks ζ pomeni koto gladine v obravnavanem času.

Robni pogoj ob dnu predstavlja splošni izvorno/ponorni člen za plavine. Ob dnu je mogoče **usedanje** plavin, kadar so dejanske strižne hitrosti ob dnu manjše od kritičnih, ali **resuspendiranje** že usedlih delcev, kadar so kritične strižne hitrosti ob dnu prekoračene. Količina materiala, ki se usede ali resuspendira, je odvisna od koncentracije plavin ob dnu, hitrosti usedanja delcev in transportne sposobnosti toka, ta pa je odvisna od razmerja med dejanskimi in kritičnimi strižnimi hitrostmi oz. napetostmi.

Kritično strižno hitrost ob dnu določimo z enačbo:

Žagar et al, 1997).

The settling velocity is inversely proportional to the concentration of suspended sediment. The most appropriate (van Rijn, 1993) empirical relation, which gives the best results within the complete concentration range, was used to reduce the settling velocity:

In the equation, W_{so} denotes the primary settling velocity and C is the suspended sediment concentration.

3.1.3 Boundary conditions

Concentrations of suspended sediment at the borders of the computational domain are also needed to solve the equation (3.1). Equations of open boundary condition and bank boundary condition are identical to the equations used within the basic PCFLOW3D model, where a detailed description can also be found (Četina, 1992).

At the free surface, the net vertical sediment flux is assumed to be zero; concentrations are determined from equation:

where ζ denotes the water surface elevation within the current time step.

The **bed boundary condition** represents the general source/sink term of suspended sediment. **Resuspension** or **settling** of suspended sediment is possible at the bottom, depending on whether critical bed-shear stress is exceeded or not. The amount of sediment being resuspended depends on the concentration in the bottom layer, the settling velocity and the transport capability of the flow, which further depends on the proportional rate between critical and actual bed-shear stresses.

Critical bed-shear stress is described by equation:

$$u_{*,cr} = \sqrt{\Theta_c \cdot (s_s - 1) \cdot g \cdot D_{50}} \quad (3.9)$$

kjer je Θ_c parameter mobilnosti, odvisen od premera zrna plavin in kinematične viskoznosti vode.

Dejanske strižne hitrosti ob dnu so posledica **tokov** in **valovanja**. Predvsem pri večjih jezerih in morju je vpliv valovanja zelo pomemben, saj so hitrosti tokov običajno razmeroma majhne, strižne napetosti ob dnu pa so v glavnem posledica oscilatornega gibanja vode med valovanjem. Vsako od komponent določimo posebej in ju nato vektorsko seštejemo, saj pri določitvi strižnih hitrosti velja princip superpozicije.

Dejanske strižne hitrosti ob dnu zaradi tokov določimo po enačbi (van Rijn, 1993):

$$u'_* = \left| \frac{\sqrt{g}}{C'} \cdot \bar{u} \right| \quad (3.10)$$

kjer pomeni C' koeficient zrnivosti plavin, $\bar{u}$ pa povprečno hitrost po vertikali, ki je rezultat hidrodinamičnega modula. Pri 3D modelu je račun strižne hitrosti ob dnu iz globinsko povprečenih hitrosti vprašljiv, saj so včasih hitrosti ob dnu za red velikosti večje od globinsko povprečenih. V modelu je za račun strižnih hitrosti upoštevana večja od obeh vrednosti.

Strižne hitrosti zaradi valovanja določimo iz parametrov valovanja (periode, višine in valovne dolžine) ter karakteristik plavin oz. sedimenta na dnu z empiričnimi enačbami (Ippen et al, 1966; van Rijn, 1993). Višino in periodo valovanja po celotni površini definicijskega območja je mogoče določiti (Ippen et al, 1966), če poznamo hitrost vetra in privetrno razdaljo, tj. dolžino območja, na katerem nastajajo valovi zaradi vetra nespremenjene hitrosti in smeri (angl.: *fetch length*). Ta je definirana kot razdalja med opazovano točko in najbližjo obalo v smeri, od koder piha veter. Nato z empiričnimi enačbami (van Rijn, 1993) izračunamo valovno dolžino, vršno hitrost in amplitudo valovanja ter koeficient trenja ob dnu.

where Θ_c denotes the mobility parameter which depends on the sediment particle diameter and the kinematic viscosity of the water.

Both currents and wind induced waves produce bed shear stress. With larger lakes and the coastal sea, where current velocities are low, the oscillatory motion of waves is the main source of bed shear stress, and, as such, it is of particularly great importance. As the principle of superposition may be used, each of the bed-shear velocity vectors is calculated separately to be totaled into the total bed-shear stress.

Actual bed-shear velocity is determined from equation (van Rijn, 1993):

where C' denotes coefficient related to grain size and $\bar{u}$ is the depth averaged velocity, which is a result of the hydrodynamic module. In the 3D model, calculation of bed shear velocity from depth averaged velocities may be unreliable, as sometimes depth-averaged velocities can be lower than the near-bed velocities for even an order of magnitude. The greater of the depth-averaged and the near-bed velocity is taken into account in the sediment module.

Empirical equations (Ippen et al, 1966; van Rijn, 1993) are used to determine the bed-shear velocity due to waves from wave parameters (wave height, wavelength) and sediment properties. Wave height and wave period throughout the computational area can be calculated (Ippen et al, 1966) if wind speed and fetch length is known. Fetch length is, by definition, the distance between the observed point and the nearest bank in the direction of the wind. Further empirical equations (van Rijn, 1993) are used to calculate wavelength, peak orbital velocity, peak orbital amplitude and bed friction coefficient.

Strižne napetosti $\tau_{b,w}$ oziroma strižno hitrost ob dnu $u_{b,w}$ zaradi valovanja izračunamo po enačbah:

Bed shear stress $\tau_{b,w}$ and bed shear velocity $u_{b,w}$ due to waves is calculated by the following equations:

$$\tau_{b,w} = 0.25 \cdot \rho \cdot (U_{d,p})^2 \cdot f_w \quad (3.11)$$

$$u_{b,w} = \sqrt{\frac{\tau_{b,w}}{\rho}} \quad (3.12)$$

kjer pomenijo oznake $U_{d,p}$ vršno hitrost valovanja, f_w koeficient trenja in ρ gostoto vode.

where $U_{d,p}$ denotes the wave peak-orbital velocity, f_w is the bed friction coefficient and ρ is the density of the water.

Pri **resuspendiranju** delcev z dna je robni pogoj podan kot koncentracija lebdečih plavin na referenčni globini a , imenovana *referenčna koncentracija*, ki jo določimo v odvisnosti od višine oblik dna ali iz hrapavosti dna (D_{90}). Običajno se privzete vrednosti za referenčno globino gibljejo med enim in desetimi odstotki celotne globine ($H/100$ do $H/10$).

When **resuspension** occurs, the bed boundary condition is represented as *near-bed reference concentration*, i.e.: the suspended sediment concentration at the representative level a . Reference concentration is determined from the height of the bed forms or the bed roughness height (D_{90}). Usually the reference level is assumed to be between 1% and 10 % of the water depth (H).

Po primerjavi meritev in različnih metod določitve referenčne koncentracije C_a , ki je enaka ravnotežni koncentraciji C_{ae} , (opisani v Garcia in Parker, 1991), je najustreznejša metoda, ki jo je predlagal van Rijn (1984). Enačba za referenčno koncentracijo ima obliko:

Results of different equations for the near-bed reference concentration C_a , which is equal to the equilibrium concentration C_{ae} , were compared with the measurements (Garcia and Parker, 1991). The equation, proposed by van Rijn (1984) was found to be the most appropriate:

$$C_{ae} = 0.015 \cdot \frac{D_{50} \cdot T^{1.5}}{a \cdot D_*^{0.3}}, \quad (3.13)$$

pri čemer pomeni T transportni parameter, odvisen od razmerja med dejanskimi in kritičnimi strižnimi hitrostmi, a referenčno globino, D_* pa parameter zrna.

where T denotes transport parameter, which depends on the proportional rate between the actual and the critical bed-shear velocity, a is the reference level and D_* is the particle parameter.

Pri **usedanju** materiala določimo koncentracije plavin ob dnu C_{bot} iz osnovne enačbe, odvisna pa je od resuspenzije z dna in transporta plavin zaradi advekcije in disperzije v prejšnjih časovnih korakih računa.

When **settling** is present, near-bed suspended sediment concentrations C_{bot} are determined from the governing equation. Near-bed concentration depends on the resuspension, inlet, transport and dispersion of suspended sediment during previous time steps.

3.1.4 Račun debeline odnešenega oz. odloženega materiala

3.1.4 Calculation of erosion / deposition thickness

Na podlagi masne bilance lebdečih plavin tik ob dnu (na referenčni globini a) v dveh

On the basis of the suspended sediment mass balance near the bed (at the reference

sosednjih časovnih korakih izračunamo količino in z upoštevanjem poroznosti oz. zbitosti tudi debelino odnešenega oziroma odloženega materiala. Pri tem je v vsakem kontrolnem volumnu upoštevana advekcija in disperzija na vseh stičnih ploskvah s sosednjimi celicami ter usedanje iz zgornje celice in v spodnjo celico. Količino lebdečih plavin v celici ob dnu primerjamo z maso, izračunano iz razlike empirično določene ravnotežne koncentracije C_{ae} in koncentracije v isti celici v prejšnjem časovnem koraku. Usedanje lebdečih plavin se pojavlja, kadar je ravnotežna koncentracija presežena, v nasprotnem primeru pa se z dna resuspendira tolikšna količina sedimenta, da je v celici dosežena ravnotežna koncentracija.

3.2 VERIFIKACIJA SEDIMENTACIJSKEGA MODULA

3.2.1 Ravnotežni profil - primerjava z analitično rešitvijo

Za ravnotežno stanje (stalni enakomerni tok) dobi osnovna enačba (3.1) obliko:

$$W_s \cdot C + D_v \cdot \frac{\partial C}{\partial z} = 0 \quad (3.14)$$

Ob parabolčno-konstantni porazdelitvi vertikalnega koeficienta turbulentne difuzije je razmerje med koncentracijo plavin C in referenčno koncentracijo plavin C_a , podano z naslednjima enačbama (Lin in Falconer, 1996; van Rijn, 1993):

$$\frac{C}{C_a} = \left[\left(\frac{a}{z} \right) \cdot \left(\frac{H-z}{H-a} \right) \right]^\lambda \rightarrow \frac{z}{H} < 0.5 \quad (3.15)$$

$$\frac{C}{C_a} = \left(\frac{a}{H-a} \right)^\lambda \cdot e^{-4\lambda \left(\frac{z}{H} - 0.5 \right)} \rightarrow \frac{z}{H} \geq 0.5 \quad (3.16)$$

pri čemer pomeni λ parameter suspendiranja in velja relacija

level a), in two consequent time steps the amount of resuspended or deposited sediment is calculated. By taking into account the porosity of bottom sediment, the thickness of the erosion or deposition can be calculated. In each finite volume advection, dispersion and settling through the cell boundaries is taken into account. The amount of suspended sediment is compared with the difference between the empirically calculated equilibrium concentration C_{ae} and the concentration in the cell in the previous time step. When the equilibrium concentration is exceeded, settling is present. Otherwise, a certain amount of sediment is being resuspended to reach the equilibrium concentration in the relevant cell.

3.2 VERIFICATION OF THE SEDIMENT TRANSPORT MODULE

3.2.1 Equilibrium concentration profile – a comparison with the analytical solution

For the equilibrium condition (steady and horizontally uniform flow), the governing equation (3.1) can be simplified to the following form:

When a constant parabolic distribution of the vertical eddy diffusivity coefficient is assumed, the relationship between suspended sediment concentration at a certain level and reference concentration is described by the following equations (Lin and Falconer, 1996; van Rijn, 1993):

where λ is the suspension parameter described as:

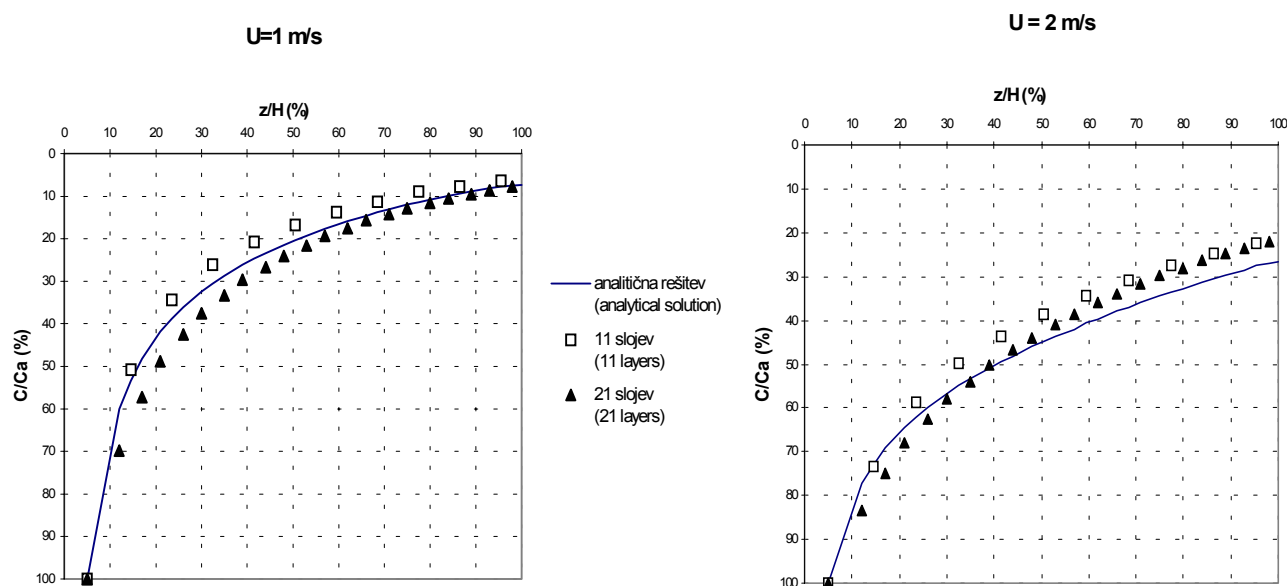
$$\lambda = \frac{W_s}{\kappa \cdot u_*} \quad (3.17)$$

Posamezne oznake pomenijo: a – referenčna globina, z – oddaljenost od dna, H – celotna globina, W_s – hitrost usedanja delcev, u_* – strižna hitrost ob dnu.

Izvedena je bila simulacija resuspendiranja materiala v pravokotnem kanalu dolžine 100 m, neskončne širine, globina kanala je znašala 1 m. Za vse testne izračune so bile izbrane plavine enotnega zrna ($D_{16}=D_{50}=D_{84}=D_{90}$), vse simulacije pa so bile izvedene na dva načina, z razdelitvijo kanala v vertikalni smeri na 11 in 21 slojev. V obeh primerih je bila debelina spodnjega sloja 10 cm, ostali sloji pa so imeli enakomerno debelino (9 oz. 4.5 cm). Referenčna globina je v vseh primerih znašala 5 odstotkov skupne globine. Vtoka plavin na levem robu kanala ni bilo, obravnavano je bilo zgolj resuspendiranje materiala z dna. Opazovani profil je bil na oddaljenosti 65 m od začetka kanala. Srednji premer zrna je znašal $D_{50} = 185 \cdot 10^{-6}$ m. Izvedeni sta bili simulaciji pri povprečni hitrosti toka $U = 1$ m/s in 2 m/s.

In the equation, a denotes the reference level, z the distance from the bottom, H is the total water depth, W_s is the settling velocity and u_* denotes the bed shear stress.

A simulation in an orthogonal channel of the following dimensions was performed: channel length equal to 100 m, width was assumed to be infinite; depth of the channel equal to 1 m. Suspended sediment of uniform grain size ($D_{16}=D_{50}=D_{84}=D_{90}$) was used in the simulations. The number of vertical layers used was 11 and 21 respectively, with the bottom layer being 10 cm thick in both cases and the thickness of the rest of the layers being uniform (9 or 4.5 cm). In both cases the reference level was set to 5 % of the total depth. There was no inlet of suspended sediment at the upstream boundary; only resuspension from the bottom was calculated. A profile at the distance of 65 m from the upstream boundary was observed. Mean particle diameter was set to $D_{50} = 185 \cdot 10^{-6}$ m. Simulations with two velocities were performed; $U = 1$ m/s in 2 m/s respectively.



Slika 3.1. Primerjava rezultatov sedimentacijskega modela z analitično rešitvijo, hitrosti toka 1 m/s in 2 m/s.

Figure 3.1. Comparison of sedimentation model results and analytical solution; flow velocities 1 m/s and 2 m/s.

Rezultati simulacije se z analitično rešitvijo zadovoljivo ujemajo (slika 3.1), saj največja napaka nikjer ne presega 10 odstotkov, povprečna napaka pa 5 odstotkov. Izvedena je bila tudi primerjava rezultatov s sorodnim sedimentacijskim modelom (Lin in Falconer, 1996), ki rešuje enačbe po drugačni numerični shemi (višjega reda točnosti), kar mu omogoča nekoliko boljše ujemanje rezultatov z analitično rešitvijo.

3.2.2 Razvoj koncentracijskega profila vzdolž kanala

V stacionarnih razmerah se pri konstantni hitrosti usedanja delcev in upoštevanju dejstva, da je v horizontalni smeri transport plavin zaradi advekcije bistveno večji od transporta zaradi difuzije, zaradi resuspendiranja v kanalu razvije koncentracijski profil, kakršen je prikazan na sliki 3.2.a. Enačba za transport plavin (enačba 3.1) dobi v tem primeru obliko:

$$U \cdot \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left(D_v \cdot \frac{\partial C}{\partial z} \right) + W_s \cdot \frac{\partial C}{\partial z} \quad (3.18)$$

Analitična rešitev enačbe (3.18) je izpeljana in razložena v literaturi (Hjelmfelt in Lenau, 1970). Predpostavljena je parabolčna porazdelitev vertikalnega koeficienta turbulentne difuzije in konstantna koncentracija na referenčni globini a . Na sliki 3.2 je prikazana primerjava rezultatov analitične in numerične rešitve, pri čemer pomeni X brezdimenzionalno razdaljo v smeri x , definirano z izrazom:

$$X = \frac{\kappa \cdot u_*}{U \cdot H} \cdot x, \quad (3.19)$$

narisane pa so izolinije relativnih koncentracij (C/C_{ae}) vzdolž kanala.

Kanal je bil enakih dimenzij kot pri prejšnji verifikaciji, po globini je bil razdeljen na 11 enako debelih slojev. Na začetnih 17 m kanala je predpisano trdno dno, opazujemo pa naslednjih 60 m dolžine.

