© *Acta hydrotechnica* **19/30 (2001)**, Ljubljana
ISSN 1581-0267

UDK / *UDC*: 504.4:519.61/.64:546.49:551.46(262.3)
Izvirni znanstveni prispevek / *Original scientific paper*

Prejeto / *Received*: 25.8.2001
Sprejeto / *Accepted*: 21.12.2001

DOLGOTRAJNA 3D SIMULACIJA TRANSPORTA IN DISPERZIJE ŽIVEGA SREBRA V TRŽAŠKEM ZALIVU
LONG-TERM 3D SIMULATION OF THE TRANSPORT AND DISPERSION OF MERCURY IN THE GULF OF TRIESTE

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Za dolgotrajno simulacijo transporta in disperzije živega srebra v raztopljeni in na delce vezani obliki smo dopolnili obstoječi tridimenzionalni matematični model PCFLOW3D, s katerim je mogoče upoštevati gibanje vode zaradi vpliva vetra, plimovanja in gibalne količine rek, ki vtekajo v zaliv ter stratifikacijo. Zbrani in prikazani so podatki o temperaturnih in slanostnih razmerah ter vetru na območju Tržaškega zaliva. Ta se skupaj s podatki o pretoku, temperaturi ter vsebnosti živega srebra v vodi in na delcih lebdečih plavin, ki dotekajo v zaliv s Sočo, predstavljajo vhodne podatke modela. Z izdelanim scenarijem za dolgotrajne simulacije, ki temelji na sezonsko povprečnih vrednostih posameznih parametrov in z dodatnimi krajšimi vložki močnega vetra in visokih pretokov Soče smo nadomestili dosedanji način simulacij s povprečnimi letnimi vrednostmi. Za verifikacijo in umerjanje izpopolnjenega modela smo uporabili meritve in opazovanja iz let 1995 – 1997. Čeprav nekateri kompleksni procesi pretvorb živega srebra še niso povsem raziskani in jih zato ni bilo mogoče upoštevati pri simulacijah, je doseženo kvalitativno dobro ujemanje rezultatov in meritev. Kjer je bila mogoča kvantitativna primerjava, je ujemanje rezultatov v okviru faktorja dve.
Ključne besede: *živo srebro, matematično modeliranje, 3D model,Tržaški zaliv*

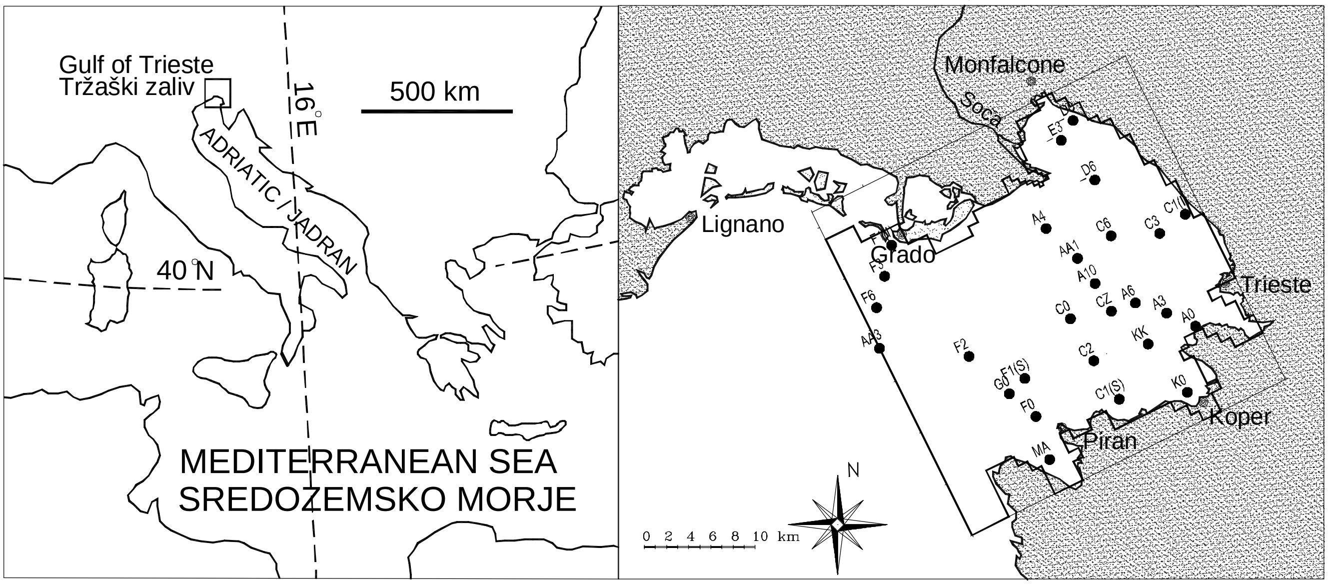
An existing three-dimensional mathematical model PCFLOW3D was upgraded to simulate long-term transport and the dispersion of mercury in its dissolved and particulate form. Hydrodynamics due to wind, tidal forcing and river inflow momentum can be simulated, and stratified conditions can be taken into account. Data on temperature and salinity fields and winds in the Gulf of Trieste, Soča River discharges, suspended sediment concentrations and temperatures were collected and interpreted. These data, together with measurements of 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 model. A scenario for long-term simulations on the basis of seasonally averaged parameters and a few shorter inserts of strong wind and high discharges of the Soča River was developed as a substitute for simulations based on annual averaged input data. Measurements and observation data from 1995 – 1997 were applied to verify and calibrate the PCFLOW3D model. Although some complex mercury transformation processes are not well known and were therefore not taken into account in the simulations, an acceptable 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 was attained.
Key words: *mercury, mathematical modelling, 3D model, Gulf of Trieste.*

1. UVOD

Tržaški zaliv, skrajni severovzhodni del Severnega Jadrana, obsega območje v obsegu 25 x 30 km (slika 1). Povprečna globina znaša okrog 16 m, v najglobljem delu pa doseže 25 m. Meritve v zalivu kažejo močno povišane koncentracije živosrebrovih (Hg) spojin v vodi, sedimentu in vodnih organizmih. Koncentracije v naravnem zaledju so v vodi in organizmih Tržaškega zaliva presežene za red, v sedimentu pa celo za dva reda velikosti. Občasne anoksije v globljih plasteh zaliva lahko pospešijo proces metilacije Hg, ki v metilirani obliki škodljivo vpliva na celotno prehransko verigo in s tem predvsem na okoliško prebivalstvo. Raziskave dokazujejo, da je glavni vir onesnaženja z živim srebrom v Tržaškem zalivu zdaj že opuščeni rudnik v Idriji. V sedimentu in lebdečih plavinah Idrijce in Soče so koncentracije Hg še vedno zelo visoke, obe reki pa to živo srebro odnašata v Tržaški zaliv.