The model results are in good agreement with the analytical solution (figure 3.1). The maximum error does not exceed 10 % and the average error is below 5 %. A comparison with a similar sedimentation model (Lin & Falconer, 1996) was also performed. In the Lin-Falconer model, equations are solved by a different numerical scheme (higher order of accuracy), which enables the results of the model to be somewhat closer to the analytical solution.

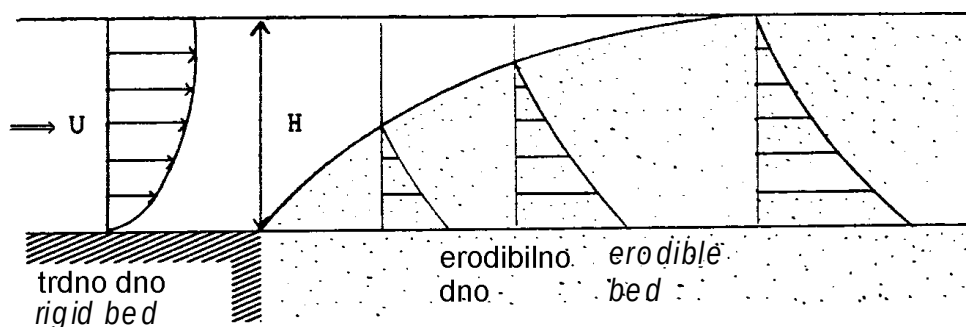
3.2.2 Development of the concentration profile along the channel

Assuming the constant settling velocity and that in the horizontal direction the mass transfer due to diffusion is much smaller than that due to advection, an adjustment of the concentration profile due to resuspension as it is evident from figure 3.2.a is present in steady flow. In that case, the governing equation (3.1) can be written as:

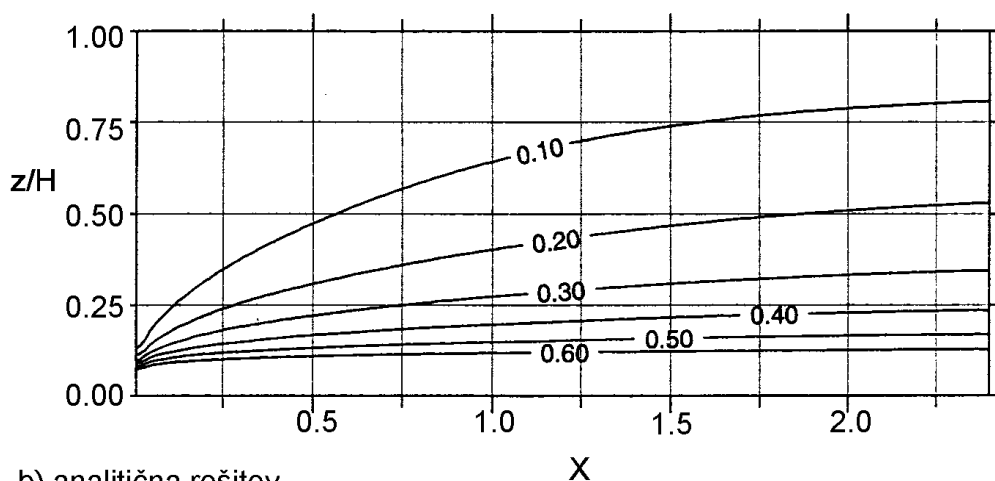
An analytical solution of the equation (3.18) is derived and explained in (Hjelmfelt and Lenau, 1970). Parabolic distribution of the vertical diffusion coefficient and constant concentration at the reference level a is assumed. Figure 3.2 shows a comparison between model results and the analytical solution, where X is the non-dimensional distance in the x direction, given by:

Isolines of relative concentrations (C/C_{ae}) along the test channel are presented.

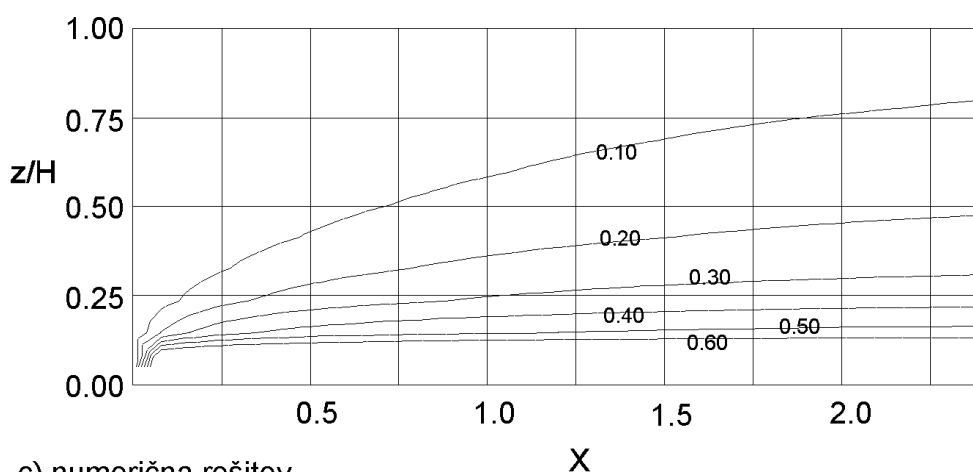
Channel of the same dimensions as used for the previous verification was chosen. Eleven vertical layers of uniform thickness were calculated. A rigid bed was assumed in the first 17 m of the channel; the following 60 m of channel with an erodible bed was observed.



a) skica kanala
 problem definition



b) analitična rešitev
 analytical solution



c) numerična rešitev
 numerical solution

Slika 3.2. Razvoj koncentracijskih profilov vzdolž kanala, primerjava z analitično rešitvijo.
 Figure 3.2. Adjustment of sediment concentration profiles along the channel; comparison to the analytical solution.

Uporabljeni so še naslednji parametri: $H = 1$ m, $U = 1$ m/s, $a = 0.05$ m, $C_a = 1$ kg/m³, $W_s = 0.02$ m/s, $u_* = 0.1$ m/s ter parameter suspendiranja $\lambda = 0.5$.

Numerična in analitična rešitev se tudi pri tej simulaciji zelo dobro ujemata. Največja napaka se pojavlja ob dnu in na začetku erodibilnega dna, sčasoma (do ravnotežnega profila) pa se napaka skoraj izniči. Tudi pri tem preizkusu se je Lin-Falconerjev model nekoliko, a ne bistveno bolje, približal rezultatom analitične rešitve.

3.2.3 Neto usedanje - primerjava z meritvami

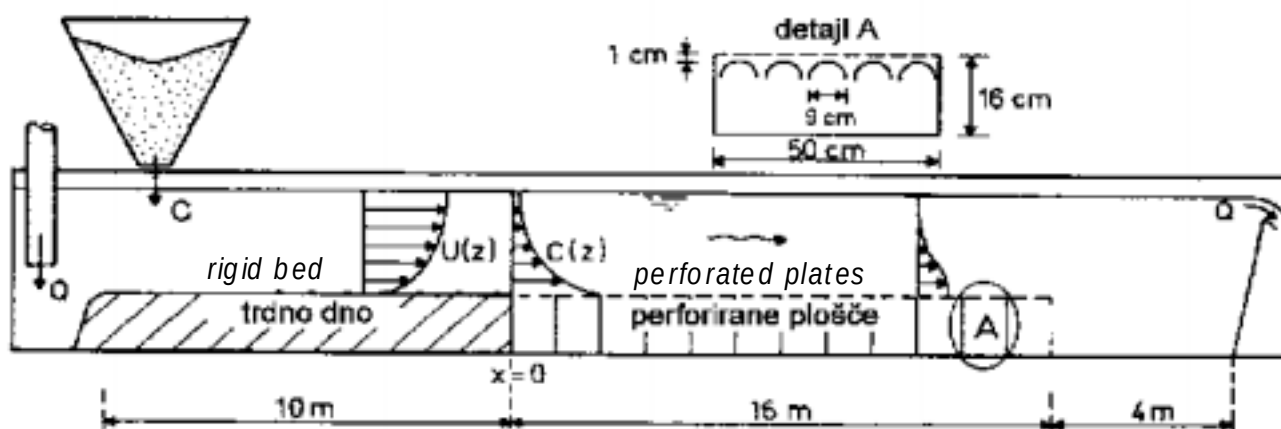
Izvedena je bila primerjava rezultatov simulacije z meritvami koncentracijskih profilov lebdečih plavin v kanalu s stalnim enakomernim tokom in luknjičastim dnom, opisanih v (Wang in Ribberink, 1986). Skica preizkusnega kanala je na sliki 3.3. Resuspendiranje delcev je onemogočeno s perforiranim dnom kanala, pod katerim ostanejo vsi usedli delci. Vzdolžni tok pod perforacijo je preprečen s prečnimi zaporami na razmaku 50 cm.

The following parameters were used: $H = 1$ m, $U = 1$ m/s, $a = 0.05$ m, $C_a = 1$ kg/m³, $W_s = 0.02$ m/s, $u_* = 0.1$ m/s and suspension parameter $\lambda = 0.5$.

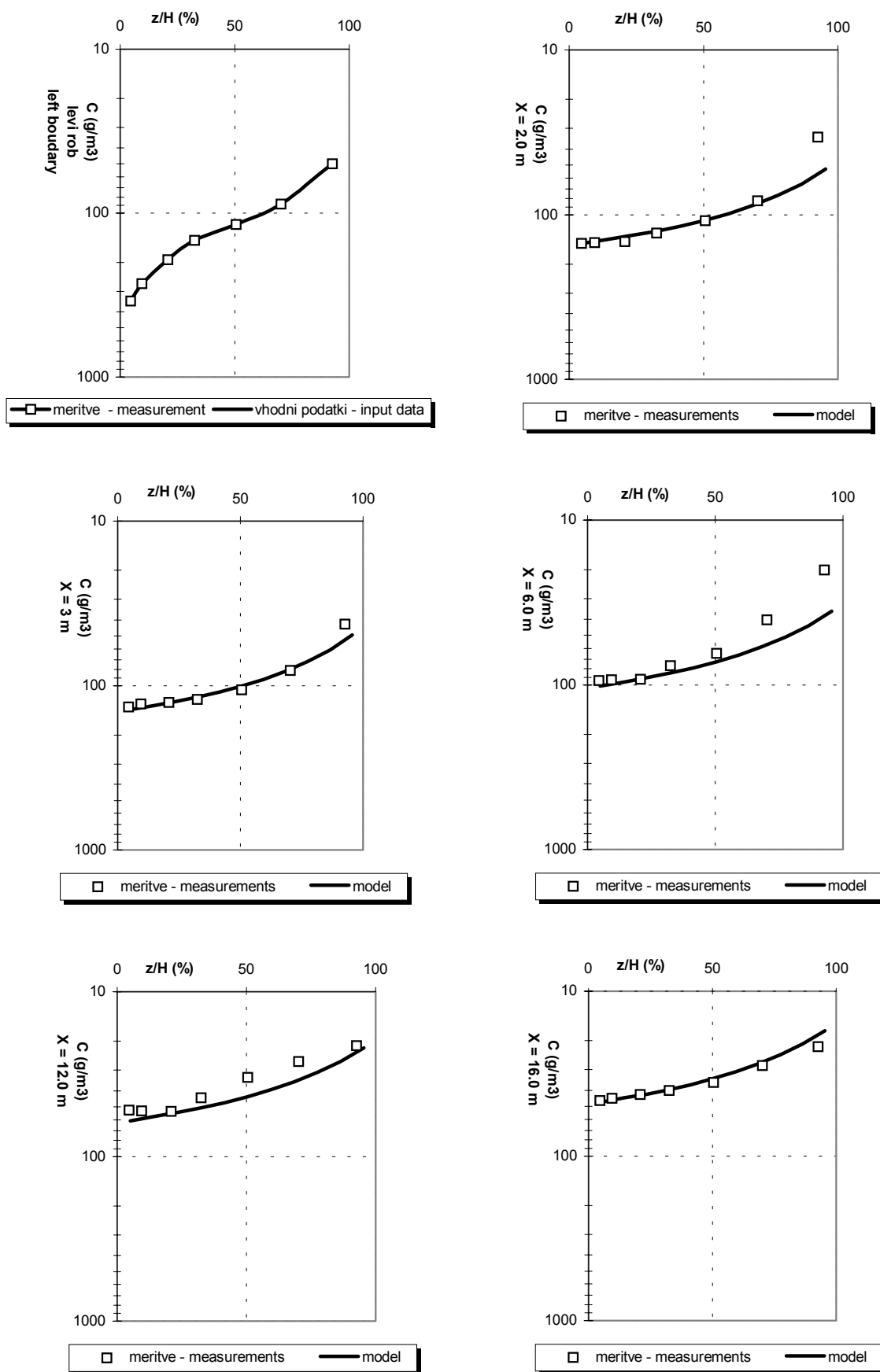
A good agreement of the numeric and analytical solution was again established. Maximal error was found to be at the bottom and at the beginning of the erodible part of the channel. The error decreases along the channel and becomes negligible at the point of the equilibrium concentration profile. Here again, the Lin-Falconer model gave somewhat, but not essentially better, results.

3.2.3 Net sedimentation – comparison to measurements

A comparison of numeric results and measured suspended sediment concentration profiles in steady state uniform flow over the perforated bottom was performed. The experiment is described in (Wang and Ribberink, 1986), an illustration of the test channel is in figure 3.3. Within the second part of the channel, where the bottom was perforated, resuspension was not possible. To avoid flow development under the perforated plates, transversal barriers were mounted at each 50 cm.



Slika 3.3. Skica preizkusnega kanala – neto usedanje.
Figure 3.3. Test channel illustration – net sedimentation.



Slika 3.4. Primerjava numeričnih rezultatov z meritvami – neto usedanje.
Figure 3.4. Comparison between numeric results and measurements – net sedimentation.

Glavni podatki eksperimenta so: $H = 0.215$ m, $U = 0.056$ m/s, $D_{50} = 100$ μ m, $W_s = 0.65$ cm/s, $u_* = 0.034$ m/s. Kot vhodni podatek simulacije so bile uporabljene koncentracije lebdečih plavin, izmerjenih na razdalji $x = 0.1$ m. V modelu smo ob dnu umetno predpisali nično resuspenzijo (pri uporabljenih podatkih se resuspendiranju drugače ni bilo mogoče izogniti). Uporabljena je bila parabolična porazdelitev vertikalnega koeficienta turbulentne difuzije.

Na sliki 3.4 je prikazana primerjava numeričnih in izmerjenih rezultatov na različnih lokacijah vzdolž kanala. Ujemanje rezultatov je v splošnem dobro, največja napaka se pojavlja pri $x = 6$ m ob gladini, v naslednjih profilih pa se napaka zopet zmanjša.

3.3 MODUL ZA SIMULACIJO TREH KONSERVATIVNIH POLUTANTOV

Izhodiščni model PCFLOW3D je vseboval advekcijsko-disperzijski enačbi, ki sta bili prvotno namenjeni računu transporta in disperzije temperature in slanosti, z enačbama pa je bilo mogoče simulirati tudi transport in disperzijo poljubnega polutanta. V primeru simulacije stratificiranega stanja pa sta enačbi že uporabljeni in potrebujemo za račun transporta in disperzije drugih polutantov dodatne advekcijsko-disperzijske enačbe (enačba 2.5).

Pri računu transporta in disperzije živega srebra se upoštevanju stratificiranega stanja ni bilo mogoče odreči, zato smo v model vgradili enačbe za simulacijo treh dodatnih polutantov. Z modelom nameravamo simulirati transport in disperzijo različnih oblik živega srebra (HgII, MMHg in DMHg), vsaka od njih pa ima različen izvorni člen in specifične robne pogoje.

Trenutno je z enačbami mogoče simulirati transport in disperzijo konservativnih polutantov, brez upoštevanja izvorno/ponornega člena *SRC*. Vse enačbe so primerne tudi za račun aktivnih polutantov in pripravljene za vgradnjo biokemijskih procesov pretvorb posameznih oblik živega srebra oz. izvorno/ponornih členov.

The main data of the experiment are: $H = 0.215$ m, $U = 0.056$ m/s, $D_{50} = 100$ μ m, $W_s = 0.65$ cm/s, $u_* = 0.034$ m/s. Suspended sediment concentration at a distance of $x = 0.1$ m was used as the input data. Zero resuspension was adopted at the bottom, as otherwise resuspension could not be avoided in the simulation with the data used. Parabolic distribution of the vertical diffusion coefficient was used.

A comparison between simulated and measured results is shown in figure 3.4. Generally good agreement of results is reached; the maximum error occurs near the water surface at $x = 6$ m, but decreases again in the following profiles.

3.3 THE MODULE FOR SIMULATION OF THREE CONSERVATIVE POLLUTANTS

Basically, the two advection-dispersion equations included within the PCFLOW3D model were used to calculate the transport and dispersion of temperature and salinity. However, the simulation of the transport of any conservative pollutant was also possible with the same equations. When stratified conditions are simulated, both equations are already employed and additional advection-dispersion equations (2.5) are needed to simulate the transport of additional pollutants.

With mercury transport and dispersion computations, stratified conditions could not be excepted; therefore, equations for three additional pollutants were built into the model. The simulation of mercury transport in different forms (HgII, MMHg and DMHg) is planned with the model, each of the forms having its own source term and specific boundary conditions.

At the moment the simulation of the transport and dispersion of conservative pollutants is possible, while the source term *SRC* has not yet been accounted for. All equations are suitable for the simulation of active pollutants and ready for an upgrade with the source term, i.e.: equations of biochemical transformation processes between individual mercury forms.

3.4 SIMULACIJA PROCESOV PRETVORB ŽIVEGA SREBRA

Živo srebro je v modelu PCFLOW3D trenutno obravnavano kot konservativni polutant, ki se lahko pojavlja v več oblikah (HgII, MMHg in DMHg), predvsem pa so mogoče simulacije transporta in disperzije živega srebra v dveh medijih, v raztopljeni in partikularni obliki.

V 3D modelu bi bilo sicer mogoče uporabiti princip, s katerim so bili simulirani procesi pretvorb (metilacija, demetilacija in redukcija) v 2D modelu (Širca, 1996), vendar pa se je med raziskavo izkazalo, da so obstoječe enačbe za opis procesov pretvorb še premalo preverjene. Simulacija v daljših časovnih obdobjih zahteva poglobljeno poznavanje dinamike biogeokemijskih procesov pretvorb v nestacionarnih razmerah v celotnem sistemu Idrijca – Soča – Tržaški zaliv. Proces pretvorb živega srebra in njegovih oblik so odvisne od lokacije, koncentracije živega srebra, temperature in tudi od drugih okoljskih parametrov, ki se med letom precej spreminjajo. Še posebno pomembno je upoštevanje hitrosti metilacije, demetilacije ter redukcije oz. oksidacije živega srebra na mejah med sedimentom in vodo ter vodo in zrakom.

Vgradnja enačb izvirnega člana, ki zajema procese pretvorb med posameznimi oblikami živega srebra, je načrtovana v naslednjem letu, ko bodo poleg novih spoznanj o procesih pretvorb predvidoma na voljo tudi dodatne meritve za kalibracijo in verifikacijo 3D modela z vgrajenimi enačbami procesov pretvorb.

4. MODELIRANJE TRANSPORTA IN DISPERZIJE ŽIVEGA SREBRA

4.1 UVOD

Rezultati 2D simulacij z modelom STATRIM so nakazali, da so kljub razmeroma dobremu ujemanju na povprečni letni ravni zmožnosti 2D modela več ali manj izrabljene,

3.4 SIMULATION OF MERCURY TRANSFORMATION PROCESSES

At this time, mercury is treated as a conservative pollutant in the PCFLOW model. Three different forms of mercury (HgII, MMHg and DMHg) in two different media (dissolved and particulate) can be simulated.

The principle used in the 2D model (Širca, 1996) to simulate mercury transformation processes (methylation, demethylation and reduction) could have been included in the 3D model. However, it was proved during the research that the existing equations of mercury transformation processes are not reliable enough to be included in the 3D model. A deeper knowledge of the dynamics of bio-geochemical transformation processes throughout the whole system (Idrijca River – Soča River – Gulf of Trieste) is required to perform long-term simulations in non-steady state conditions. Mercury transformation processes depend on location, mercury concentration, temperature and other environmental parameters, which are far from being uniform through the seasons. Determination of the methylation, demethylation and reduction/oxidation rates at the sediment-water and water-air contact is of particularly great importance.

A further upgrade of the PCFLOW3D model with the source term equation, where the transformation processes between individual mercury forms are included, is planned for the next year. Besides the new mercury processes relationships, additional measurements are expected to be available next year for an additional calibration and verification of the model.

4. MODELLING OF MERCURY TRANSPORT AND DISPERSION

4.1 INTRODUCTION

In spite of relatively good agreement at an annually averaged level, it is pointed out from the results of STATRIM simulations that the feasibility of the 2D model has been more or

saj bi nadaljnje izboljšave modela zahtevale preveč posegov v model ob premajhnem učinku prenovljenega modela.

Najbolj očitne pomanjkljivosti stacionarnega 2D modela, ki so razvidne iz rezultatov simulacij, so:

1. Povprečenje parametrov po vertikali kot omejitev, ki je z dvodimenzionalnim modelom ne moremo preseči,
2. Premajhna disperzija živega srebra, ki je v naravi večja zaradi nestacionarnosti hidrodinamičnih in transportno-disperzijskih procesov.
3. Slabše ujemanje rezultatov ob izlivu reke Soče v Tržaški zaliv zaradi preredke numerične mreže v neposredni okolici izliva.

Kot rešitev prvih dveh pomanjkljivosti smo uporabili nestacionarni 3D model, numerično mrežo v zalivu pa smo s prvotnega koraka $\Delta x = \Delta y = 1800$ m zgostili na mrežo s korakom $\Delta x = \Delta y = 900$ m, ob ustju Soče še dodatno na $\Delta x = \Delta y = 300$ m. S tem je bilo hkrati doseženo natančnejše ujemanje gibalne količine in pretoka na izlivu ter natančnejši račun dogajanja v bližini izliva.

V vertikalni smeri je bilo izvedenih več poizkusov z različnimi debelinami in številom slojev. Po primerjavi rezultatov več simulacij z različnim številom in debelinami slojev smo izbrali 25 enakomerno debelih slojev debeline 1m. Dimenzije končne numerične mreže Tržaškega zaliva so torej $43 \times 42 \times 25$, kar je sprejemljivo tako s stališča računskega časa kot tudi dosežene natančnosti rezultatov.

Pri simulacijah s 3D modelom je bil poleg popolnoma nestacionarnega modeliranja (modeliranja v realnem času oz. *real-time modelling*) uporabljen tudi tako imenovani *kvazi-stacionarni* pristop, pri katerem ob večjih spremembah vhodnih parametrov račun nekaj časa poteka povsem nestacionarno. Ko pa se hitrosti, potek gladine in tlaki ter porazdelitev gostote, temperature in slanosti ustalijo, jih fiksiramo in računamo transport

less exploited. Further modifications of the model are not reasonable, as the improvement of the results of such upgraded 2D models would not be proportional to the investment.

The following deficiencies of the steady state 2D model, evident from the results of the simulations, were found to be the most important:

1. Depth averaging of all parameters, which cannot be avoided using a 2D model.
2. Too low dispersion of mercury forms which, in nature, is higher due to the non-steady state nature of the hydrodynamic and transport processes.
3. A relatively worse agreement of results near the Soča River mouth due to a too coarse numerical grid in its vicinity.

A non-steady state 3D model was used as an answer to the first two deficiencies. The numerical grid in the Gulf was also refined from $\Delta x = \Delta y = 1800$ m, used with the 2D model to $\Delta x = \Delta y = 900$ m, and, additionally, to $\Delta x = \Delta y = 300$ m near the Soča River mouth. The last modification contributed to a better agreement of Soča River momentum and discharge as well as to a more accurate computation near the river mouth.

Several attempts with different numbers and thicknesses of layers in the vertical direction were performed. Finally, according to a comparison of the results, 25 layers of uniform thickness, each being 1 m thick, was adopted. Consequently, the numerical grid in the Gulf of Trieste consists of $43 \times 42 \times 25$ cells, which results in an acceptable computational time, as well as acceptable accuracy of the simulation results.

Besides full non-steady state simulations (real-time modelling), the quasi-steady state principle was used with the 3D modelling. Here, a non-steady state simulation is performed for a certain period of time after input parameters have been changed significantly. Afterwards, when the velocity field, free surface elevations, pressure, density distribution, temperature and salinity field are stabilised, they are treated as fixed, and only the transport of the pollutant is further calculated. This way the computational time is

polutantov s stacionarnimi hidrodinamičnimi količinami. S tem se čas računanja bistveno skrajša, saj za izračun hidrodinamičnih količin, ob upoštevanju gostotnih gibanj in gostote stratifikacije, porabimo več kot 80 odstotkov računskega časa. Popoln nestacionarni račun transporta in disperzije živega srebra z izbrano numerično mrežo za območje Tržaškega zaliva in z upoštevanjem vseh parametrov je trenutno tudi na najzmogljivejših osebnih računalnikih še neizvedljiv, saj računski čas večkrat presega trajanje obdobja, ki ga želimo simulirati.

Za modeliranje dolgotrajnih procesov običajno zadoščajo časovno povprečni podatki za daljša obdobja, kalibracija in verifikacija modela pa zahtevata simulacije v realnem času za kratkotrajna obdobja, v katerih so bile izvedene meritve. Pri kalibraciji kompleksnega modela, kakršen je izpopolnjeni model PCFLOW3D, pa je bilo treba obe metodi kombinirati. Nestacionarni 3D model namreč zahteva za delovanje mnogo vhodnih podatkov, ki jih je na razmeroma velikem območju, kakršen je Tržaški zaliv, zelo težko meriti na dovolj merskih točkah sočasno.

Za kalibracijo in verifikacijo modela so bile izvedene tri simulacije:

1. Transport in disperzija celokupnega raztopljenega živega srebra za obdobje od 1.11.1994 do 25.6.1995. Rezultate simulacije smo primerjali z rezultati meritev, opravljenih 25.6.1995.
2. Transport in disperzija lebdečih plavin in na delce vezanega živega srebra v času trajanja visokovodnega vala Soče novembra 1997. Izvedena je bila kvalitativna primerjava rezultatov simulacije z izmerjenimi koncentracijami živega srebra v sedimentu na dnu Tržaškega zaliva.
3. Simulacija resuspendiranja sedimenta z dna zaliva z računom debeline erozije med dvodnevni obdobjem močne burje (13 m/s). Rezultate simulacije smo vnovič primerjali z izmerjenimi koncentracijami živega srebra v sedimentu na dnu zaliva.

essentially reduced, as about 80 % of total computational time needed is used for the hydrodynamics computation when density driven flow and stratified conditions are taken into account. At this time, a full real-time computation of mercury transport and dispersion using the adopted numerical grid of the Gulf of Trieste and accounting for all parameters is impossible, even with the most efficient personal computers, as the computational time severely exceeds the time being simulated.

Usually steady state simulations with time-averaged input data are sufficient for the modelling of long-term processes, while real-time simulations over the short time periods of the measurements must be performed to calibrate and verify the model. However, to calibrate such a complex 3D model, a combination of both methods had to be used. The non-steady state 3D model needs a large amount of input data to work properly. In a relatively large area, such as the Gulf of Trieste, it is very difficult to measure all the parameters simultaneously in enough sampling points.

Three simulations were performed in order to calibrate and verify the model:

1. Transport and dispersion of total dissolved mercury between 1 November, 1994 and 25 June, 1995. Results of the simulation were compared with the measurements performed on 25 June, 1995.
2. Transport and dispersion of suspended sediment and particulate mercury during the Soča River flood wave in November, 1997. A qualitative comparison was made with the measured distribution of mercury concentrations in the bottom sediments of the Gulf of Trieste.
3. Simulation of resuspension, bottom sediment erosion and transport due to a two-day period of strong *burja* wind (NE, 13 m/s) was performed. Again, a qualitative comparison with the measured distribution of mercury concentrations in the bottom sediments of the Gulf was made.

4.2 MODELIRANJE RAZTOPLJENEGA ŽIVEGA SREBRA IN PRIMERJAVA Z MERITVAMI – JUNIJ 1995

Najprej smo na podlagi uradnih statističnih podatkov Hidrometeorološkega zavoda Republike Slovenije izdelali scenarij za tipično leto, pri čemer smo ga razdelili na štiri glavne sezone, ki tako rekoč sovpadajo s koledarskimi letnimi časi. Za glavne sezone so bile nato na podlagi statističnih podatkov izračunane povprečne sezonske vrednosti posameznih parametrov. Glavnim sezonam smo dodali še vložke močnega vetra in visokovodnih valov Soče, ki se z visoko stopnjo verjetnosti pojavljajo vsako leto ob skoraj istem času.

Prav ti vložki pomenijo bistveno izboljšavo v primerjavi z dosedanjim modeliranjem s stacionarnimi modeli. Znano je namreč, da največji del (več kot 90 odstotkov) lebdečih plavin prinesejo v Tržaški zaliv prav visoke vode, ki se praviloma pojavljajo ob pomladanskem in jesenskem deževju. Prav tako je znano, da je premeščanje sedimenta v samem zalivu (resuspendiranje z dna, transport plavin in vnovično usedanje na dno) večinoma posledica močnega vetra in z njim neposredno povezanega valovanja, ki se praviloma pojavlja v hladnejšem delu leta, med novembrom in februarjem.

V končni fazi je tipično leto razdeljeno na 12 sekvenc (slika 4.2), ki jih simuliramo zaporedno; krajše (nekajdnevne) popolnoma nestacionarno, za daljše (nekaj tednov ali mesecev) pa uporabimo že omenjeni kvazi-stacionarni pristop.

4.2.1 Podatki

Veter

Smer in jakost povprečnih sezonskih vetrov je bila za postajo Beli Križ določena iz podatkov Hidrometeorološkega zavoda Republike Slovenije (na voljo so bile urne vrednosti jakosti in smeri vetra za celotno obdobje med letoma 1975 in 1990) z metodo VECTRA (Širca, 1996).

4.2 MODELLING OF DISSOLVED MERCURY AND COMPARISON WITH MEASUREMENTS – JUNE, 1995

First of all, a scenario for a typical year was prepared on the basis of official statistical data (Hydrometeorological service). Four main seasons, which were more or less identical to the calendar seasons, were accounted for. On the basis of official statistical data, seasonally averaged values of parameters during these main seasons were calculated. A few inserts of strong wind and the river Soča flood-peaks, which statistically occur with high probability at approximately the same time every year, were added to the main seasons.

These inserts are of great importance, as they represent a significant step forward in comparison with the previously performed steady state modelling. It is known that over 90 % of the annual inflow of suspended sediment and mercury are flushed into the Gulf with two flood waves, usually during spring and autumn rains. It is also known that strong wind and wind driven waves are the most important cause of the transport processes of bottom sediment in the Gulf (resuspension, transport with currents and repeated sedimentation). This latest phenomenon mostly occurs during the winter months between November and February.

Finally, a typical year was divided into 12 sequences (Figure 4.2), which were simulated successively. With the shorter (up to a few days long) sequences, non-steady state calculations were used, while with the longer (a few weeks to a few months long), the quasi-steady state principle, as described above, was used.

4.2.1 Input data

Wind

Seasonally averaged wind force and direction above the Gulf was evaluated from the official data for the Beli Križ Measuring Station (measured hourly values of wind force and direction for the period from 1975 to 1990 were available) using the VECTRA method (Širca, 1996).

Preglednica 4.1. Sezonski povprečni veter nad Tržaškim zalivom.
Table 4.1. Seasonally averaged wind above the Gulf of Trieste.

Sezona <i>Season</i>	Smer <i>Direction</i>	Hitrost <i>Velocity</i>
	[°]	[m/s]
Zima (jan., feb., mar.) <i>Winter (Jan., Feb., Mar.)</i>	66.6	2.2
Pomlad (apr., maj., jun.) <i>Spring (Apr., May, June)</i>	101.6	1.1
Poletje (jul., avg., sep.) <i>Summer (July, Aug., Sep.)</i>	64.7	1.0
Jesen (okt., nov., dec.) <i>Autumn (Oct., Nov., Dec.)</i>	69.8	2.3

Beli Križ se je že pri dosedanjem modeliranju (Širca, 1996; Širca in Rajar, 1997a) izkazal za najbolj reprezentativno mersko postajo na območju Tržaškega zaliva. Stoji na vzpetini in zato topografija terena manj vpliva na smer in jakost vetra kot pri merski postaji v Trstu. Hkrati je bilo prav za Beli Križ na voljo največ podatkov, zato so izračunane sezonske vrednosti bolj reprezentativne od vrednosti, ki smo jih izračunali za mersko postajo v Trstu in so bile tudi uporabljene kot vhodni podatek za simulacije.

Glede na pogostnost se v tipičnem letu pojavljata dva letna maksimuma trajanja burje (smer NE), in sicer februarja in novembra, ki hkrati skoraj točno sovpadata z maksimumoma jakosti.

As Beli Križ is considered to be the most representative measuring site near the Gulf, the data from this station were also used in our previous modelling (Širca, 1996; Širca and Rajar, 1997a). It is positioned on the top of a rise and thus wind force and direction is less influenced by the topography of the surrounding land than with the station in Trieste. Additionally, the data was collected more frequently at the Beli Križ Station, and thus the calculated seasonally averaged values are more representative than the ones from the Trieste station. These values were used as the input data for the main seasons in all the performed simulations.

Regarding the frequency of occurrence, there are two peaks of *burja* wind (NE) during a typical year. These two peaks in February and November almost exactly coincide with the wind force peaks.

Preglednica 4.2. Vložki vetra (merska postaja Beli Križ).
Table 4.2 Wind inserts (Beli Križ measuring station).

Smer <i>Direction</i>	Mesec <i>Month</i>	Pogostnost <i>Frequency</i>	Trajanje <i>Duration</i>	Hitrost <i>Velocity</i>
		[%]	[dni - days]	[m/s]
NE	Februar <i>February</i>	37.4	11	6.4
NE	November <i>November</i>	32.8	10	6.2

Veter iz nekoliko bolj vzhodne smeri (ENE) ima na Belem Križu v februarju in novembru sicer višjo povprečno hitrost (6.6 m/s), vendar je pogostnost te smeri samo 9.7 odstotka (v februarju) oziroma 10.7 odstotka (v novembru). Za simulacije sta bila uporabljena najdaljša vložka, dolžine 10 in 11 dni, ki zaradi svojega trajanja nedvomno prispevata največ k premeščanju sedimenta v zalivu.

Soča

Sezonski pretoki in visokovodni vložki Soče temeljijo na meritvah, opravljenih na vodomerni postaji Solkan (preglednica 4.3). Med Solkanom in izlivom Soče v Tržaški zaliv dotekata v Sočo še dva večja pritoka (slika 1.1), Vipava in Ter (Torre). Podatki za Vipavo so razvidni iz preglednice 4.3, hidrologija italijanskega dela Soče pa je slabše raziskana, saj po razpoložljivih podatkih pretokov nihče ne meri. V spodnjem toku Soče obdelavo podatkov otežuje tudi kompleksen sistem nadzemnih in podzemnih tokov v vzhodnem delu Furlanske nižine in Krasa ob slovensko-italijanski meji. Največja neznanka v tem delu ostaja reka Ter, ki se ji (odvisno od gladine talne vode) vzdolž toka pretok povečuje ali zmanjšuje in poleti občasno sploh ne priteče do sotočja s Sočo (Mosetti, 1983, Širca et al, 1999b). Skupna prispevna površina porečja Soče nad Solkanom znaša 2235 km², pod Solkanom pa 1065 km², zato je pretok ob ustju določen kot 1.5-kratni skupni pretok Soče in Vipave. Povprečni letni pretok na izlivu v Tržaški zaliv tako znaša 168 m³/s, ta številka pa se dobro ujema z vrednostmi drugih avtorjev, ki znašajo med 165 m³/s (Mosetti, 1983) in 172 m³/s (Benini, 1974).

Sezonski povprečni pretoki so določeni iz povprečnih mesečnih pretokov, podanih v literaturi (za Solkan v VGI (1982), za Miren pa v Vodnogospodarskih osnovah (1978)).

In February and November, winds from the ENE direction are stronger (6.6 m/s) at the Beli Križ Station; however, the frequency is only 9.7 % (in February) and 10.7 % (in November). The longest inserts (10 and 11 days long) were assumed, as they contribute the most to the sediment transport in the Gulf of Trieste.