1. INTRODUCTION

The Gulf of Trieste is situated in the eastern part of the Northern Adriatic Sea. It covers an area of about 25 x 30 km (Figure 1). The average depth is about 16 m and reaches 25 m in the central part. Recent measurements in the Gulf have shown greatly increased mercury (Hg) concentrations in the water, sediment and some marine organisms. 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. Occasional anoxia at the bottom of the Gulf may increase the methylation of Hg; thus, there is a potential impact on the humans living near the Gulf. Recent studies have shown that the former Idrija Mercury Mine, where mining was active for about 500 years, is the main source of the Hg pollution in the Gulf of Trieste. The suspended and bottom sediment of both rivers, the Idrijca River and the Soča River is highly contaminated with the Hg, which is carried away to the Gulf of Trieste.



Slika 1. Lega Tržaškega zaliva (levo), definicijsko območje modeliranja in merske točke v Tržaškem zalivu (desno).
Figure 1. The Gulf of Trieste: location (left) and the extent of the computational domain and measuring points (right).

Še 10 let po zaprtju rudnika v Idriji se koncentracije živega srebra v rečnih plavinah ter vodi in sedimentu Tržaškega zaliva niso znatno znižale (Horvat et al. 1999; Horvat et al. 1998, Žagar in Širca, 2001). Zato je v teku obsežna raziskava o kroženju živega srebra v Tržaškem zalivu, pri kateri za določitev fizikalnih, bioloških in kemičnih parametrov poleg meritev uporabljamo tudi matematično modeliranje. Sprva smo za simulacijo hidrodinamičnih parametrov ter transporta in pretvorb živega srebra razvili in uporabili dvodimenzionalni (2D) stacionarni model STATRIM. Rezultati 2D simulacij so predstavljeni v Rajar et al. (1997) in v Širca in Rajar (1997b). Z 2D modelom pa ni bilo mogoče izračunati porazdelitve posameznih parametrov po vodnem stolpcu, zato smo za nadaljnje simulacije nadgradili obstoječi tridimenzionalni (3D) nestacionarni model PCFLOW3D in ga uporabili za simulacijo transporta in disperzije živega srebra v Tržaškem zalivu. Večina živega srebra v zalivu je vezanega na delce lebdečih plavin, zato je bilo treba razviti nov modul za transport lebdečih plavin. Opis prvotnega modela, sedimentacijskega modula in nekatere simulacije transporta lebdečih plavin so podrobno opisane v Rajar et al. (2000), Rajar et al. (1998) ter Rajar in Četina (1997).

2. OPIS TRIDIMENZIONALNEGA MODELA PCFLOW3D

Prvotni model PCFLOW3D za račun hidrodinamičnih parametrov ter transporta in diperzije, izdelan na FGG, je bil že večkrat verificiran in uporabljen za reševanje praktičnih problemov (modeliranje tokov in širjenja polutantov) v Sloveniji in tujini. PCFLOW3D je nestacionarni nelinearni baroklini model, sestavljen iz hidro-dinamičnega (HD), transportno-disperzijskega (TD) in novega sedimentacijskega (ST) modula. Diagram poteka modela je prikazan na sliki 2, v nadaljevanju pa je podan kratek opis posameznih modulov.

Even 10 years after the closure of the Idrija Mercury Mine, concentrations in river sediments, water and the sediment at the bottom of the Gulf do not show a significant decrease (Horvat et al. 1999, Horvat et al. 1998, Žagar and Širca, 2001). Therefore, extensive research on Hg cycling in the Gulf is in progress. Besides the measurements of physical, chemical and biological parameters, mathematical modelling was also used to simulate Hg cycling in the Gulf of Trieste. A two-dimensional (2D) steady-state model STATRIM was developed first for the simulation of hydrodynamic circulation and Hg transport and fate. Some of the results of the 2D simulations using annually averaged input data are described in Rajar et al. (1997) and in Širca and Rajar (1997b). The simulation of vertical distribution of the parameters was not possible with the 2D model; therefore an existing three-dimensional (3D) unsteady state model PCFLOW3D was upgraded and used to simulate the transport and dispersion of Hg in the Gulf of Trieste. As most of the Hg flowing to the Gulf, is bound to suspended sediment particles, a new sediment transport module was first developed and included into the model. The basic model, the new sediment transport module and some simulations of the transport of suspended sediment are described in detail in Rajar et al. (2000), Rajar et al. (1998) and Rajar and Četina (1997).

2. DESCRIPTION OF THE THREE-DIMENSIONAL MODEL

The PCFLOW3D hydrodynamic and transport-dispersion model was developed at the Faculty of Civil and Geodetic Engineering of the University of Ljubljana. It has already been applied to many practical hydrodynamic and pollutant dispersion problems in Slovenia and abroad. It is a non-linear baroclinic model composed of three modules: a hydrodynamic (HD) module, a transport-dispersion (TD) module, and a recently developed sediment-transport (ST) module. Figure 2 shows the flow chart of the model and a short description of the modules is given below.

2.1 HIDRODINAMIČNI IN TRANSPORTNO-DISPERZIJSKI MODUL

Diskretizacija diferencialnih enačb poteka po metodi kontrolnih volumnov, sistem enačb pa rešujemo s pomočjo hibridne implicitne numerične sheme. Koeficienta turbulentne viskoznosti in difuzije sta v horizontalni smeri konstantna, v vertikalni smeri pa je uporabljen Koutitasov model turbulence. Z modelom je mogoča tudi simulacija nekaterih biokemičnih procesov.

Enačbe obeh modulov rešujemo sočasno, saj izračunana porazdelitev temperature, slanosti in poljubnega polutanta, ki lahko vpliva na gostoto vode, hkrati vpliva tudi na hitrostno polje. Tako lahko z modelom upoštevamo tudi gostotne tokove in stratifikacijo, ki je običajno izrazitejša v toplejši polovici leta. Z modelom je mogoča tudi simulacija toplotnega onesnaženja; vgrajene so enačbe za račun transporta in disperzije toplote iz atmosfere ali drugih virov. Transportno enačbo v modelu lahko rešujemo po metodi končnih razlik (MKR) ali po metodi sledenja delcev (MSD), kar je odvisno od konkretnega problema, ki ga rešujemo. Za račun transporta živega srebra smo uporabili MKR.

V 3D modelu še niso vključene enačbe za simulacijo procesov pretvorb živega srebra. Z modelom je trenutno mogoče računati transport in disperzijo nemetiliranega in metil-živega srebra v raztopljeni in partikularni (vezani na delce lebdečih plavin) obliki.

2.1 HYDRODYNAMIC AND TRANSPORT-DISPERSION MODULES

The HD and TD modules are both based on the finite volume method; the system of differential equations is solved using a hybrid implicit scheme. In the horizontal plane, the eddy viscosity and diffusivity are constant, while in the vertical direction the simplified one-equation turbulence model of Koutitas is included. The simulation of some biochemical processes has also been included.