The Soča River

Seasonally averaged discharges, as well as the Soča River flood-peak inserts, are based on measurements in the cross-section at Solkan (Table 4.3). There are another two important tributaries of the Soča River between Solkan and the river mouth (Figure 1.1): the Vipava River, which mainly flows through Slovenian territory, and is well elaborated (Table 4.3); and the river Torre. The hydrology of the Italian part of the Soča River watershed is less known. Continuous measurements are not available downstream of Solkan. Moreover, a complex system of surface and groundwater flows exists in the eastern part of the Friuli plain and the karst area of Kras at the Slovenian – Italian border. The most important unknown of the lower reach represents the Torre River, which, according to the saturation conditions of the plain, either loses or gains water along its flow and sometimes, during the summer months, even disappears underground (Mosetti, 1983, Širca et al, 1999b). The total catchment area of the Soča River in Slovenia is 2235 km², while the catchment area in Italy is 1065 km². The mean discharge at the river mouth is, therefore, considered to be equal to 150 % of the sum of the mean discharges at Solkan and Miren. The annually averaged discharge of the Soča River at its mouth was thus set to 168 m³/s. The number can be compared with the values of other authors, which are between 165 m³/s (Mosetti, 1983) and 172 m³/s (Benini, 1974).

Seasonally averaged discharges are evaluated from measurements (monthly averaged discharges) from other authors (for Solkan in VGI (1982); for Miren in Vodnogospodarske osnove (1978)).

Preglednica 4.3. Mesečni in sezonski povprečni pretoki Soče.
Table 4.3. Monthly and seasonally averaged discharges of the Soča River.

Mesec Month	Pretoki Discharges				
	Soča (Solkan)	Vipava (Miren)	Σ Soča + Vipava	Soča na ustju <i>The Soča River mouth</i>	Sezonski povprečni <i>Seasonally averaged</i>
	[m ³ /s]	[m ³ /s]	[m ³ /s]	[m ³ /s]	[m ³ /s]
January	72	22	94	141	
February	70	20	90	135	150
March	94	21	115	173	
April	109	20	129	194	
May	116	16	132	192	190
June	109	13	122	183	
July	69	9	78	117	
August	59	7	66	99	120
September	82	14	96	144	
October	109	20	129	194	
November	144	27	171	257	209
December	94	26	120	180	
Povprečni letni Annually averaged	94	18	112	168	168

Opisana metoda ekstrapolacije pretokov je za kratkotrajneša obdobja manj zanesljiva, kljub temu pa je bil isti princip uporabljen tudi za račun visokovodnih vložkov. Intenziteta vložkov je bila določena s pomočjo srednjih visokih pretokov, tj. povprečja visokih pretokov v nekem daljšem (dolgoletnem) obdobju. Gledano po mesecih, imajo mesečni srednji visoki pretoki (prvi stolpec preglednice 4.4) v Solkanu za obdobje od 1926 do 1975 dva maksimuma, ki se pojavljata maja in novembra.

Po verjetnostni analizi predstavljata zgornji vrednosti za oba meseca visoka pretoka s povratno dobo 2.5 leti ($Q_{2.5}$), kar pokaže interpolacija med Q_2 in Q_5 (2. in 3. stolpec preglednice 4.4). To sicer pomeni, da se dogodek zgodi le na 2.5 leta, vendar s približevanjem Q_1 statistične analize izgubljajo smisel. Petdnevno obdobje s pretokom 473 m³/s ima povratno dobo dve leti, zato je

Although with a lower reliability for shorter events, the same relationship between discharges as described above was used to determine discharges during the flood-peak inserts. Intensity of the inserts was evaluated from the mean high discharges (i.e. an average of high discharges during a longer period). The mean high discharges for individual months (the first column in Table 4.4) at Solkan, between the years 1926 and 1975, have two peaks, which occur in May and November respectively.

According to probability analysis these values represent an event with a recurrence of 2.5 years ($Q_{2.5}$), for both May and November, as is evident from interpolation between Q_2 and Q_5 (the second and the third column in Table 4.4). As statistical analyses for events with a recurrence of only one year (Q_1) are aimless, $Q_{2.5}$ was used in simulations, although such an event statistically occurs only every 2.5 years. The recurrence of a five day long insert with a 473 m³/s discharge is two years;

upoštevana dolžina pomladnega vložka 5 dni. Trajanje jesenskega vložka je krajše, saj bi imelo petdnevno obdobje s pretokom $950 \text{ m}^3/\text{s}$ povratno dobo kar 50 let. Upoštevana dolžina jesenskega vložka je tako 2 dni.

therefore, the length of the spring-insert was set to five days. The autumn-insert is shorter, as the recurrence of a five day long insert with $950 \text{ m}^3/\text{s}$ discharge is about 50 years. A two day long autumnal insert was adopted.

Preglednica 4.4. Visokovodni vložki Soče (meritve - Solkan).
Table 4.4. The Soča River flood-peak inserts (measurements - Solkan).

Mesec <i>Month</i>	srQ_v	Q_2	Q_5	Trajanje <i>Duration</i>
	$[\text{m}^3/\text{s}]$	$[\text{m}^3/\text{s}]$	$[\text{m}^3/\text{s}]$	[dni – <i>days</i>]
<i>May</i>	476	416	687	5
<i>November</i>	914	821	1299	2

Dvodnevnu vložku z najvišjim pretokom sta dodana še dan prej in dan kasneje s pretokom $230 \text{ m}^3/\text{s}$. Tako imata pomladni in jesenski vložek Soče v Solkanu približno enak volumen odtoka, ki znaša okrog 200 milijonov m^3 (VGI, 1982). Dimenzije majskega vložka potrjuje tudi obdelava odvisnosti med volumnom in pretokom v Solkanu (VGI, 1982), iz katere je razvidno, da znaša srednji pretok petdnevnega visokovodnega vala s povratno dobo 2 leti okrog $475 \text{ m}^3/\text{s}$, odtekli volumen pa nekoliko presega 200 milijonov m^3 . Jesenski vložek lahko primerjamo z registriranim visokovodnim valom novembra 1997, katerega povratna doba pa znaša po različnih podatkih od 5 do 30 let. Pod sotočjem z Vipavo je bil takrat v dveh glavnih dneh odtekli volumen okrog 200 milijonov m^3 , če upoštevamo še naraščanje pretoka dan prej in upadanje nazaj na normalni novembrski pretok, ki je trajalo še štiri dni, je bil skupni odtekli volumen pod sotočjem Soče z Vipavo v enem tednu novembra 1997 približno 380 milijonov m^3 .

V modelu so bili kot vhodni podatki ob visokovodnih vložkih uporabljeni pretoki Soče na ustju, kot so navedeni v preglednici 4.5.

A day before and a day after with a discharge of $230 \text{ m}^3/\text{s}$ were added to the two day long autumn-insert. Thus, both flood-peak inserts have approximately the same volume of about 200 millions m^3 (VGI, 1982). The volume of the spring-insert was also confirmed by the relationship between discharge and flood-wave volume for the cross-section in Solkan (VGI, 1982). It is evident that the mean discharge of a five day long flood-wave with a recurrence of about two years is approximately $475 \text{ m}^3/\text{s}$, and the volume of the flood-wave somewhat exceeds 200 millions m^3 . The autumn-insert can be compared with the observed flood wave of the Soča River in November, 1997, which had a recurrence of between 5 and 30 years from different sources. Below the confluence of the Soča and Vipava rivers, the volume of the main flood wave (in a duration of two days) was about 200 million m^3 . Taking into account one day of water rising before and four days of returning back to the normal November discharge, the total volume of flood wave in a single week in November, 1997 was about 380 million m^3 .

The data from Table 4.5 (discharges at the Soča River mouth) were used as the input data for flood-peak insert simulations.

Preglednica 4.5. Visokovodni vložki Soče na ustju (vhodni podatki za model).
 Table 4.5. Flood-peak inserts at the Soča River mouth (input data for simulations).

Mesec (vložek) Month (insert)	Pretok na ustju Discharge at the river mouth	Trajanje Duration
	[m ³ /s]	[dni - days]
maj (celoten vložek) May (complete insert)	714	5
november (1.dan) November (1 st day)	345	1
november (2. in 3. dan) November (2 nd and 3 rd day)	1371	2
november (4.dan) November (4 th day)	345	1

Za simulacije v stratificiranem stanju je pomemben tudi podatek o temperaturi Soče na ustju. Na voljo so bile meritve temperature pod zadnjim mostom pred ustjem Soče (manj kot kilometer od izliva Soče) v približno dvotedenskih intervalih med leti 1974 in 1995. Največja gostota meritev je bila med leti 1978 in 1987. Za nameravane simulacije s 3D modelom so bile iz podatkov statistično izračunane povprečne sezonske vrednosti (preglednica 4.6).

Water temperature of the Soča River at its mouth is another important data to simulate the stratified conditions. Measurements of water temperature under the last bridge, situated less than one km from the river mouth, were available. Temperature was measured in about two-week intervals between the years 1974 and 1995, the most frequently between the years 1978 and 1987. Seasonally averaged water temperatures were statistically evaluated from measurements (Table 4.6) and used in 3-D modelling.

Preglednica 4.6. Povprečne sezonske temperature vode v Soči (most pred izlivom).
 Table 4.6. Seasonally averaged water temperature in the Soča River (the nearest bridge to the river mouth).

Sezona Season	Temperatura Temperature
	[°C]
Zima Winter	7.7
Pomlad Spring	12.9
Poletje Summer	16.3
Jesen Autumn	9.2

Meritve raztopljenega živega srebra v Soči pri nizkih pretokih oktobra 1997, med visokovodnim valom novembra 1997 in ob srednje nizkih pretokih decembra 1998 ter v Tržaškem zalivu ob ustju Soče maja in septembra 1995 (Horvat et al, 1999) kažejo, da so koncentracije raztopljenega živega srebra v Soči in Tržaškem zalivu le malo odvisne od pretoka Soče in letnega časa in znašajo pri vseh meritvah v Soči od 1.6 do 3.5 ng/l, v zalivu blizu ustja (morska točka D6 na sliki 4.1) pa od 4.5 do 5 ng/l. Višje koncentracije v morju so posledica kemijskega procesa sproščanja živega srebra iz partikularne v raztopljeno obliko v območju mešanja sladke in slane vode. Procesu ni bilo mogoče neposredno vključiti v model, zato je pri vseh simulacijah in v vseh letnih časih upoštevana koncentracija na ustju 5 ng/l.

Tržaški zaliv

Plimovanje pri simulacijah s 3D modelom ni bilo upoštevano, saj so rezidualni tokovi zaradi plimovanja v zalivu vsaj za red velikosti manjši od rezidualnih tokov zaradi vetra, ki je glavni vzrok gibanja vode (Širca, 1996). Že napaka zaradi numerične difuzije, ki se ji z obstoječo numerično shemo ne moremo izogniti, je bistveno večja od vpliva plimovanja, zato upoštevanje le-tega ne bi bilo smiselno.

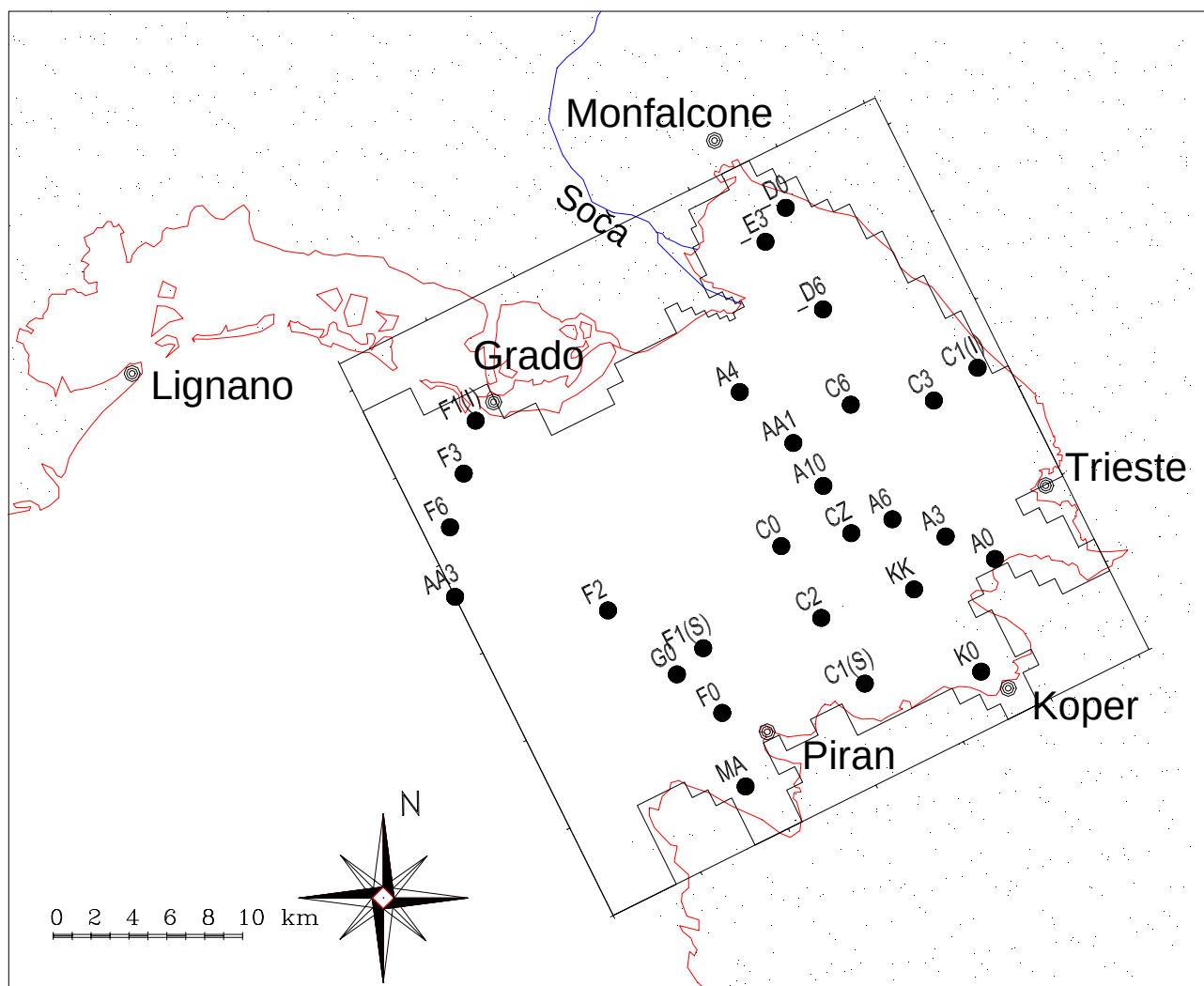
Predvsem v toplejšem delu leta na disperzijo živega srebra v vertikalni smeri vplivajo tudi stratificirane razmere v zalivu. Za simulacije je bilo potrebno za vsako sezono zagotoviti podatke o porazdelitvi temperatur in slanosti v vseh točkah računske mreže.

There were several measurements of dissolved mercury in the Soča River available: during the flood-wave in November, 1997, the mean low discharge in December, 1998 and the low discharge in October, 1997 respectively (Horvat et al, 1999). In the Gulf of Trieste, measurements were performed in May and November, 1995 (Horvat et al, 1999). It is evident from the data that the interdependence between the discharge of the Soča River and the concentrations of dissolved mercury is very low. In the Soča River, concentrations vary between the range of 1.6 and 3.5 ng/l, while in the Gulf, near the river mouth (point D6 in Figure 4.1), concentrations between 4.5 and 5 ng/l were measured. Higher concentrations in the seawater are due to mercury release from particulate to its dissolved form within the freshwater and saltwater mixing zone. It was not possible to include the process itself in the model; therefore, a mercury concentration of 5 ng/l was taken into account with all simulations in any season.

The Gulf of Trieste

The effect of tide on the circulation in the Gulf was not taken into account with the 3D simulations. Typical tide-induced residual currents in the Gulf were, at least for an order of magnitude, smaller than the wind-induced residual currents (Širca, 1996). Moreover, the error due to tidal forcing exclusion is significantly exceeded by the error caused by false diffusion, which can not be avoided using the existing numerical scheme. Therefore, the inclusion of tidal forcing in the model would not improve the accuracy of results and was not performed.

Stratified conditions within the Gulf and their impact on the dispersion of mercury along the water column are also a very important factor, particularly during the warmer half of the year. Therefore, temperature and salinity distribution along the entire computational domain had to be evaluated for the four main seasons.



Slika 4.1. Definicijsko območje modeliranja in merske točke v Tržaškem zalivu (temperatura in slanost).

V zalivu so bile izmerjene temperature in slanosti sredi posameznih letnih časov (februar, maj, avgust, november) sočasno v 27 točkah zaliva (slika 4.1) v 5-metrskih intervalih po globini. Z linearno interpolacijo so bile nato iz podatkov meritev določene vrednosti temperature in slanosti po posameznih slojih za vse merske točke, iz teh pa so bile z orodjem *QuickSurf* določene vrednosti v vseh kontrolnih volumnih celotnega definicijskega območja za vsako sezono.

Temperature and salinity were measured simultaneously in 27 sampling points within the Gulf (Figure 4.1), in the middle of each main season (February, May, August, November) in 5-m intervals along the depth. Afterwards, temperature and salinity in all layers along the depth was interpolated from measured data in each sampling point. From these values, the temperature and salinity distribution along the entire computational domain for four main seasons was calculated using *QuickSurf* software.

daljših časovnih obdobjih, upoštevali smo jih le kot začetni pogoj za posamezno sezono. Meritve v 27 točkah namreč ne zadoščajo za dovolj natančen opis razmer na celotnem območju zaliva, napaka interpolacij in ekstrapolacij pa je ob tako majhnem številu merskih točk lahko velika. Zaradi napačnih vrednosti se v posameznih delih zaliva pojavijo močni gostotni tokovi, ki lahko povsem pokvarijo sliko hidrodinamičnih parametrov, pri čemer izgubimo vso prednost 3D modela pred enostavnejšimi modeli. Izkušnje z gostotnimi gibanji (Rajar et al, 1997) kažejo tudi, da je potrebno 'glajenje' rezultatov meritev temperatur in slanosti, sicer se pri simulacijah lahko pojavijo problemi s stabilnostjo numerične sheme. Poleg tega bi bila pri simulaciji dolgotrajnih procesov končna slika temperatur in slanosti nerealna zaradi vtoka Soče, gostotnega gibanja in disperzije temperature in slanosti zaradi gibanja vodnih mas.

Glajenje matrike izvedemo na dva načina: pri prvem izključimo vse druge izvore gibanja in določen čas upoštevamo samo gostotno gibanje, dokler na celotnem definicijskem območju ne dosežemo pričakovanih hitrosti, pri drugem pa hkrati z gostotnimi gibanji upoštevamo tudi druge izvore gibanja vode (veter, vtok rek, plimovanje). Če v nadaljevanju simuliramo močno nestacionarne procese, je primernejši drugi način, ki je bil uporabljen tudi pri simulacijah transporta raztopljenega živega srebra v Tržaškem zalivu.