The TD module, which is solved coupled with the HD module, simulates temperature, salinity or any contaminant which can influence water density and, at the same time, the velocity field. Therefore, stratified conditions during the warmer half of the year, as well as density-driven flow, can be simulated using the model. The simulation of transport and the dispersion of heat from heat sources and from the atmosphere has also recently been included to enable the simulation of thermal pollution in surface waters. There are two methods of solving the transport equation in the model, a Eulerian finite difference method (FDM) and a Lagrangean particle tracking method (PTM). Each of them has its benefits as well as its deficiencies. The FDM was used for the Hg transport simulations.

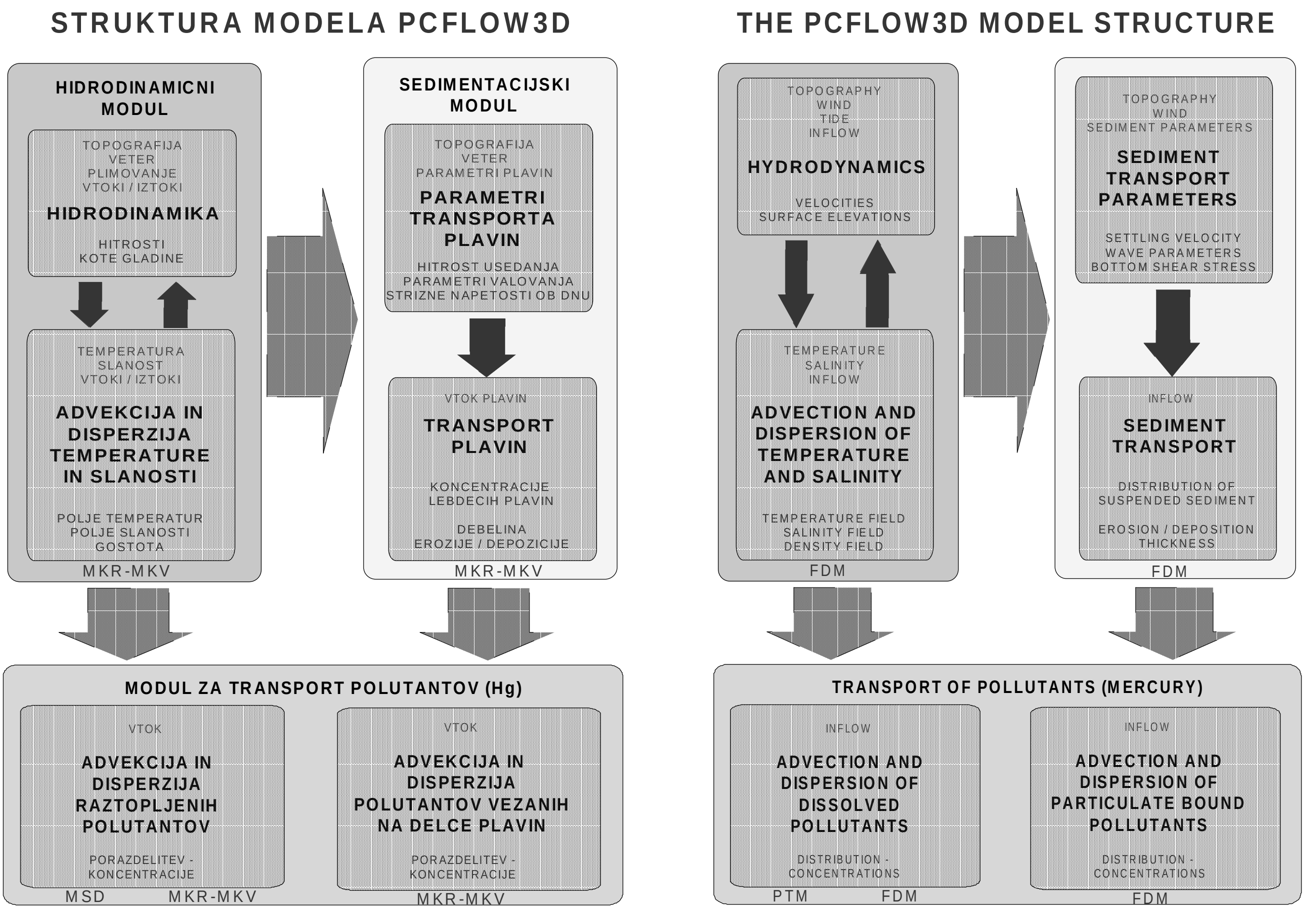
Hg transformation equations have not yet been included in the 3D model. In the present state, the transport of dissolved and particle-bound Hg in both non-methylated and methylated forms was simulated.

2.2 MODUL ZA TRANSPORT PLAVIN

Z modulom za transport plavin, ki temelji na enačbah iz literature (van Rijn, 1993), so mogoče simulacije za nevezane delce plavin. Temelj sedimentacijskega modula predstavlja advekcijsko-disperzijska enačba, zapisana za koncentracijo lebdečih plavin, pri čemer upoštevamo empirično rešitev za hitrost usedanja delcev (van Rijn, 1993). Robni pogoj ob dnu predstavlja usedanje oz. resuspenzija delcev, ki je odvisna od strižnih hitrosti ob dnu zaradi vpliva tokov (rezultat HD modula) in valovanja. Za izračun debeline nanešenega oz. odnešenega materiala uporabimo kontinuitetno enačbo za plavine.

2.2 THE SEDIMENT-TRANSPORT MODULE

The sediment transport module is based on the equations of van Rijn (1993). Non-cohesive sediment material can be simulated. The module basically resolves the advection-diffusion equation for suspended sediment concentration, where the empirical equation for the sedimentation velocity of the particles is accounted for (van Rijn, 1993). As the bottom boundary condition, resuspension or settling of the suspended sediment which depends on the bottom shear stress caused by current velocities (result of the HD module) and wave parameters is calculated. The mass conservation equation for the sediment is used to calculate erosion/deposition thickness at the bottom.



Slika 2. Diagram poteka modela PCFLOW3D
Figure 2. Flow-chart of the PCFLOW3D model.

3. DOLGOTRAJNE SIMULACIJE

3.1 OSNOVNI PRINCIP

Za pravilno delovanje nestacionarnega 3D modela moramo zagotoviti veliko količino vhodnih podatkov. Na relativno velikem območju Tržaškega zaliva je sočasno merjenje vseh parametrov v zadostnem številu merskih točk tako rekoč neizvedljivo.

Pri modeliranju dolgotrajnih procesov običajno zadoščajo stacionarne simulacije s časovno povprečnimi vhodnimi podatki za daljša časovna obdobja, kalibracija in verifikacija modela pa zahtevata simulacije v realnem času za krajša obdobja, za katera imamo na voljo rezultate meritev. Transport in disperzija živega srebra pa je izrazito nestacionaren proces. Več kot 90 odstotkov letnega vnosa lebdečih plavin, ki jih v zaliv prinese Soča, je posledica dveh visokovodnih valov, ki se praviloma pojavljata ob pomladanskem in jesenskem deževju. Prav tako so najpomembnejši vzrok za premeščanje plavin obdobja močnega vetra (burje), ki ponavadi nastopajo pozimi, med novembrom in februarjem.

Popolna nestacionarna simulacija za obdobje več mesecev kljub številnim meritvam različnih vhodnih parametrov modela ni bila izvedljiva, zato smo uporabili nov pristop. Povprečne letne vhodne podatke smo nadomestili s sezonsko povprečnimi, pri čemer smo upoštevali štiri glavne sezone, ki bolj ali manj sovpadajo z letnimi časi. Dodali smo še vložke močnega vetra in visokovodnih valov Soče, ki se z visoko stopnjo verjetnosti pojavljajo vsako leto ob skoraj istem času. Prav ti vložki so zelo pomembni, saj predstavljajo bistveno izboljšavo v primerjavi z dosedanjim modeliranjem s stacionarnimi modeli.

Poleg tega smo popolnoma nestacionarne simulacije nadomestili s t.i. kvazi-stacionarnimi simulacijami. Pri tem načinu ob vsaki bistveni spremembi vhodnih parametrov nekaj časa računamo popolnoma nestacionarno stanje. Po določenem času pa, ko se hidrodinamični parametri ter temperaturna in slanostna polja ustalijo, jih fiksiramo in v

3. LONG-TERM SIMULATIONS

3.1 THE BASIC PRINCIPLE

The unsteady state 3D model needs a very 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.

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, Hg transport and dispersion was found to be a highly unsteady state process. It is known that over 90 % of the annual inflow of suspended sediment and Hg are flushed into the Gulf with two flood waves of the Soča River, usually during spring and autumn rains. It is also known that strong wind is the most important cause of the transport processes in the Gulf. This latest phenomenon mostly occurs during the winter months between November and February.

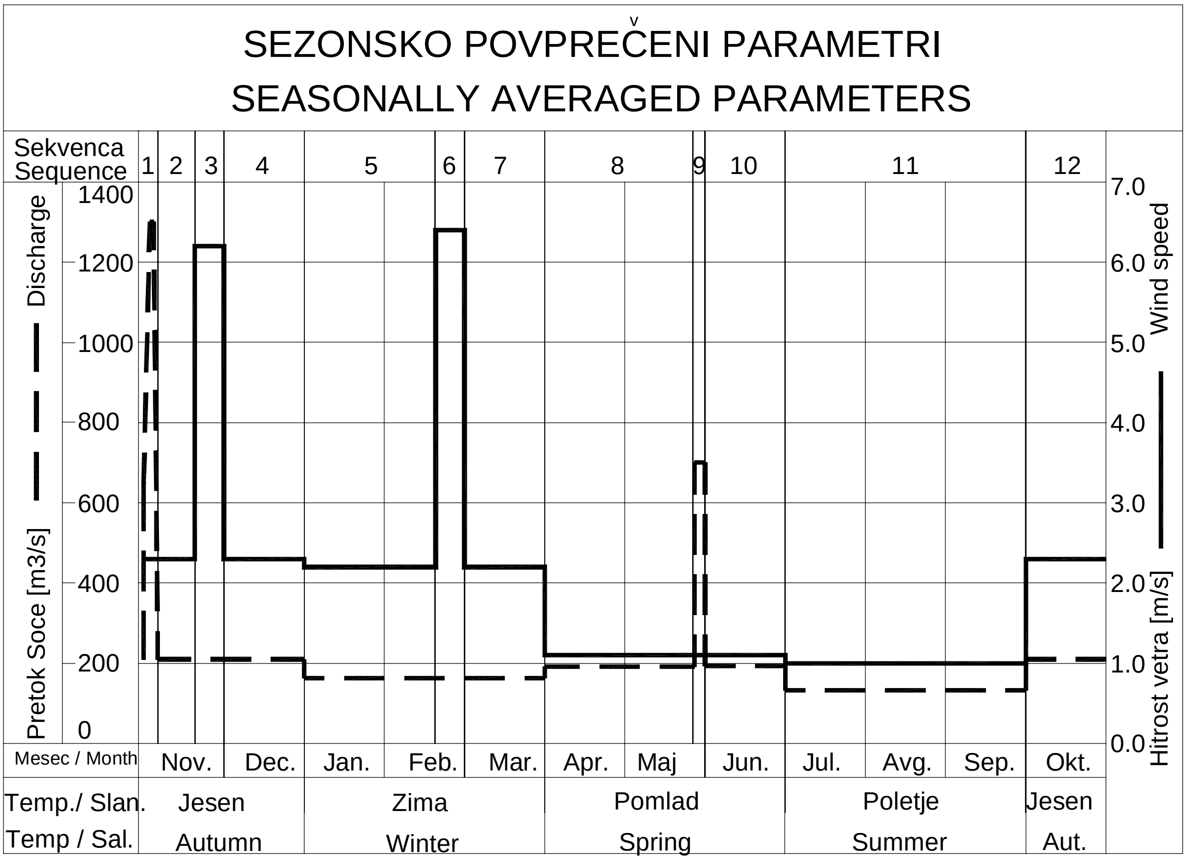
Despite numerous measurements of different parameters, it was not possible to perform fully unsteady state simulations over several months; therefore, a new approach was used. Annually averaged input data were replaced with seasonally averaged input data. Four main seasons, more or less identical to the calendar seasons, were accounted for. A few inserts of strong wind and the Soča River 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.

Furthermore, real-time modelling was replaced by the quasi-steady state principle. Here, an unsteady state simulation is performed for a certain period of time after input parameters have been changed significantly. Afterwards, when the hydrodynamic parameters and temperature and nadaljnjem računu obravnavamo kot nespremenljiva. Od tod naprej računamo samo transport in disperzijo živega srebra. Na ta način močno zmanjšamo čas računa, saj za račun hidrodinamičnih parametrov z upoštevanjem gostotnih tokov in stratifikacije porabimo okrog 80 odstotkov skupnega časa računa.

Tipično leto smo na koncu razdelili na 12 sekvenc (slika 3), ki jih računamo zaporedno; krajše (nekajdnevne) računamo popolnoma nestacionarno, pri daljših (nekaj tednov do nekaj mesecev) pa uporabimo že omenjeni kvazistacionarni pristop.

salinity fields are stabilised, they are treated as fixed, and only the transport of Hg is further calculated. In this way the computational time is also essentially reduced, as about 80 % of the total computational time needed is used for the hydrodynamics computation when density driven flow and stratified conditions are taken into account.