Koncentracije živega srebra v sedimentu na dnu Tržaškega zaliva so zelo visoke, ob ustju Soče dosegaajo 25-30 $\mu\text{g/g}$ suhe teže. Iz sedimenta se živo srebro sčasoma izloči v porne vode in zaradi difuzije prehaja v okoliško vodo. Porne vode so zato pomemben vir raztopljenega živega srebra še dolgo časa po zmanjšanju ali celo prenehanju dotoka živega srebra v okolje. V letih 1995 in 1996 so bile v merski točki AA1 (slika 4.1) izvedene meritve koncentracij živega srebra v pornih vodah v sedimentu na mestu samem z bentoško komoro (*benthic chamber*) (Covelli

for long-term steady-state simulations; thus, they were only used as an initial condition for each main season. Measurements in only 27 sampling points are not sufficient to describe conditions within the whole area of the Gulf and the interpolation / extrapolation unreliability can be significant with such a small number of sampling points. Strong density-driven flows can occur in some parts of the Gulf due to inaccurate temperature and/or salinity distribution. The influence of these currents on the hydrodynamic parameters can nullify all the advantages of 3D modelling over other simpler models. It is also evident from previous density-driven flow modelling (Rajar et al, 1997) that the values calculated from measurements need to be 'smoothed' to avoid stability problems of the numerical scheme during computation. Additionally, with long-term simulations, the final distribution of temperature and salinity would be unreal due to the Soča River inflow, density-driven flows and, most importantly, due to advection.

There are two possibilities for 'smoothing' a matrix: in the first, all other forcing factors are excluded and only density-driven flow is calculated; while in the second, all forcing factors (wind, river inflows, tidal forcing and density-driven flow) are taken into account. The computation is then performed for a certain amount of time, until the expected velocities are reached within the entire computational domain. The second method was found to give more appropriate results with simulations of highly non-steady state processes, and has, therefore, been used to simulate the transport of mercury in its dissolved form within the Gulf of Trieste.

In the bottom sediment of the Gulf, mercury concentrations are highly increased and reach about 25-30 $\mu\text{g/g}$ dry weight near the Soča River mouth. Mercury bound to sediment particles is gradually being released into the pore water and, due to molecular diffusion, also proceeded to the surrounding water. Therefore, pore waters are an important source of dissolved mercury for a long time after the inflow of mercury has begun being reduced or has even ceased. Mercury concentrations in the pore water of the bottom sediment of the Gulf were determined by an in situ benthic chamber experiment at location AA1 (Figure 4.1) during 1995 and 1996 (Covelli et al, 1999b).

These measured values cannot be applied to

et al, 1999b).

Meritev je bila zaradi zahtevnosti postopka in visoke cene izvedena v eni sami točki zaliva, zato številke nikakor ne moremo posplošiti na celotno obravnavano območje. Če primerjamo podatke različnih avtorjev o količini živega srebra, ki se v enem letu usede na dno zaliva (*downward flux*), so vrednosti precej različne, od 3.10 mg/m²/leto v globini 20 m v južnem delu zaliva (Planinc in Faganeli, 1993), 2.96 mg/m²/leto v globini 21 m v sredini zaliva (Covelli et al, 1999b) do 1.29 mg/m²/leto v globini 10 m v južnem delu zaliva (Planinc in Faganeli, 1993). Na različnih mestih zaliva lahko torej pričakujemo tudi precejšnje razlike v količini izločenega živega srebra, ki je odvisna od globine, biokemičnih razmer ob dnu, granulometrijske sestave, geološkega porekla ter vsebnosti živega srebra v sedimentu.

Podatek o sproščanju (*upward flux*) 0.78 mg/m²/leto (Covelli et al, 1999b) celokupnega živega srebra ob predpostavki, da je vrednost po celotnem zalivu enaka, pomeni letno količino približno 470 kg živega srebra (Širca et al, 1999b), ki iz sedimenta izhaja nazaj v zaliv, kar je bistveno več od 10 kg raztopljenega živega srebra, ki ga letno v zaliv prinese Soča. Sproščeno živo srebro pa večinoma ostane v bentoškem pasu tik nad dnom. Opazovanja in meritve potrjujejo, da so koncentracije približno pol metra nad dnom vsaj za red velikosti nižje od koncentracij tik nad dnom in tudi do dva reda velikosti nižje od koncentracij v pornih vodah, nekaj centimetrov pod dnom. Tanek sloj vode ob dnu lahko hidravlično opišemo kot mejno plast, na katero advekcija nima vpliva, kot edini vzrok za transport živega srebra navzgor po vodnem stolpcu pa ostane molekularna difuzija. Globina na lokaciji eksperimenta (21 m) je dovolj velika, da do dna ne seže niti oscilatorno gibanje zaradi valovanja ob močnem vetru, ki bi lahko prispevalo k mešanju. Slika v plitvejšem (severnem) delu zaliva je verjetno precej drugačna, kar pa morajo potrditi dodatne meritve.

the whole area of the Gulf, as only one location was observed, due to the difficulty and expense of the experiment. Comparison of the downward mercury flux values and the total amount of suspended mercury by different authors shows a wide range of results for the Gulf of Trieste. The highest value of downward flux, 3.10 mg/m²/year at the depth of 20 m in the southern part of the Gulf was determined by Planinc and Faganeli, (1993); according to Covelli et al, (1999b), the downward flux was 2.96 mg/m²/year at a depth of 21 m in the middle of the Gulf, and according to Planinc and Faganeli, (1993), 1.29 mg/m²/year at a depth of 10 m in the southern part of the Gulf. Therefore, significantly different upward fluxes may also be expected at different locations in the Gulf. Upward fluxes depend on depth, biochemical conditions at the bottom, granulometric characteristics of the bottom sediment, its geological origin and mercury concentrations in the bottom sediment.

If the rate of Covelli et al, (1999b), for upward flux (0.78 mg/m²/year) is applied with an assumption of constant upward flux over the whole area of the Gulf, 470 kg of total mercury would be released annually from the bottom of the Gulf. This amount significantly exceeds the amount of total dissolved mercury which is carried into the Gulf by the Soča River (10 kg/year). However, the released mercury remains mostly in the thin benthic zone near the sea-bottom. It was confirmed by observations and measurements that mercury concentrations about 50 cm above the sea-bottom are, for at least an order of magnitude lower than the concentrations a few centimetres above the bottom and up to two orders of magnitude lower than the concentrations in pore water a few centimetres below the sea-bottom. Therefore, the thin layer of water near the bottom can be hydraulically considered as a boundary layer, where the impact of advection is negligible. Mercury is only transported upwards in the water column due to molecular diffusion. The impact of oscillatory water motion due to wind-driven waves which could contribute to the mixing and upward transport of mercury, is negligible, as well, as at the location of the experiment, the water reaches a depth of 21 m. Substantially different conditions may occur in the shallower (northern) part of the Gulf; however, additional measurements are needed to confirm this supposition.

Vsekakor je količina živega srebra, ki se sprošča iz sedimenta ob dnu, dovolj velika, da jo bo treba v prihodnje upoštevati pri modeliranju, predvsem pa je zaskrbljujoče dejstvo, da je skoraj četrtina sproščenega živega srebra v metilirani obliki (slika 1.2), in tako predstavlja glavni vir metiliranega živega srebra v zalivu.

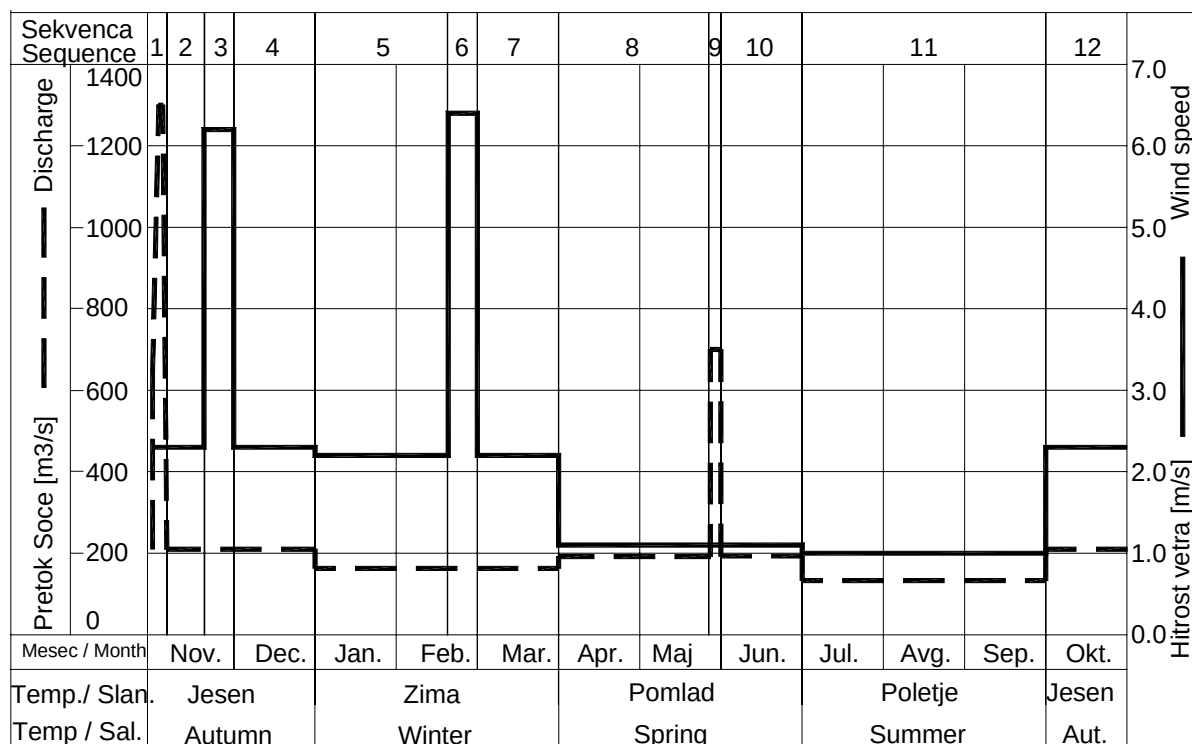
4.2.2 Simulacija, rezultati in primerjava z meritvami

Z zbranimi podatki smo izdelali končno razdelitev tipičnega leta na sekvence in pripravili podatke za simulacijo. Krajša obdobja smo obravnavali popolnoma nestacionarno, račun je potekal v realnem času, pri daljših pa smo uporabili kvazistacionarni pristop. Čas nestacionarne obravnave je v posameznih daljših sekvencah različen, odvisen pa je od pretoka Soče, hitrosti vetra in začetnih temperaturnih in slanostnih pogojev v zalivu. Traja lahko od 8 ur, v primeru močnejšega vetra in/ali visokega pretoka Soče, do nekaj dni pri šibkem vetru in nizkem pretoku Soče.

By all means, the high amount of mercury being released from the bottom sediment is very important and needs to be taken into account with future modelling and simulations. Moreover, almost 25 % of the mercury released by benthic fluxes appears in its methylated form (Figure 1.2), and, as such, represents the most important source of methylated mercury for the Gulf of Trieste.

4.2.2 Simulation, results and comparison to measurement

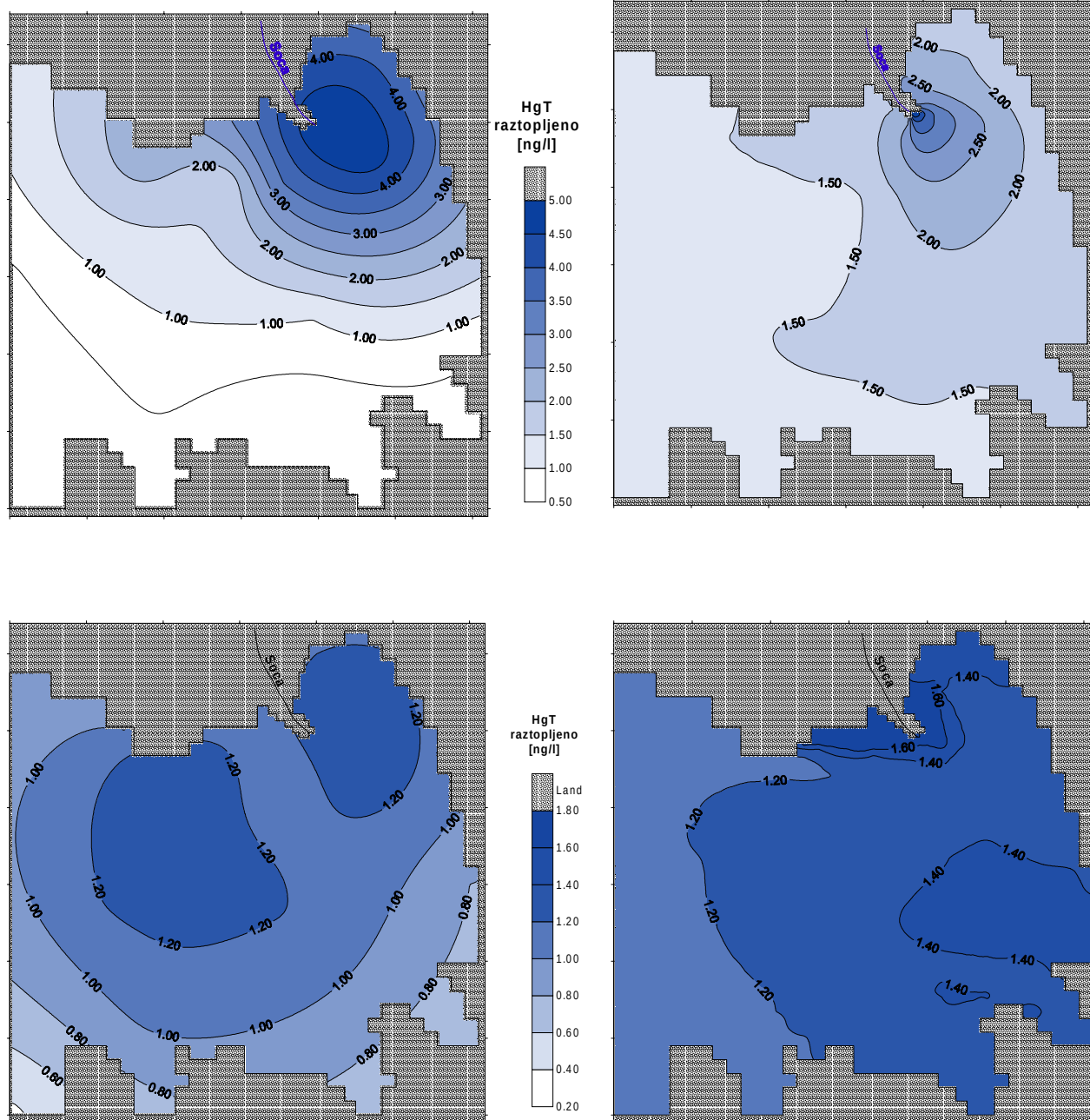
Input data for the simulations were prepared and the final partitioning of a typical year was done using the collected data. Fully non-steady state simulations (real-time modelling) were applied with the shorter sequences and quasi-steady state modelling with the longer ones. The duration of non-steady state treatment was different with individual longer sequences, as it depends on the discharge of the Soča River, the wind force and temperature / salinity conditions in the Gulf, respectively. Non-steady state simulations in duration from 8 hours with strong wind and/or high discharge of the Soča River, up to a few days with weak wind and lower discharges were applied.



Slika 4.2. Sezonsko povprečni parametri v Tržaškem zalivu.
Figure 4.2. Seasonally averaged parameters in the Gulf of Trieste.

Meritve celokupnega raztopljenega živega srebra so bile opravljene 25. junija 1995 (Horvat et al, 1995) v 14 točkah na površini in ob dnu, primerjava rezultatov modela in merjenih vrednosti pa je podana na sliki 4.3

Measurement of total dissolved mercury was performed on 25 June, 1995 in 14 sampling sites at the surface and at the bottom. Figure 4.3 shows a comparison between measurements and the results of the model simulation.



Slika 4.3. Primerjava merjenih in izračunanih koncentracij celokupnega raztopljenega živega srebra (junij 1995) v površinskem sloju (zgoraj) in sloju ob dnu (spodaj).
 Figure 4.3. Comparison of measured and simulated concentrations of total dissolved mercury (June, 1995) in the surface layer (above) and the bottom layer (below).

Iz primerjave rezultatov simulacije in meritev lahko sklepamo naslednje:

1. Kvalitativno je ujemanje rezultatov na površini zelo dobro. Dobro je vidno širjenje sladke vode iz Soče v pravilni smeri. Kvantitativno je ujemanje na površini dokaj dobro, povsod v mejah faktorja dve, kar je bistven napredek v primerjavi z rezultati 2D simulacij. Disperzija živega srebra v površinskem sloju je nekoliko prevelika, kar je predvsem posledica numerične difuzije, ki pa se ji s trenutno vgrajeno numerično shemo ni mogoče izogniti.
2. Kljub zvišanju koncentracij raztopljenega živega srebra v Soči je ujemanje v bližini ustja slabše, saj z modelom še ne moremo upoštevati sproščanja živega srebra z delcev plavin, ki je prisotno v območju mešanja sladke in slane vode. Proces še ni dovolj dobro raziskan, da bi ga bilo mogoče vključiti v model.
3. Ujemanje ob dnu je nekoliko slabše, še vedno pa je v mejah faktorja dve. Omeniti pa je treba, da tudi na rezultate meritev pri tako nizkih koncentracijah vpliva cela vrsta dejavnikov in je zato zanesljivost meritev v mejah ± 20 odstotkov. Če torej upoštevamo nezanesljivost analiznih metod in napako pri modeliranju, lahko zaključimo, da je ujemanje rezultatov dobro.
4. Poleg numerične difuzije na rezultate modela nekoliko vpliva tudi uporaba razmeroma preprostega modela turbulence. Slednji kljub zmanjšanju vertikalnega koeficienta turbulentne difuzije v stratificiranih razmerah daje nekoliko previsoke vrednosti koeficientov, predvsem pri šibkejšem vetru. Prednostna naloga pred nadaljnjim modeliranjem je torej vgradnja izpopolnjenega modela turbulence z dvema enačbama (k - ε model) in numerične shema višjega reda točnosti (npr. *Quickest*).
5. V modelu še ni upoštevano zvišanje koncentracij ob dnu zaradi sproščanja živega srebra iz pornih vod v sedimentu, ki lahko precej spremeni sliko koncentracij ob dnu.