Finally, a typical year was partitioned into 12 sequences (Figure 3), which were simulated successively. With the shorter (up to a few days long) sequences, unsteady 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.



Slika 3. Sezonsko povprečni parametri v Tržaškem zalivu
Figure 3. Seasonally averaged parameters in the Gulf of Trieste.

3.2 VHODNI PODATKI

3.2.1 VETER

Smer in jakost sezonsko povprečnih vetrov nad Tržaškim zalivom (preglednica 1) je bila določena z metodo VECTRA (Širca, 1996; Širca in Rajar, 1997a), pri kateri za izračun upoštevamo vektorsko vsoto posameznih značilnih vetrov (*unit winds*). Pri izračunu smo upoštevali uradne (HMZ RS) merjene urne vrednosti jakosti in smeri vetra za obdobje od 1975 do 1990 za postajo Beli Križ.

Pozimi nad Tržaškim zalivom burja (smer NE) pogosto doseže najvišje hitrosti tudi nad 30 m/s, za modeliranje pa je pomembnejši podatek, da lahko s hitrostjo 16 m/s piha neprekinjeno tudi več dni. Iz podatkov meritev je razvidno, da se v hladnejši polovici tipičnega leta glede na pogostost pojavljata dva maksimuma burje (februarja in novembra), ki hkrati skoraj točno sovpadata tudi z maksimumoma jakosti (preglednica 2). Zaradi razmeroma velike dolžine nedvomno največ prispevata k transportu živega srebra v Tržaškem zalivu. Za določitev jakosti in smeri vetra je bila uporabljena ista metoda kot za določitev povprečnih sezonskih vetrov.

3.2 INPUT DATA

3.2.1 WIND

Seasonally averaged wind force and direction above the Gulf of Trieste (Table 1) was evaluated using the VECTRA method, which takes into account vectorial sum of the unit winds (Širca, 1996; Širca and Rajar, 1997a). The official data for the Beli Križ Measuring Station (hourly measured wind directions and speed for the period from 1975 to 1990) were used for calculation.

In winter time the *burja* wind (direction NE) above the Gulf of Trieste often reaches peak velocities over 30 m/s, and, even more important for modelling, it can blow with a velocity of 16 m/s for several days continuously. It is evident from the official measurements that during the colder half of a typical year, there are two peaks of the *burja* wind (in February and November). These two peaks coincide almost exactly with the wind force peaks (Table 2), and, due to their length, the two peak-wind inserts undoubtedly contribute the most to the Hg transport in the Gulf. The same method as described above was also used to evaluate the wind direction and velocity of the wind peaks.

Preglednica 1. Sezonski povprečni veter nad Tržaškim zalivom
Table 1. Seasonally averaged wind above the Gulf of Trieste

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

Preglednica 2. Vložki vetra (merska postaja Beli Križ)
Table 2. Wind inserts (Beli Križ measuring station)

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

3.2.2 SOČA

Sezonski pretoki in visokovodni vložki Soče temeljijo na meritvah, opravljenih na vodomerni postaji Solkan, tik pred slovensko-italijansko mejo (preglednica 3). Med Solkanom in izlivom Soče v Tržaški zaliv dotekata v Sočo še dva večja pritoka, Vipava in Ter (Torre). Podatki za Vipavo so razvidni iz preglednice 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, 1999). Skupna prispevna površina porečja Soče nad Solkanom znaša 2235 km^2, pod Solkanom pa 1065 km^2, 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 m^3/s, ta številka pa se dobro ujema z vrednostmi drugih avtorjev, ki znašajo od 165 m^3/s (Mosetti, 1983) do 172 m^3/s (Benini, 1974).

3.2.2 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 3). There are another two important tributaries of the Soča River between Solkan and the river mouth: the River Vipava, which mainly flows through Slovenian territory, and is well elaborated (Table 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, 1999). The total catchment area of the Soča River in Slovenia is 2235 km^2, while the catchment area in Italy is 1065 km^2. 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 m^3/s. The number can be compared with the values of other authors, which are between 165 m^3/s (Mosetti, 1983) and 172 m^3/s (Benini, 1974).

Preglednica 3. Mesečni in sezonski povprečni pretoki Soče
Table 3. Monthly and seasonally averaged discharges of the Soča River

Mesec Month	Pretoki Discharge Soča (Solkan)	Vipava (Miren)	Σ Soča + Vipava	**Soča na ustju** ***The Soča River mouth***	**Sezonski povprečni** ***Seasonally averaged***
	[m^3/s]	[m^3/s]	[m^3/s]	[m^3/s]	[m^3/s]
Jan	72	22	94	**141**	
Feb	70	20	90	**135**	**150**
Mar	94	21	115	**173**	
Apr	109	20	129	**194**	
Maj / May	116	16	132	**192**	**190**
Jun	109	13	122	**183**	
Jul	69	9	78	**117**	
Avg / Aug	59	7	66	**99**	**120**
Sep	82	14	96	**144**	
Okt / Oct	109	20	129	**194**	
Nov	144	27	171	**257**	**209**
Dec	94	26	120	**180**	
Povprečni letni ***Annually averaged***	**94**	**18**	**112**	**168**	**168**

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

Opisana metoda ekstrapolacije pretokov je za kratkotrajna obdobja manj zanesljiva, kljub temu pa je bil isti princip uporabljen tudi za račun visokovodnih vložkov. Najprej smo iz statističnih podatkov ugotovili trajanje in intenziteto tipičnih vložkov. Tipični majski visokovodni val traja okrog 5 dni, novembrski pa okrog 4 dni. Intenziteta 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) v Solkanu za obdobje od 1926 do 1975 dva maksimuma, ki se pojavljata maja in novembra.

Seasonally averaged discharges are evaluated from measurements (monthly averaged discharges) from other authors (for Solkan in the VGI (1982); for Miren in the water management plans (ZVSS, 1978)).

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. First, the duration and intensity of typical flood peak inserts was determined. The typically observed duration of the May and November flood-peak was about 5 days and about 4 days respectively. The 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 averaged for individual months (the first column in Table 4) at Solkan, between the years 1926 and 1975, have two peaks, which occur in May and November respectively.

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). To sicer pomeni, da se dogodek zgodi le na 2.5 leta, vendar pa smo na ta način z modelom upoštevali tudi vpliv manj pogostih dogodkov, ki pa imajo velik vpliv na dotok živega srebra v Tržaški zaliv. Petdnevno obdobje s povprečnim pretokom 473 m^3/s ima povratno dobo dve leti, zato je upoštevana dolžina pomladnega vložka 5 dni. Trajanje jesenskega vložka je krajše, saj bi imelo petdnevno obdobje s povprečnim pretokom 950 m^3/s povratno dobo kar 50 let. Upoštevana dolžina jesenskega vložka je tako 2 dni.