The following conclusions can be made from the results of the simulation and measurements:

1. At the surface, a very good qualitative agreement of modelling results and measurements was achieved. Relatively good quantitative agreement, everywhere within a factor of two, was a significant improvement in comparison with the 2D modelling. The dispersion of mercury at the surface was somewhat too high, mostly due to false diffusion, which cannot be avoided using the existing numerical scheme.
2. In spite of an additional increase of dissolved mercury concentrations in the Soča River, agreement of the measurements with the simulation is worse near the river mouth. Additional research of the of mercury release from particulate matter to its dissolved form in the freshwater / saltwater mixing zone is needed to include the process in the 3D model.
3. Agreement in the bottom layer is somewhat worse, but still within a factor of two. However, the reliability of the measurements with such low concentrations is limited by several factors, and the accuracy does not exceed the limits of ± 20 %. By taking into account both the unreliability of the analytical methods and the inaccuracy of the modelling, the agreement of the results and measurements can be considered good.
4. Besides the false diffusion, the results are also influenced by the use of a relatively simple model of turbulence. In spite of adapting the eddy diffusivity to stratified conditions, values of the vertical coefficients are somewhat too high, particularly in weak wind conditions. A two-equation turbulence model (k - ε model) and a numerical scheme of a higher order of accuracy (e.g. *Quickest*) must be included in the model as soon as possible.
5. Increase of concentrations at the sea-bottom due to benthic fluxes, which can significantly change the mercury concentrations within the bottom layer, was not taken into account at the present state of the model.

4.3 MODELIRANJE TRANSPORTA IN DISPERZIJE LEBDEČIH PLAVIN OB VISOKOVODNEM VALU SOČE NOVEMBRA 1997

Z modelom je bil simuliran ekstremni dogodek, jesenski visokovodni val Soče med 6. in 14. novembrom 1997, za katerega je bilo na voljo dovolj meritev in opazovanj.

4.3.1 Podatki

Upoštevane so normalne jesenske razmere v zalivu, ko po obdobju močnejšega vetra nastopi premešano stanje, temperatura je po globini enakomerna in znaša 8°C , slanost pa 37.8 promila. Izveden je bil račun s povprečnim jesenskim vetrom jakosti 2.3 m/s iz smeri ENE ($69^{\circ} 48'$).

Opazovani visokovodni val je imel dve konici, ob prvi so znašali pretoki na ustju okrog $2500\text{ m}^3/\text{s}$, ob drugi pa okrog $2200\text{ m}^3/\text{s}$ (slika 4.4). Takšni pretoki predstavljajo visoko vodo s povratno dobo približno 5 let.

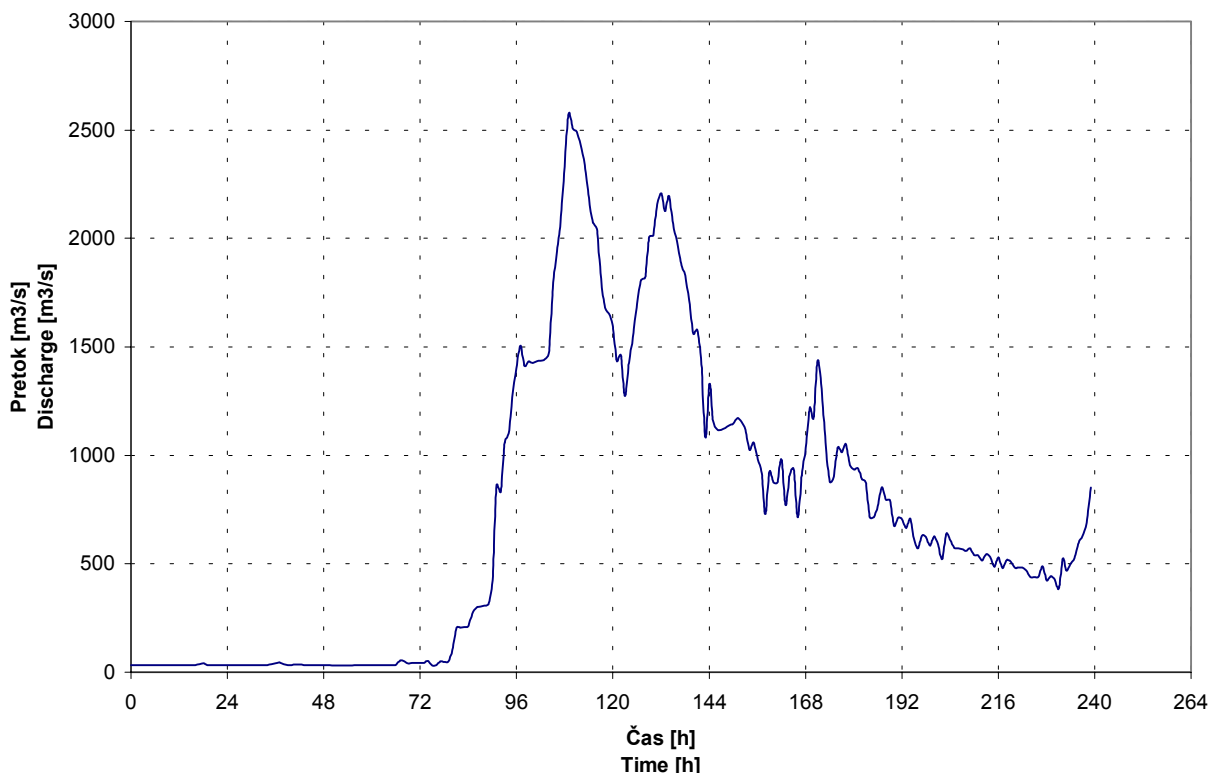
4.3 TRANSPORT AND DISPERSION OF SUSPENDED SEDIMENT DURING THE FLOOD-WAVE OF THE SOČA RIVER IN NOVEMBER, 1997

An extreme event was simulated with the model: the autumnal flood-wave of the Soča River between 6 and 14 November, 1997, when measurements of several different parameters were performed.

4.3.1 Input data

Normal winter conditions within the Gulf were taken into account, when, after a certain period of strong wind, well-mixed conditions occurred. A constant temperature of 8°C and a salinity of 37.8 ppt along the depth was supposed. An average autumnal wind from the ENE direction ($69^{\circ} 48'$) of 2.3 m/s was taken into account.

The observed flood-wave had two peaks; the discharge of the Soča River was about $2500\text{ m}^3/\text{s}$ with the first peak and about $2200\text{ m}^3/\text{s}$ with the second (Figure 4.4). Such discharges represent a flood-wave with a recurrence of approximately 5 years.



Slika 4.4. Pretoki Soče ob visokovodnem valu novembra 1997.

Figure 4.4. The Soča River discharge during the flood wave in November, 1997.

Vzorci lebdečih plavin so bili odvzeti pri pretoku okrog 1600 m³/s med obema vrhovoma vala. Gostota delcev znaša 2500 kg/m³, rezultati granulometrijske analize vzorcev pa so: srednji premer zrna D_{50} je 15 µm, premer D_{16} znaša 6.5 µm, premer D_{84} je enak 33 µm in D_{90} 40 µm. Povprečna koncentracija lebdečih plavin v vodi je znašala 360 g/m³.

Skupna količina lebdečih plavin, ki jih je v zaliv prinesla Soča med 6. in 14. novembrom tako znaša okrog 95.000 ton (Širca, 1999b), kar je slaba polovica povprečne letne količine, ki znaša nekaj nad 200.000 tonami (Širca, 1996). Za potrebe modeliranja je bila na podlagi masne bilance plavin ocenjena odvisnost med pretokom in koncentracijo lebdečih plavin, na voljo so bile namreč le meritve koncentracij ob treh različnih pretokih. Dve sta bili opravljeni pri zelo nizkih pretokih Soče (pod 100 m³/s), tretja pa pri pretoku 1600 m³/s.

Povprečna koncentracija živega srebra, izmerjena na lebdečih plavinah, je znašala 49 µg/g (Horvat et al, 1999). Skupna količina partikularnega živega srebra, ki ga je v zaliv prinesla Soča med dogodkom, tako znaša okrog 4700 kg (Širca et al, 1999b) in je precej nad povprečno letno vrednostjo (približno 1508 kg). Upoštevati pa moramo, da gre za dogodek s povratno dobo približno 5 let in je zato tako visoka vrednost pričakovana. Drugi podatek o koncentraciji živega srebra na lebdečih plavinah (41 µg/g) izvira iz meritev opravljenih junija 1995, ko je bila to največja izmerjena vrednost. V simulaciji je zato upoštevana povprečna koncentracija 40 µg/g živega srebra na lebdečih plavinah, s katero je pomnožena koncentracija lebdečih plavin.

4.3.2 Simulacija in rezultati

Izvedena je bila povsem nestacionarna simulacija za celotno trajanje visokovodnega vala (9 dni). Na sliki 4.5 so prikazane koncentracije celokupnega partikularnega živega srebra v sloju ob dnu zaliva po 96 urah simulacije, to je v času 144 ur na diagramu pretokov (slika 4.4) oz. 27 ur po najvišjem

Suspended sediment concentrations were sampled at the discharge of about 1600 m³/s between both peaks of the flood-wave. The density of the sediment particles was 2500 kg/m³, and the results of a granulometric analysis were: mean particle diameter D_{50} was 15 µm, diameter D_{16} was 6.5 µm, D_{84} was 33 µm and D_{90} , 40 µm, respectively. The average suspended sediment concentration in the water was 360 g/m³.

The total calculated amount of suspended sediment brought into the Gulf between 6 and 14, November was about 95.000 tons (Širca, 1999b). This value represents a little less than half of the annually averaged suspended sediment inflow, which is supposed to be somewhat above 200.000 tons (Širca, 1996). The relationship between the discharge and the suspended sediment concentration was estimated from the annual mass balance of suspended sediment, as there were only three measurements performed. Two were done at very low river discharge (below 100 m³/s), and the third, at the discharge of 1600 m³/s.

The average concentration of mercury bound to suspended sediment was 49 µg/g (Horvat et al, 1999). Therefore, the total amount of mercury in its particulate form carried into the Gulf by the Soča River during the observed event was about 4700 kg (Širca et al, 1999b), which significantly exceeds the annually averaged amount (about 1508 kg). However, the recurrence of such an event is about 5 years and such a high result was not unexpected. In June, 1995, when another measurement was performed, the highest concentration of mercury bound to suspended sediment was 41 µg/g. Taking into account both measurements, simulations with a value of 40 µg/g were performed, and the suspended sediment concentration was multiplied by the mercury concentrations to get the results.

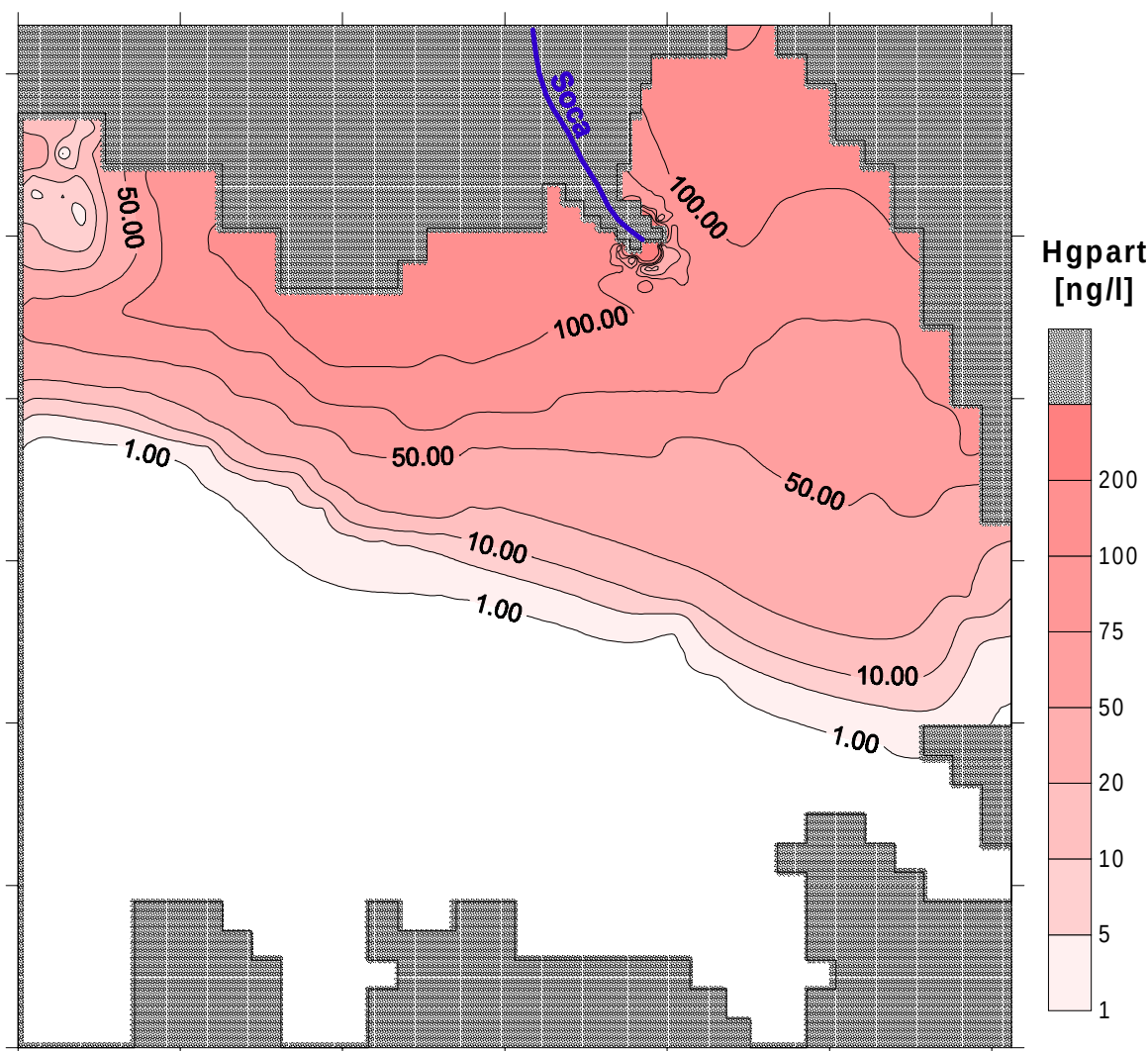
4.3.2 Simulation and results

A real time simulation for the whole flood-wave duration (9 days) was performed. Figure 4.5 shows the concentrations of total particulate mercury in the bottom layer of the Gulf after 96 hours of simulation (27 hours after the Soča River peak discharge), which is equal to the 144 hours in Figure 4.4.

pretoku Soče.

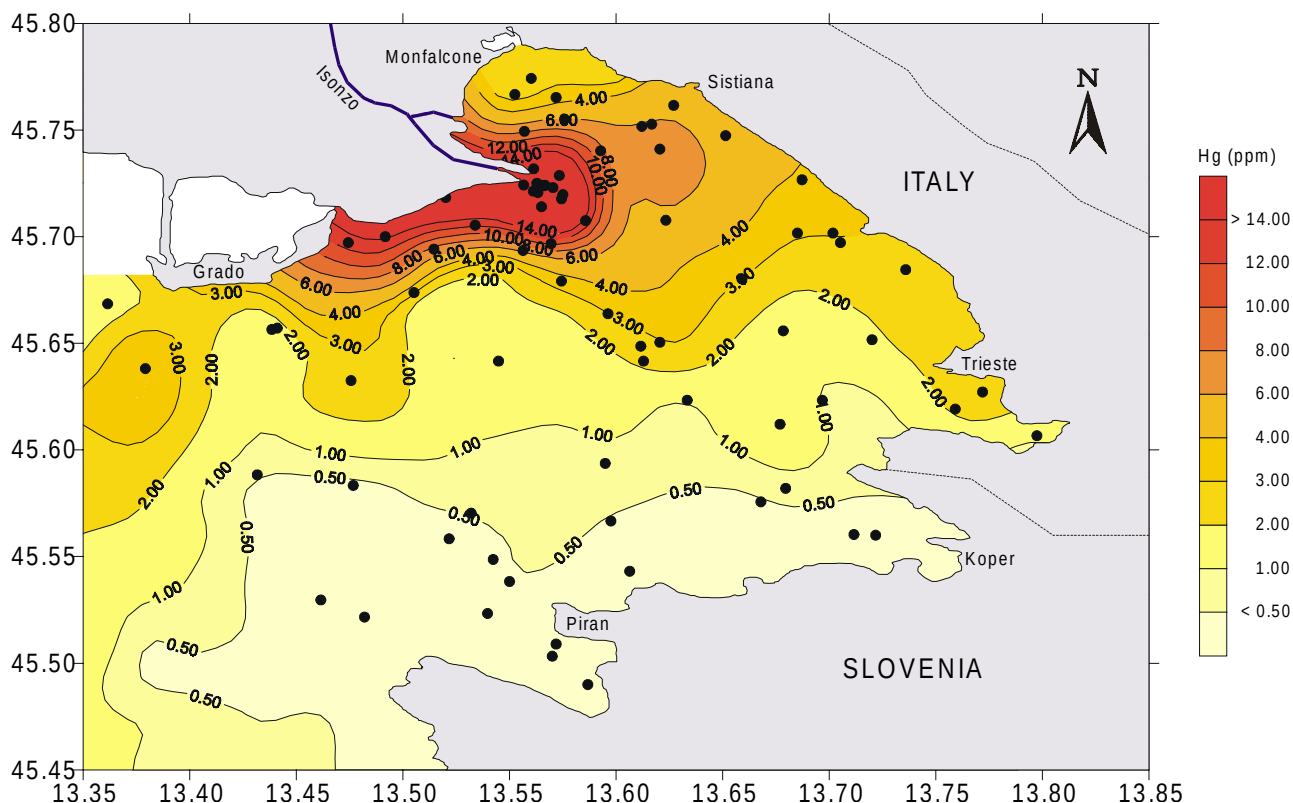
Iz rezultatov na sliki 4.5 sta vidna vpliv gibalne količine Soče, ki povzroča širjenje koncentracij proč od izliva, in vpliv šibke burje, ki obrne del dotoka ob severni obali zaliva proti zahodu. Ob upoštevanju, da večina plavin in z njimi tudi partikularnega živega srebra doteka v zaliv s Sočo in da se zaradi hitrega zmanjšanja hitrosti ob vtoku v zaliv večinoma tudi usede na dno blizu ustja Soče, je mogoče sklepati, da je količina živega srebra v sedimentu proporcionalna količini odloženega sedimenta, s tem pa tudi količini lebdečih plavin v sloju ob dnu.