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 the interpolation between Q_2 and Q_5 (the second and the third column in Table 4.4). Such discharges ($Q_{2.5}$) were used in model simulations, as also, in that manner, less frequent events with a significant influence on mercury transport in the Gulf were taken into account. The recurrence of a five-day long insert with a mean discharge of 473 m^3/s is two years; 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 a mean discharge of 950 m^3/s is about 50 years. A two-day long autumnal insert was adopted.

Preglednica 4. Visokovodni vložki Soče (meritve - Solkan)
Table 4. The Soča River flood-peak inserts (measurements – Solkan)

Mesec *Month*	$_{sr}Q_v$	Q_2	Q_5	Trajanje [dni]
	[m^3/s]	[m^3/s]	[m^3/s]	[dni – *days*]
Maj / *May*	476	416	687	5
November	914	821	1299	2

Dvodnevnemu vložku z najvišjim pretokom sta dodana še dan prej in dan kasneje s pretokom 230 m^3/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 m^3/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.

A day before and a day after, with a discharge of 230 m^3/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 the 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 m^3/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 the flood wave in a single week in November, 1997 was about 380 million m^3.

V modelu so bili kot vhodni podatki ob visokovodnih vložkih uporabljeni pretoki Soče na ustju, kot so navedeni v preglednici 5.

The data from Table 5 (discharges at the Soča River mouth) were used as the input data for flood-peak insert simulations.

Preglednica 5. Visokovodni vložki Soče na ustju (vhodni podatki za model).
Table 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 (1st day)*	345	1
november (2. in 3. Dan) *November (2nd and 3rd day)*	1371	2
november (4.dan) *November (4th day)*	345	1

Preglednica 6. Povprečne sezonske temperature vode v Soči (most pred izlivom)
Table 6. Seasonally averaged water temperature in the Soča River

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

Za simulacije stratificiranega stanja 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 od leta 1974 do 1995. Največja gostota meritev je bila od leta 1978 do 1987. Za nameravane simulacije s 3D modelom so bile iz podatkov statistično izračunane povprečne sezonske vrednosti (preglednica 6).

The water temperature of the Soča River at its mouth is another important factor in the simulation of the stratified conditions. Measurements of water temperature under the last bridge, situated less than one kilometre from the river mouth, were available. Temperature was measured in about two-week intervals between the years 1974 and 1995, and more frequently between the years 1978 and 1987. Seasonally averaged water temperatures were statistically evaluated from the measurements (Table 6) and used in the 3D modelling.

Na voljo so bili podatki meritev 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). Iz meritev je razvidno, 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 (merska točka D6 na sliki 1) pa od 4.5 do 5 ng/l. Višje koncentracije v morju so posledica sproščanja živega srebra iz partikularne v raztopljeno obliko na območju mešanja sladke in slane vode. Procesa ni bilo mogoče neposredno vključiti v model, zato je pri vseh simulacijah in v vseh letnih časih upoštevana koncentracija na ustju 5 ng/l.

3.2.3 TRŽAŠKI ZALIV

Rezidualni tokovi zaradi plimovanja v Tržaškem zalivu so reda velikosti 1 mm/s, hitrosti rezidualnega toka zaradi vpliva vetra pa dosegajo vrednosti 2 do 3 cm/s (Širca, 1996). Vpliv plimovanja na gibanje vode v zalivu pri simulacijah s 3D modelom ni bil upoštevan, saj so rezidualni tokovi zaradi plimovanja v zalivu vsaj za red velikosti manjši od rezidualnih tokov zaradi vetra, ki je glavni vzrok gibanja vode. Poleg tega pri dolgotrajnih simulacijah, predvsem v obdobjih šibkega vetra in nizkih pretokov Soče, že napaka, ki nastane pri računu koncentracij polutanta zaradi numerične difuzije, ki se ji z uporabo obstoječe numerične sheme ne moremo izogniti, bistveno presega napako zaradi neupoštevanja plimovanja.

Predvsem v toplejšem delu leta na disperzijo živega srebra v vertikalni smeri vplivajo tudi stratificirane razmere v zalivu. Za simulacije je bilo treba za vsako sezono zagotoviti podatke o porazdelitvi temperatur in slanosti v vseh točkah računske mreže. V celotnem zalivu so bile izmerjene temperature in slanosti sredi posameznih letnih časov (februar, maj, avgust, november) sočasno v 27 točkah zaliva (slika 1) v 5 m intervalih po globini.

There were several measurements of dissolved Hg 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. 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 Hg 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 1), concentrations between 4.5 and 5 ng/l were measured. Higher concentrations in the seawater are due to Hg 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 Hg concentration of 5 ng/l was taken into account with all simulations in any season.

3.2.3 THE GULF OF TRIESTE

Typical tide-induced residual currents in the Gulf were of the order of 1 mm/s, while typical wind-induced residual currents reached 2 to 3 cm/s (Širca, 1996). As the tide-induced currents were at least for an order of magnitude smaller than the wind-induced residual currents, the effect of the tide on the circulation in the Gulf was not taken into account with the 3D simulations. Moreover, by computation of the concentrations of pollutants with long-term simulations, particularly during calm periods, the error due to tidal forcing exclusion was significantly exceeded by the error caused by false diffusion, which could not be avoided using the existing numerical scheme.

Stratified conditions within the Gulf and their impact on the dispersion of Hg along the water column were also a very important factor, particularly during the warmer half of the year. Temperature and salinity distribution along the entire computational domain had to be evaluated for the four main seasons. Measurements were performed simultaneously in 27 sampling points within the Gulf (Figure 1), in the middle of each main season (February, May, August, November) in 5-m intervals along the depth.

Pri simulacijah smo uporabili numerično mrežo, kjer smo definicijsko območje po globini razdelili na 25 slojev, debeline 1 m. V horizontalni ravnini smo območje razdelili na 43 × 42 celic, z dimenzijami od 300 × 300 m ob ustju Soče do največ 900 × 900 m. Za vsako računsko celico smo morali zagotoviti podatka o temperaturi in slanosti.

Najprej smo iz podatkov meritev z linearno interpolacijo izračunali temperaturo in slanost pod merskimi točkami v vsakem sloju. Nato smo nad vsakim slojem z uporabo trikotne mreže napeli ploskev temperatur in slanosti z orodjem *Quicksurf*, s katerim smo tudi izvrednotili celotne matrike temperatur in slanosti v vsaki celici definicijskega območja za vse štiri sezone.