Both influences, the inflow momentum of the Soča River, which spreads the plume away from the river mouth, and the influence of the weak *burja* wind, which directs part of the plume towards the west, along the coast, can be seen from Figure 4.5. As it was proven that most of the sediments and particle bound mercury is carried into the Gulf by the Soča River and as most of the suspended sediment is settled near the river mouth due to the rapid decrease of velocity in the Gulf, the concentration of mercury in the bottom sediment is presumably proportional to the amount of settled sediment, and also to the suspended sediment concentration in the bottom layer.



Slika 4.5. Z modelom izračunane koncentracije živega srebra v sloju ob dnu po 96 urah
 – simulacija visokovodnega vala Soče novembra 1997.

Figure 4.5. Simulated concentration of particulate mercury at the bottom of the Gulf after 96 hours
 – simulation of the Soča River flood-wave in November, 1997.



Slika 4.6. Merjene koncentracije živega srebra v sedimentu na dnu Tržaškega zaliva v $\mu\text{g/g}$ suhe teže (Covelli et al, 1999b).

Figure 4.6. Measured concentration of mercury in the bottom sediment of the Gulf of Trieste in $\mu\text{g/g}$ dry weight (source: Covelli et al, 1999b).

Meritve, ki bi omogočale kvantitativno primerjavo, še niso bile opravljene, vsekakor pa je mogoča kvalitativna primerjava koncentracij živega srebra v sloju ob dnu (slika 4.5) z merjenimi koncentracijami živega srebra v sedimentu na dnu (slika 4.6). Iz podobnosti slik lahko sklepamo na kvalitativno pravilnost rezultatov modela, za kvantifikacijo primerjave pa bodo potrebne dodatne meritve koncentracij plavin in partikularnega živega srebra v zalivu med in neposredno po visokovodnem valu Soče, hkrati pa tudi v sami Soči. Slednje bi pripomoglo tudi k bolj točni ugotovitvi relacije med pretokom in količino lebdečih plavin v rečni vodi, ki je bila pri tokratnem računu opravljena s pomanjkljivimi podatki.

Due to lack of measurements, a quantitative comparison was not possible; however, a qualitative comparison of mercury concentrations in the bottom layer of the Gulf (Figure 4.5) with the concentrations of mercury in the bottom sediment (Figure 4.6) was performed. A good qualitative accuracy of the model simulations can be concluded from the similarity of concentration patterns; however, additional measurements of suspended sediment concentrations and particulate mercury in the Gulf during and after a similar flood-wave are needed to quantify the comparison. Measurements of suspended sediment in the Soča River are also of great importance, as they would contribute to a more accurate relationship between the Soča River discharge and sediment concentration.

4.4 MODELIRANJE RESUSPENDIRANJA SEDIMENTA Z DNA ZALIVA OB MOČNEM VETRU V ZIMSKEM ČASU

Na območju Tržaškega zaliva predvsem v zimskih razmerah pogosto pihajo močni vetrovi. Burja doseže v sunkih hitrosti tudi nad 30 m/s, za modeliranje pa je pomembnejši podatek, da lahko s hitrostjo 16 m/s piha neprekinjeno tudi več dni. Z modelom smo simulirali večdnevno obdobje močnega vetra, za katerega je velika verjetnost, da se pojavlja vsako leto. Po statističnih podatkih je bila primerna hitrost vetra 13 m/s, smer ENE (66° 40'), trajanje pa 2 dni. Takšne razmere se lahko v zalivu pojavljajo večkrat vsako zimo.

4.4.1 Podatki

V simulaciji je bil upoštevan povprečni zimski pretok Soče 150 m³/s. Količino lebdečih plavin, ki ob tem razmeroma nizkem pretoku Soče doteka v zaliv, smo namerno izključili, da bi bila iz rezultatov jasno vidna količina resuspendiranega materiala. Ostali podatki simulacije so: gostota sedimenta v suhem stanju 2500 kg/m³, poroznost 0.6, srednji premer zrna D_{50} 15 µm, premeri D_{16} 6.5 µm, D_{84} 33 µm in D_{90} 40 µm. V zalivu so predpostavljene normalne poznojesenske oz. zimske razmere, premešano stanje z enakomerno temperaturo 7.8 °C in slanostjo 37.8 promila.

4.4.2 Rezultati simulacije

Veter hitrosti 13 m/s povzroči v zimskih nestratificiranih razmerah precej močno gibanje vode po vsej globini. V plitvejšem delu zaliva ob severni obali dosežejo hitrosti ob dnu okrog 15 do 20 cm/s, povprečne hitrosti po globini pa do 35 cm/s. Posledica tako močnih tokov so velike strižne napetosti ob dnu, ki že brez dodatnega vpliva valovanja povzročajo resuspendiranje sedimenta.

4.4 RESUSPENSION OF BOTTOM SEDIMENT DUE TO STRONG WIND IN WINTER CONDITIONS

Strong winds often blow above the Gulf of Trieste in winter conditions. Gusts of *burja* wind sometimes reach over 30 m/s, and, even more important for the purpose of modelling, the *burja* wind can blow with a velocity of 16 m/s for several days continuously. A longer insert with the high probability of occurrence every year was simulated. According to the statistical data, an appropriate wind speed of 13 m/s from the ENE (66° 40') for a duration of two days was chosen. Such conditions may occur above the Gulf several times each winter.

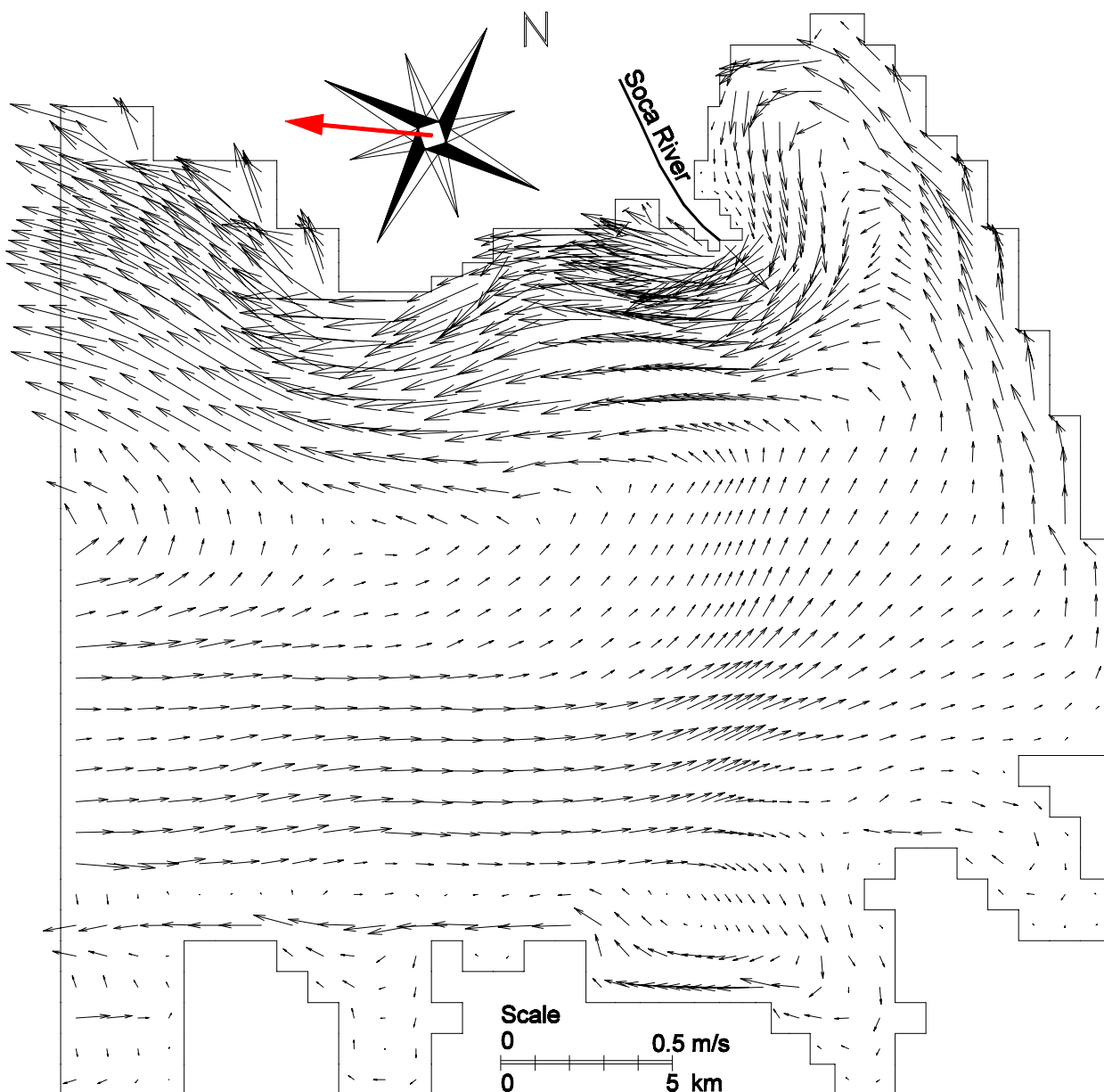
4.4.1 Input data

The seasonally averaged Soča River discharge during the winter (150 m³/s) was taken into account. With this relatively low discharge, the inflow of suspended sediment with the Soča River was set to zero to observe the phenomenon (resuspension) more clearly.

Other input data for the simulation were: sediment density 2500 kg/m³, porosity 0.6, the mean diameter of sediment particles, D_{50} , was set to 15 µm, the diameter D_{16} was 6.5 µm, D_{84} was 33 µm and D_{90} was 40 µm. Normal late autumn / winter conditions within the Gulf were supposed: well mixed conditions, a constant temperature of 7.8 °C and a salinity of 37.8 ppt along the depth.

4.4.2 Results

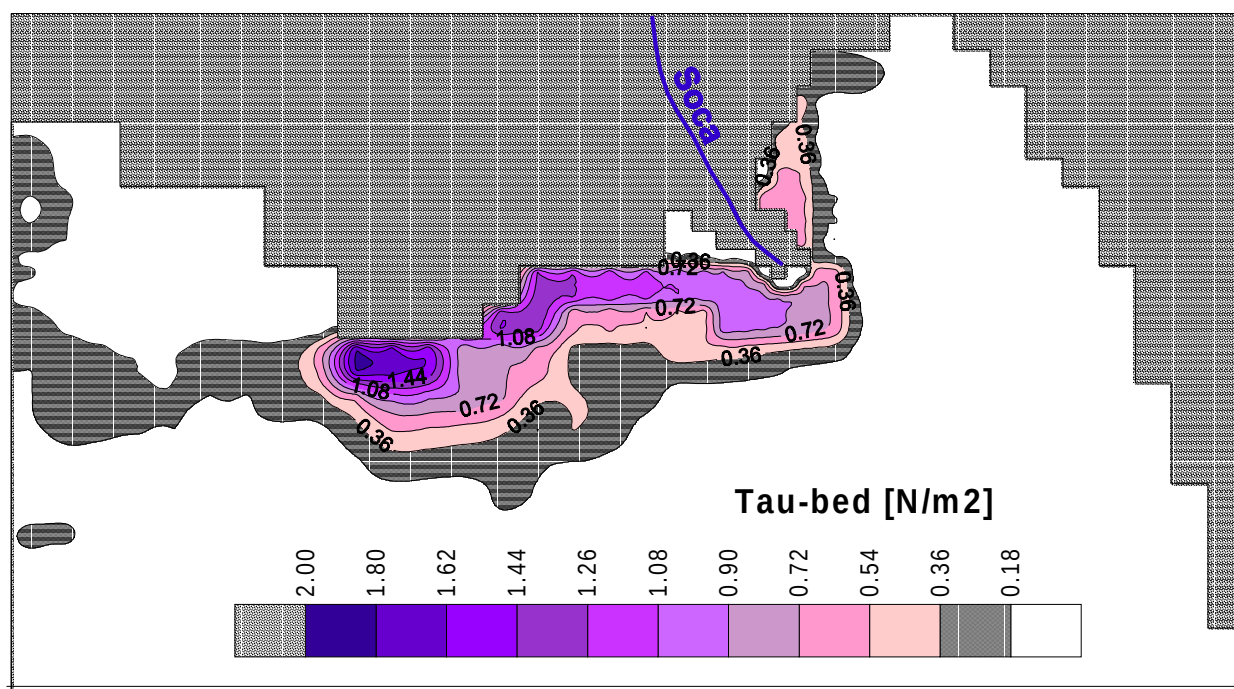
A relatively strong motion of water along the whole water column was caused by the strong wind in non-stratified winter conditions. Bottom layer velocities in the shallower part of the Gulf near the northern shore were about 15 to 20 cm/s, while depth averaged velocities reached values up to 35 cm/s. In consequence, critical shear stress at the bottom was exceeded, which resulted in the resuspension of the bottom sediment even without taking into account the shear stress due to wind-driven waves.



Slika 4.7. Globinsko povprečne hitrosti – ekstremne zimske razmere (veter ENE 13 m/s).
 Figure 4.7. Depth averaged velocities – extreme winter conditions (wind ENE 13 m/s).

Oscilatorno gibanje valov, nastalih zaradi vetra, strižne napetosti še poveča. Z modelom izračunana višina valov v zalivu znaša na odprtem robu okrog 1.80 m in se zmanjšuje proti vzhodni obali zaliva. Skupne strižne napetosti ob dnu presegajo kritične v večjem delu plitvega dela zaliva ob severni obali, kjer se pojavlja močna resuspenzija materiala. Izračunana kritična strižna napetost, ob kateri se začne resuspendiranje materiala, je pri izbranih parametrih 0.179 N/m^2 in je lokalno tudi do desetkrat presežena.

The oscillatory motion of wind-driven waves additionally increases bottom shear stress. Simulated wave-height at the open boundary was about 1.80 m, decreasing towards the eastern shore of the Gulf. Due to the combined influence of currents and waves, critical bed shear stress is exceeded in the majority of the shallower parts of the Gulf along the northern coast, where strong resuspension occurs. Calculated critical bed shear stress with chosen parameters, 0.179 N/m^2 , was locally exceeded up to ten times.



Slika 4.8. Strižne napetosti ob dnu zaliva – veter ENE 13 m/s.
Figure 4.8. Bottom shear stress in the Gulf – wind ENE 13 m/s.

Koncentracije resuspendiranih lebdečih plavin v sloju ob dnu dosegaajo vrednosti do 150 g/m^3 , na večjem delu območja ob severni obali pa presegajo 50 g/m^3 , kar je povprečna letna koncentracija lebdečih plavin, ki jih v zaliv prinese Soča.

Z modelom smo izračunali debelino odnešenega oz. odloženega materiala na območju premeščanja sedimenta ob severni obali zaliva (slika 4.9). Ob statistično razmeroma pogostem dogodku, debelina erozije dna in odloženega materiala lokalno presegata 1 cm, iz nove razporeditve sedimenta po končani simulaciji pa je razvidno, da močni zimski vetrovi povzročajo premeščanje sedimenta od ustja Soče ob severni obali zaliva proti zahodu.

V poglavju 4.3 smo pokazali, da se lebdeče plavine, ki jih v zaliv prinese Soča, odlagajo razmeroma blizu ob ustju. Iz meritev je razvidno, da je vsebnost živega srebra v plavinah Soče višja od vsebnosti v sedimentu na dnu zaliva (povprečna vrednost meritev novembra 1997 znaša $49 \text{ } \mu\text{g/g}$ (Horvat et al, 1999), v zalivu ob ustju pa $25\text{--}30 \text{ } \mu\text{g/g}$ (Covelli

Suspended sediment concentrations in the bottom layer due to resuspension reached up to 150 g/m^3 and exceeded 50 g/m^3 , which is the annually averaged concentration in the water of the Soča River, within most of the area near the northern shore of the Gulf.

Erosion and deposition thickness in the area of bottom sediment displacement along the northern shore of the Gulf was also modelled (Figure 4.9). With a statistically relatively frequent event, the thickness of the eroded and deposited material exceeds 1 cm locally. It is also evident from the distribution of bottom sediment after the simulation, that the bottom sediment was displaced from the river mouth along the northern shore towards the west by strong winter winds.

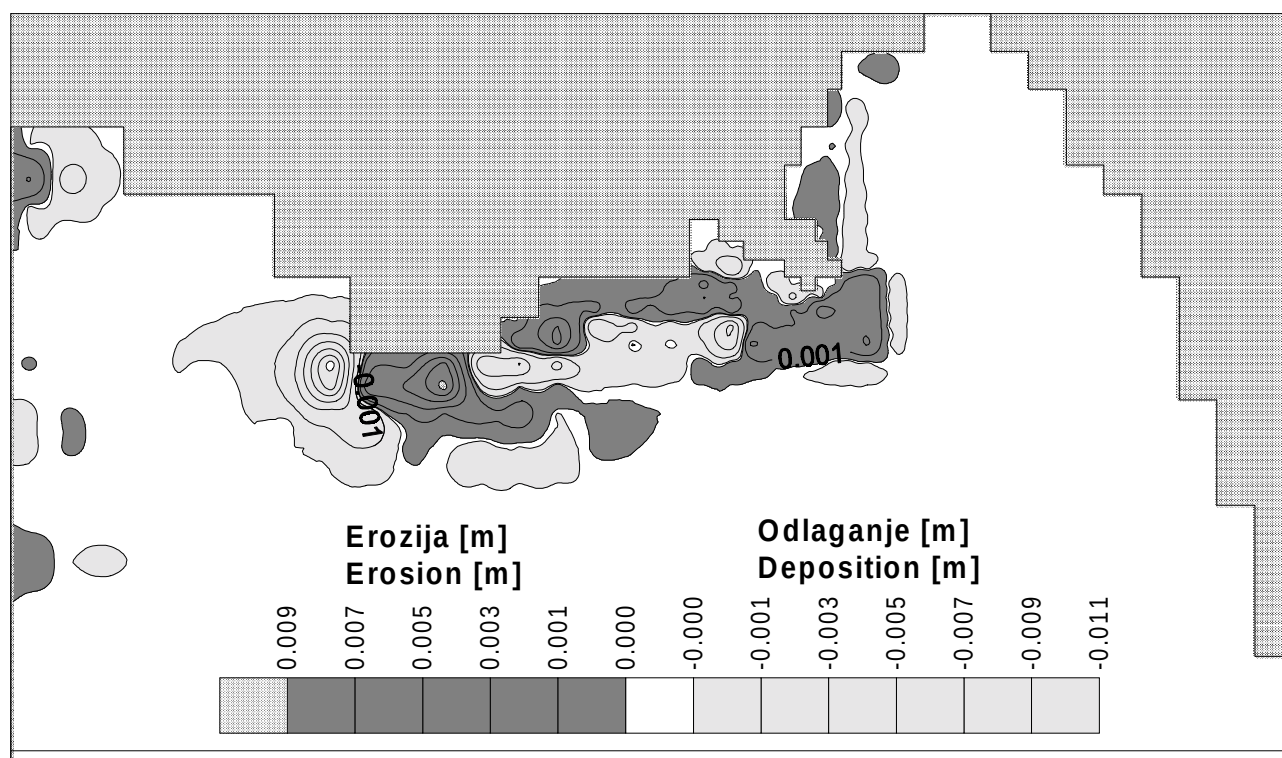
It was stated in Chapter 4.3, that the suspended sediment brought to the Gulf by the Soča River is mostly deposited near the river mouth. It is also evident from the measurements, that the mercury concentration in the suspended sediment of the Soča River is higher than the concentration in the bottom sediment of the Gulf (an average value of $49 \text{ } \mu\text{g/g}$ was measured in the Soča River in November, 1997 (Horvat et al, 1999), while in the bottom sediment near the river mouth, it was $25\text{--}30 \text{ } \mu\text{g/g}$ (Covelli et al, 1999b)).

et al, 1999b)). Iz navedenega lahko sklepamo, da mora biti porazdelitev koncentracij živega srebra v sedimentu podobna porazdelitvi sedimenta po premeščanju, saj so v 'svežem' sedimentu, premeščenem od ustja Soče proti zahodu, koncentracije živega srebra višje. Če primerjamo porazdelitev sedimenta po končani simulaciji (slika 4.9) s sliko merjenih koncentracij živega srebra v sedimentu na dnu (slika 4.6), podobnost obeh slik potrjuje kvalitativno pravilnost rezultatov modeliranja, za kvantifikacijo pa bodo potrebne dodatne meritve (*sediment trap*).

Z rezultati simulacije smo celo uspeli pojasniti pojav, ki iz samih meritev ni bil povsem razumljiv – visoke koncentracije živega srebra v sedimentu ob vhodu v Laguno di Grado. Rezultati simulacije kažejo, da na tem mestu transportna sposobnost upade, ker se dno zaliva naglo poglobi. Posledica je naglo usedanje lebdečih plavin z višjo vsebnostjo živega srebra, prinesenih od ustja Soče, kar je verjetni vzrok za višje koncentracije živega srebra v sedimentu na tem mestu.

Therefore, it can be concluded that the distribution of mercury in the bottom sediment must be similar to the distribution of settled sediment after it has been displaced, as the concentration of mercury is higher in the 'fresh' sediment carried from the river mouth towards the west. Again, the great similarity between the distribution of sediment after the simulation (Figure 4.9) and the concentration of mercury in the bottom sediment of the Gulf (Figure 4.6) confirms qualitatively the correctness of the model results. However, additional measurements with a sediment trap will be needed to quantify the comparison.

The results of the simulation have even helped to clarify a phenomenon which was not completely clear from the measurements – high concentrations of mercury in the bottom sediment at the entrance of Laguna di Grado (Figure 4.6). At this location, the simulation showed a high decrease of transport capability due to the rapid deepening of the Gulf. As a consequence, an immediate settling of mercury rich sediment brought from the river mouth occurs, which is most likely the reason for the increased mercury concentration at the observed location.



Slika 4.9. Debelina odnešenega / nanešenega materiala, veter ENE 13 m/s.
Figure 4.9. Erosion / deposition thickness - wind ENE 13 m/s.

5. ZAKLJUČKI IN NAPOTKI ZA NADALJNJE DELO

Z izpopolnitvijo modela in izvedenimi simulacijami smo se modelu, s katerim bi bilo mogoče simulirati celotno gibanje živega srebra v morskem okolju vključno s transportom in vsemi procesi pretvorb, približali za pomemben korak.

Izdelan in verificiran je bil sedimentacijski modul z upoštevanjem vpliva stratifikacije, usedanja in resuspendiranja delcev, ki je uporaben kot del ekološkega modela in za modeliranje drugih primerov iz inženirske prakse.

Model je bil dopolnjen z modulom za račun transporta živega srebra v več različnih oblikah in dveh medijih in je pripravljen za nadaljnjo vgradnjo specifičnih robnih pogojev in enačb procesov pretvorb živega srebra.

Izdelan je bil scenarij za dolgotrajne simulacije, v katerem je mogoče uporabiti kombinacijo sezon in krajših vložkov, ki bistveno prispevajo k transportu in posredno tudi procesom pretvorb živega srebra v Tržaškem zalivu, pridobili smo podatke, potrebne za dolgotrajne simulacije (veter, temperatura in slanost v zalivu, pretoki, temperatura in koncentracije živega srebra v Soči).

Rezultati izvedenih simulacij se kvalitativno dobro ujemajo z meritvami, kar dokazuje pravilen pristop in razumevanje problematike, kljub temu da kvantitativna primerjava ni bila vedno mogoča. Dosežen je velik napredek v primerjavi z 2D modeliranjem. Z rezultati modeliranja smo celo uspeli pojasniti pojav višjih koncentracij živega srebra v sedimentu ob vhodu v Laguno di Grado, ki iz samih meritev ni bil povsem jasen.

Prednost 3D modela pred 2D modelom je kljub večjim zahtevam glede količine in kakovosti vhodnih podatkov nedvoumna; s tridimenzionalnim modelom je mogoče opisati in izračunati porazdelitev vseh parametrov tudi

5. CONCLUSIONS AND FURTHER RESEARCH

With the upgrading of the model, a significant step forward was made towards a model which would be capable of simulating complete mercury cycling in the marine environment, including the transport of mercury and all its transformational processes.

A new sediment transport module which is capable of simulating stratified conditions, sediment settling and resuspension was developed. The module can be used as a part of an ecological model, as well as for solving other different practical problems connected to sediments.

The model was upgraded with a new module which can simulate the transport of mercury in several different forms and in two different media. The module is ready for an additional upgrade with the specific boundary conditions, as well as the specific mercury transformation equations.

A new scenario for long-term simulations where a combination of seasons and shorter inserts is possible was developed. These inserts contribute greatly to the transport of mercury and also indirectly to the transformational processes in the Gulf. A large amount of data needed for the long-term simulations was collected (wind, temperature and salinity distribution in the Gulf; discharge, temperature and mercury concentration of the Soča River).

Although a quantitative comparison was not always possible, qualitatively, a good agreement between the simulated and measured results was achieved. This confirms the correct understanding, as well as the correct assessment of the problem. A significant step forward was made in the comparison with 2D modelling. Simulations even helped to clarify the reason for high concentration of mercury in the bottom sediment at the entrance to the Laguna di Grado, which was not completely understandable from the measurements.

In spite of demanding more input data of a higher accuracy, the advantage of the 3D model over the 2D model is evident, as with the 3D model it is possible to simulate the distribution of all the parameters along the

po globini.

Glavni vzrok visokih koncentracij živega srebra ob severni obali zaliva je veter, ki povzroča resuspendiranje sedimenta in njegov transport ob severni obali zaliva proti zahodu. Vzrok pojava iz meritev ni razviden, rezultati modela pa so ga nedvoumno dokazali. To je hkrati potrditev predvidevanja, da je resuspendiranje zelo pomemben dejavnik pri transportu živega srebra in ga je pri modeliranju treba upoštevati.

Kratki vložki močnega vetra in visokovodnih valov Soče so zelo pomembni za pravilen račun transporta živega srebra v Tržaškem zalivu. Resuspendiranje se dogaja ob močnih vetrovih, večina lebdečih plavin in na njih vezanega živega srebra pa doteka v zaliv ob višjih pretokih Soče.

Izločanje živega srebra iz pornih vod v sedimentu na dnu zaliva (*benthic flux*) je pomembno in ga je v prihodnje treba vključiti v model. Trenutno so na voljo le meritve v eni točki, kar za modeliranje ne zadošča, iz meritev pa je jasno razvidno, da so koncentracije MMHg v pornih vodah višje kot v plavinah Soče in bistveno prispevajo k celotni količini MMHg v zalivu.

Za uspešnejše in bolj točno modeliranje transporta in procesov pretvorb živega srebra v prihodnje so potrebne še številne izboljšave modela in dodatne meritve.

Numerični difuziji, ki precej vpliva na točnost rezultatov dolgotrajnih simulacij, se je treba izogniti z uporabo numerične sheme višjega reda točnosti in/ali izpopolniti metodo sledenja delcev, da jo bo mogoče uporabiti v dolgotrajnih simulacijah.

V 3D model je treba vgraditi enačbe procesov pretvorb med posameznimi oblikami živega srebra. Spoznanja ob izpopolnjevanju modela in izvedenih simulacijah kažejo, da zahteva prenos enačb v 3D model dodatne raziskave v zvezi z dinamiko procesov pretvorb v nestacionarnem okolju.

Za nadaljnjo verifikacijo in kalibracijo modela so potrebne nadaljnje meritve

water column.

Wind was found to be the main reason of increased mercury concentration along the northern coast of the Gulf. The reason itself is not clearly visible from the measurements; however, it was pointed out by the results of the simulation. At the same time, our supposition about the importance of resuspension in the mercury transport process has been confirmed.

Short inserts of strong wind and the Soča River flood-peak inserts are very important for an accurate simulation of the mercury transport in the Gulf of Trieste. Resuspension is mostly caused by strong winds and the most of suspended sediment is carried into the Gulf with the higher discharges of the Soča River.

Mercury release from the pore water (*benthic flux*) is of great importance and must be included in the model in the future. At the present state, measurements at a single location only are available, which is not sufficient for the purpose of modelling. Still it is clearly evident from the measurements that the concentration of MMHg in the pore water is higher than in the Soča River suspended sediment. Therefore, the *benthic flux* contributes greatly to the total amount of MMHg in the Gulf.

Numerous further improvements of the model, as well as additional measurements, are needed in the future to simulate the transport and processes of mercury with higher accuracy.

False diffusion, which significantly affects the results of long-term simulations, must be excluded from the model. A numerical scheme of a higher order of accuracy must be used and/or a particle-tracking method must be improved and used with the long-term simulations.

Mercury transformation equations must be included in the 3D model. During the improvement of the 3D model it was pointed out that additional research about the dynamics of the transformation processes in non-steady state conditions is needed to include the processes in the 3D model.

Additional measurements of mercury concentrations in the water column, suspended sediment, bottom sediment, pore water and biota in different seasons is needed for further calibration and verification of the model. In

koncentracij živega srebra v vodnem stolpcu, lebdečih plavinah, sedimentu na dnu, pornih vodah in organizmih v zalivu v različnih obdobjih koledarskega leta. Potrebne so še dodatne meritve koncentracij lebdečih plavin v Soči ob različnih pretokih za bolj točno določitev medsebojne odvisnosti. Potrebne so tudi dodatne meritve koncentracij vseh oblik živega srebra v vodi, plavinah in v sedimentu rek Soče in Idrijce v različnih obdobjih leta in ob različnih pretokih, hkrati z meritvami koncentracij v coni mešanja sladke in slane vode, kjer del živega srebra, vezanega na delce, prehaja v raztopljeno obliko.

Poleg meritev koncentracij je nujno potrebno tudi bolj poglobljeno poznavanje biogeokemijskih procesov pretvorb v celotnem sistemu Idrijca – Soča – Tržaški zaliv, ki so odvisne od lokacije, koncentracije živega srebra, temperature in drugih okoljskih parametrov.

Problemатiko onesnaževanja z živim srebrom je treba obravnavati s čim širšega vidika. Spoznati je treba transport živega srebra po zraku, izpiranje materiala po rečnem sistemu Idrijca – Soča, vključno z odlaganjem in vnovičnim izpiranjem s poplavnih območij, vse do sedimenta na dnu zaliva. Končni cilj celotnega sklopa modeliranja je ugotovitev koncentracij živega srebra v ribah in v drugih morskih organizmih, ki predstavljajo pomemben vir prehrane in dohodka okoliškemu prebivalstvu in tudi širšemu zaledju, ugotovitev posledic onesnaževanja s sociološko-ekonomskega vidika in iskanje ustreznih rešitev.

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addition, measurements of suspended sediment concentration in the Soča River at different discharges is needed to determine the relationship with greater accuracy. Measurements of the concentration of all forms of mercury in the water, suspended and bottom sediment of the Soča and Idrijca Rivers during different seasons and different discharges are also needed, together with the mercury concentration in the freshwater / saltwater mixing zone, where a portion of sediment bound mercury is being released into its dissolved form.

Besides measurements, a deeper knowledge of biogeochemical transformation processes throughout the entire system: the Idrijca River – the Soča River – the Gulf of Trieste is required. The processes depend on the location, mercury concentration, temperature and other environmental parameters.

The problem of mercury pollution must be observed in wider aspects. The amount of mercury transported through the air must be known, as well as the amount of mercury being washed away by the Soča and Idrijca Rivers, including the deposition and re-entering into suspension at the flooding areas. Mercury must be observed all the way from its source until it has settled at the bottom of the Gulf. The final goal of the research and modelling is to determine the mercury concentration in fish and other marine organisms. These represent an important source of food and also an important economic category for the people living near the Gulf, as well as for the people in the hinterland. The consequences of mercury pollution from the socio-economic viewpoint must be determined and the appropriate solutions must be found.

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NAVODILA ZA PRIPRAVO PRISPEVKOV

1. Prispevki za Acta hydrotechnica

- 1.1 Acta hydrotechnica je znanstveno-strokovna periodična publikacija, katere izdajatelj in založnik je Univerza v Ljubljani, Hidrotehnična smer Fakultete za gradbeništvo in geodezijo (FGG), ki jo sestavljajo Katedra za mehaniko tekočin z laboratorijem (LMTe), Katedra za splošno hidrotehniko (KSH) in Inštitut za zdravstveno hidrotehniko (IZH). Predstavniki omenjenih enot tudi sestavljajo izdajateljski odbor revije.
- 1.2 Acta hydrotechnica izhaja dvakrat na leto v obliki zaporednih števil, dodatno razvrščenih v letnik.
- 1.3 Acta hydrotechnica je namenjena objavam prispevkov strokovnjakov in raziskovalcev s področja vodarstva in hidrotehnike. Acta hydrotechnica objavlja prispevke s področja vodarstva in hidrotehnike v obliki izvirnih in preglednih znanstvenih člankov, preliminarne objav in strokovnih člankov.
- 1.4 Prispevki so napisani enakovredno v slovenskem in angleškem jeziku, kar zagotavlja ohranjanje in razvijanje slovenskega strokovnega izrazoslovja na področju vodarstva in hidrotehnike ter obenem zagotavlja berljivost revije v tujini. Dolžina prispevka je omejena na 30 000 znakov. Dolžina prispevka, ki je povzetek magistrske naloge ali doktorskega dela, je omejena na 100 000 znakov. Prednost pri objavi imajo krajši prispevki.
- 1.5 Prispevke je treba oddati v elektronski in pisni obliki na uredništvo Acta hydrotechnica.
- 1.6 Vsi prispevki so oblikovno podvrženi uredniški recenziji v skladu s temi navodili in vsebinsko podvrženi recenziji dveh strokovnjakov s področja prispevka.
- 1.7 Pri oblikovanju prispevkov za Acta hydrotechnica je treba upoštevati slovenske standarde za dokumentacijo in informatiko.
- 1.8 Za vsebino prispevkov in prevod v angleški jezik odgovarjajo avtorji.
- 1.9 Vsi prispevki so lektorirani, tako slovensko kakor tudi angleško besedilo.

2. Oblikovanje prispevkov za Acta hydrotechnica

- 2.1 Vsak prispevek mora biti sestavljen iz naslednjih enot, enakovredno podanih v slovenskem in angleškem jeziku:
 - ☐ naslov prispevka
 - ☐ podatki o avtorju ali avtorjih
 - ☐ izvleček (abstract) in ključne besede (key-words)
 - ☐ glavno besedilo
 - ☐ zahvala (acknowledgements) naročniku naloge, raziskave ali študije (neobvezno)
 - ☐ pregled uporabljenih izrazov (terminology) in oznak (notations) (neobvezno)
 - ☐ viri (references)Njihov natančnejši opis je podan v naslednjih odstavkih.
- 2.2 Naslov prispevka naj bo jasen, jedrnat in naj izraža bistvo prispevka. Dolžina naslova je največ 90 znakov, razen ko gre za povzetke magistrskih in doktorskih del, kjer je lahko naslov prispevka enak uradnemu naslovu dela.
- 2.3 Podatki o avtorju obsegajo ime in priimek, opis znanstvene strokovne stopnje in poln naslov delovnega mesta.
- 2.4 Vsak prispevek mora spremljati izvleček (abstract) v obsegu okoli 150 besed v vsakem od obeh jezikov. Izvlečka morata strnjeno podati celoten prispevek vključno z zaključki. Avtor naj navede do 8 ključnih besed.
- 2.5 Glavno besedilo naj bo razdeljeno po decimalnem sistemu (1. PRVO POGLAVJE, 1.1 PRVO PODPOGLAVJE, 1.1.1 Zadnja poddelitev). Vire v besedilu navedemo z imenom avtorja in letnico objave (Manning, 1892), (Strickler & Nikuradse, 1924b), (Einstein et al., 1951), (Colebrook, 1932; 1934). Merske enote naj bodo v skladu z veljavnim sistemom SI. Datum naj bo podan po naslednjem vrstnem redu : dan-mesec-leto (23.4.1998).

Kratice in opombe pod črto naj se uporabljajo le izjemoma.

Ilustracije (preglednice in slike) v besedilu naj bodo skozi vse besedilo enotno oštevilčene z arabskimi številkami in naj se ne okrajšujejo (preglednica 1, slika 14, Table 2, Figure 4). Praviloma mora biti ilustracija dvojezična. Če je ilustracija privzeta iz drugega že objavljenega dela, je potrebno ob njenem opisu dodati tudi njen izvor.

Enačbe v besedilu naj bodo oštevilčene z arabskimi številkami v okroglih oklepajih enotno skozi vse besedilo, pri daljših prispevkih (več kakor 1 avtorsko polo) lahko tudi enotno za vsako poglavje posebej. Navajanje enačb naj v besedilu ne bo okrajšano (enačba (11), enačba (2.17)).

2.6 V besedilu uporabljeni viri morajo biti navedeni v abecednem vrstnem redu in neoštevilčeno, na koncu prispevka, enotno za oba jezika. Če je vir pisan v jeziku, ki ni angleški, naj naslovu vira v oklepaju sledi prevod naslova v angleščino, na koncu navedbe pa dostavek, v katerem jeziku je pisan, npr. (in Slovenian). Glede na vrsto mora avtor navesti vire takole:

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