Dosedanje izkušnje z gostotnimi gibanji (Rajar et al. 1997) kažejo, da je potrebno 'glajenje' matrik temperatur in slanosti, dobljenih z interpolacijami iz meritev, sicer se pri simulacijah lahko pojavijo težave s stabilnostjo numerične sheme. Poleg tega bi bila pri simulaciji dolgotrajnih procesov končna slika temperatur in slanosti nerealna tudi zaradi vtoka Soče, gostotnega gibanja in disperzije temperature in slanosti zaradi gibanja vodnih mas. Vhodne podatke modela (začetno stanje) smo izboljšali tako, da smo za vsako od glavnih sezon izvedli simulacijo hidrodinamičnih parametrov ter advekcije in disperzije temperature in slanosti ob hkratnem upoštevanju vseh dejavnikov, ki vplivajo na gibanje vode (veter, vtok Soče in gostotno gibanje). Simulirali smo izbrano časovno obdobje (od 8 h ob močnem vetru in/ali visokem pretoku Soče do dveh dni ob šibkem vetru in nizkih pretokih), dokler na celotnem definicijskem območju niso bile dosežene pričakovane hitrosti. Takšno porazdelitev slanosti in temperatur smo v nadaljevanju uporabili kot začetno stanje za račun transporta in disperzije raztopljenega živega srebra.

Koncentracije živega srebra v sedimentu na dnu Tržaškega zaliva so zelo visoke, ob ustju Soče dosegajo 25-30 μg/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

The computational grid with a maximum of 25 layers, each 1 m thick, was used. In the horizontal plane, the computational area was divided into 43 × 42 cells, with dimensions from 300 × 300 m near the Soča River mouth to 900 × 900 m. Temperature and salinity values in each cell of the computational grid had to be provided.

First, temperature and salinity values in each layer below the sampling points were calculated using linear interpolation. Afterwards, an envelope of temperature and salinity concentrations for each layer was constructed on the basis of a triangular grid using *Quicksurf* software. Finally, with the same tool, complete temperature and salinity matrices in each cell of the computational domain for all four seasons were calculated.

Temperature and salinity matrices calculated in that manner need to be 'smoothed' to avoid stability problems with the numerical scheme during computation (Rajar et al. 1997). 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. To get the best possible initial state for each of the main seasons, simulations of hydrodynamic quantities and the advection and dispersion of temperature and salinity, with all forcing factors taken into account (wind, river inflow and density-driven flow) were performed. Computations for set amounts of time (from 8 hours with strong wind and/or high discharge of the Soča River, up to two days with weak wind and lower discharges) were performed, until the expected velocities were reached within the entire computational domain. Such matrices of temperature and salinity distribution were finally used as an initial state to simulate the transport of Hg in its dissolved form.

In the bottom sediment of the Gulf**,** Hg concentrations are highly increased, and reach about 25-30 μg/g dry weight near the Soča River mouth. Hg bound to sediment particles is gradually being released into the pore water and, due to molecular diffusion, also proceeds to the surrounding water. Therefore, pore po zmanjšanju ali celo prenehanju dotoka živega srebra v okolje. V letih 1995 in 1996 so bile v merski točki AA1 (slika 1) izvedene meritve koncentracij živega srebra v pornih vodah v sedimentu na mestu samem z bentoško komoro (*benthic chamber*) (Covelli et al. 1999).

Meritev je bila zaradi zahtevnosti postopka in visoke cene izvedena v eni sami točki zaliva, zato rezultatov meritev ne moremo posplošiti na celotno obravnavano območje. Vsekakor pa je jasno, da je količina živega srebra, ki se sprošča z dna (po Covelli et al. znaša okoli 470 kg/leto) dovolj velika, da jo bo treba v prihodnje upoštevati pri modelnih simulacijah.

3.3 REZULTATI SIMULACIJE

Z zbranimi podatki smo izdelali končno razdelitev tipičnega leta na sekvence in pripravili podatke za simulacijo (slika 3). S temi podatki smo izvedli simulacijo za obdobje od 1.novembra 1994 do 1.julija 1995. Krajše sekvence smo obravnavali popolnoma nestacionarno, račun je potekal v realnem času, pri daljših pa smo uporabili kvazi-stacionarni pristop. Čas nestacionarne obravnave je bil v posameznih daljših sekvencah različen, odvisen pa je bil od pretoka Soče, hitrosti vetra in začetnih temperaturnih in slanostnih pogojev v zalivu. Nestacionarne simulacije so tako trajale od 8 ur v primeru močnejšega vetra in/ali visokega pretoka Soče, do nekaj dni pri šibkem vetru in nizkem pretoku Soče.

Meritve celokupnega raztopljenega živega srebra so bile opravljene 25. junija 1995 (Horvat et al. 1999) v 14 točkah na površini in ob dnu, primerjava rezultatov modela in merjenih vrednosti pa je prikazana na sliki 4 in v preglednici 7.

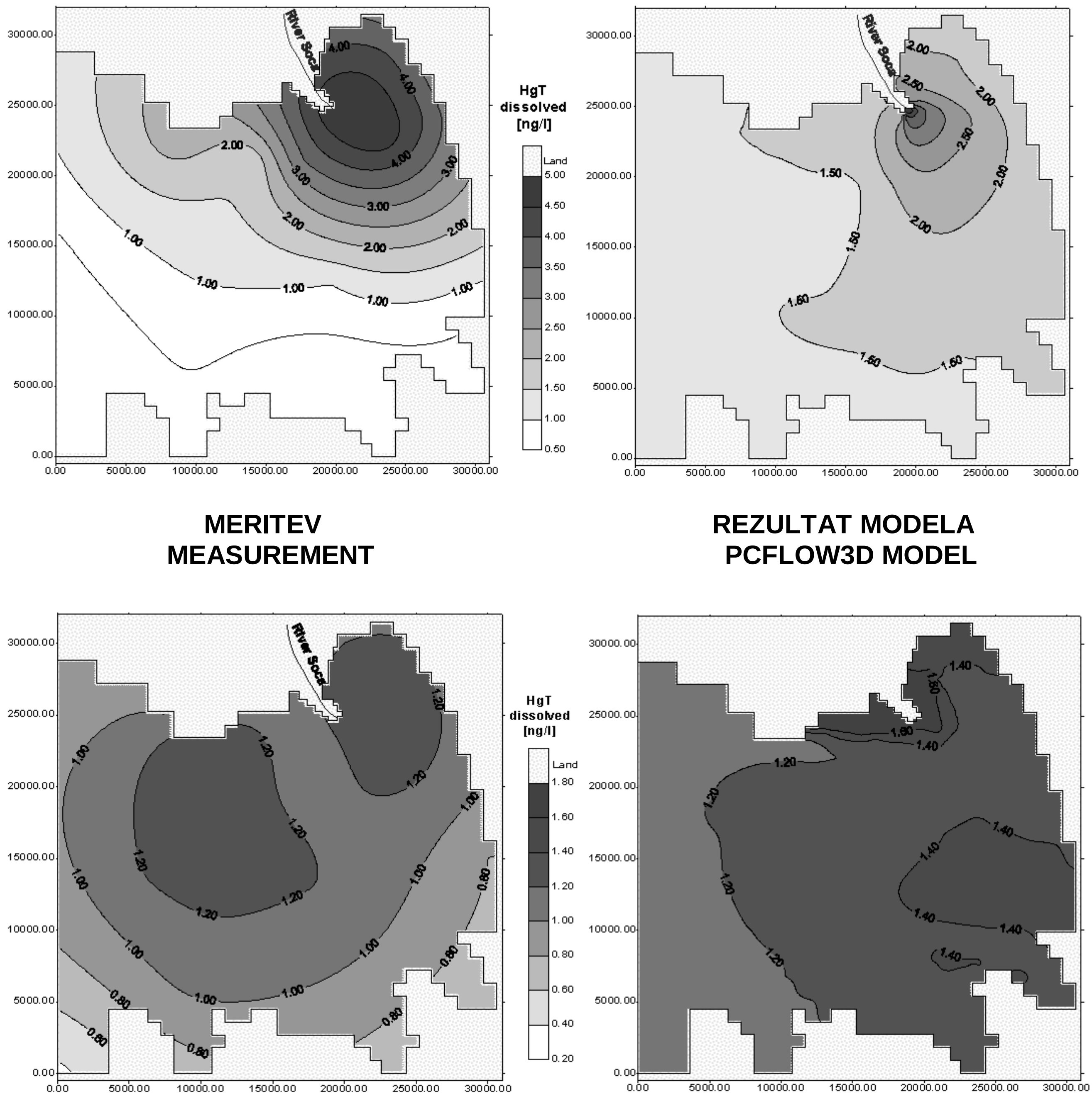
waters are a significant source of dissolved Hg for a long time after the inflow of Hg has begun to reduce or has even ceased. Hg concentrations in the pore water of the bottom sediment of the Gulf were determined by an in situ benthic chamber experiment at location AA1 (Figure 1) during 1995 and 1996 (Covelli et al. 1999).

These measured values cannot be applied to the whole area of the Gulf, as only one location was observed, due to the difficulty and expense of the experiment. The high amount of Hg being released (according to Covelli et al. about 470 kg/year) from the bottom sediment is very significant, and needs to be taken into account with future modelling and simulations.

3.3 RESULTS OF THE SIMULATION

Input data for the simulations were prepared and the final partitioning of a typical year was carried out using the collected data (Figure 3). With these data a simulation for the period between 1 November, 1994 and 1 July, 1995 was performed. Fully unsteady state simulations (real-time modelling) were applied with the shorter sequences and quasi-steady state modelling with the longer ones. The duration of the unsteady 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. Unsteady 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.

Measurement of total dissolved Hg was performed on 25 June, 1995 (Horvat et al. 1999) in 14 sampling sites at the surface and at the bottom. In Figure 4 and Table 7 a comparison between the measurements and the results of the model simulation is given.



Slika 4: Primerjava merjenih in izračunanih koncentracij celokupnega raztopljenega živega srebra (junij 1995) v površinskem sloju (zgoraj) in v sloju ob dnu (spodaj).

Figure 4: Comparison of measured and simulated concentrations of total dissolved mercury (June, 1995) in the surface layer (above) and the bottom layer (below).

Preglednica 7. Primerjava merjenih in izračunanih koncentracij celokupnega raztopljenega živega srebra (junij 1995) v površinskem sloju in v sloju ob dnu
Table 7. Comparison of measured and simulated concentrations of total dissolved mercury (June, 1995) in the surface layer and the bottom layer

Merska točka *Sampling point*	Globina *Depth* [m]	Merjena koncentracija *Measured concentration* [ng/l]	Izračunana koncentracija *Calculated concentration* [ng/l]	Odstopanje *Ratio* [-]
D6 ↑	0.5	4.90	3.45	-30 %
D6 ↓	3.5	1.31	1.53	+17 %
A4 ↑	0.5	3.47	2.25	-35 %
A4 ↓	11.5	1.08	1.35	+25 %
A29 ↑	0.5	1.53	1.68	+10 %
A29 ↓	9.5	1.28	1.21	-5.5 %
A20 ↑	0.5	2.31	1.52	-34 %
A20 ↓	3.5	1.34	1.16	-13 %
CZ ↑	0.5	0.97	1.72	+77 %
CZ ↓	23.5	1.18	1.43	+21 %
F2 ↑	0.5	0.95	1.33	+40 %
F2 ↓	20.5	1.23	1.21	- 1.6 %
F0 ↑	0.5	0.68	1.38	+103 %
F0 ↓	20.5	1.09	1.18	+ 8.3 %

4. ZAKLJUČKI

Iz primerjave rezultatov simulacije in meritev lahko sklepamo naslednje:

Kvalitativno je ujemanje rezultatov na površini zelo dobro. Relativno dobro kvantitativno ujemanje, povsod v mejah faktorja dve, 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.

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 sproščanja živega srebra iz partikularne v raztopjleno obliko še ni dovolj dobro raziskan, da bi ga bilo mogoče vključiti v model.

4. CONCLUSIONS

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

At the surface, a very good qualitative agreement of modelling results and measurements was achieved. Relatively good quantitative agreement, always within a factor of two, was a significant improvement in comparison with the 2D modelling. The dispersion of Hg at the surface was somewhat too high, mostly due to false diffusion, which cannot be avoided using the existing numerical scheme.

In spite of an additional increase of dissolved Hg concentrations in the Soča River due to the Hg release from particulate to dissolved form, agreement of the measurements with the simulation is less accurate near the river mouth. Additional research of the Hg release from particulate matter to its dissolved form in the freshwater / saltwater mixing zone is needed before including the process in the 3D model.

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. Zato je ujemanje ob dnu kvalitativno nekoliko slabše, kvantitativno pa še vedno v mejah faktorja dve. Omeniti pa je treba, da tudi na rezultate meritev pri tako nizkih koncentracijah vpliva mnogo dejavnikov in je zato zanesljivost meritev v mejah ± 20 % (Horvat et al., 1999). Če torej upoštevamo nezanesljivost analiznih metod in vhodnih potatkov ter napako pri modeliranju, lahko zaključimo, da je ujemanje rezultatov dobro.

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*).

The increase of concentrations at the sea-bottom due to benthic fluxes, which can significantly change Hg concentrations within the bottom layer, was not taken into account in the present state of the model. Therefore, qualitative agreement in the bottom layer is somewhat less accurate, but quantitatively 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 % (Horvat et al., 1999). By taking into account the unreliability of the analytical methods, uncertainty of the input data and the inaccuracy of the modelling, the agreement of the results and measurements can be considered good.

Besides the false diffusion, the results are also influenced by the use of a relatively simple model of turbulence. Despite adapting the eddy diffusivity to stratified conditions, the 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*) will be included in the model as soon as possible.

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