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MODELIRANJE HIDRODINAMIKE IN TRANSPORTA ŽIVEGA SREBRA V VELENJSKEM JEZERU – 2. DEL: MODELIRANJE IN PREVERJANJE MODELA

MODELLING OF HYDRODYNAMICS AND MERCURY TRANSPORT IN LAKE VELENJE – PART 2: MODELLING AND MODEL VERIFICATION

Jože KOTNIK, Dušan ŽAGAR, Rudi RAJAR, Milena HORVAT

Tridimenzionalni matematični model PCFLOW3D, razvit na katedri za mehaniko tekočin Fakultete za gradbeništvo in geodezijo, smo uporabili za simulacije hidrodinamike in transporta živega srebra v Velenjskem jezeru. Popolnoma nelinearen hidrodinamični modul daje kot rezultat tri komponente hitrosti, potek gladine vode in tlake. S transportno-disperzijskima enačbama izračunamo prostorsko porazdelitev slanosti in temperature (in/ali poljubnega polutanta). Iz rezultatov simulacij je razvidno, da so glavni vir živega srebra v Velenjskem jezeru vtoki. Hidrodinamične simulacije so pokazale, da vtoki in iztoki površinskih in podzemnih voda nimajo velikega vpliva na cirkulacijo vode v jezeru. Glavni vzrok za gibanje vode sta veter in temperatura vode in okolice. Simulacije transporta živega srebra z modelom PCFLOW3D se dobro ujemajo z merjenimi koncentracijami različnih oblik Hg in metil-Hg v Velenjskem jezeru. Izračunane tokove vode smo preverili s primerjavo z meritvami izotopov $\delta^{18}O$ *in* $\delta^{2}H$ *ter meritvami različnih oblik živega srebra in metil živega srebra. Porazdelitev posameznih zvrsti in oblik živega srebra ter izotopska sestava v vodnem okolju Velenjskega jezera je opisana v prvem delu članka.*

Ključne besede: *modeliranje, sladkovodno jezero, transport, disperzija, hidrodinamika, živo srebro, metil živo srebro*

PCFLOW3D – a three-dimensional mathematical model that was developed at the Chair of Fluid Mechanics of the Faculty of Civil and Geodetic Engineering, University of Ljubljana, was used for hydrodynamic and Hg transport simulations in Lake Velenje. The model is fully non-linear and computes three velocity components, water elevation and pressure. Transport-dispersion equations for salinity and heat (and/or any pollutant) are further used to compute the distributions of these parameters. The results show that the major sources of mercury in Lake Velenje are lake inflows. The hydrodynamic simulations revealed that ground and/or surface water inflow and outflow do not have much influence on water cycling in the lake basin. Wind and ambient temperature seem to have the greatest influence on water movement in the lake. Mercury transport simulations performed by PCFLOW3D show good agreement with the measured distribution of different Hg and MeHg forms in Lake Velenje. Verification of water flow was done by isotope tracers $\delta^{18}O$ *and* $\delta^{2}H$ *and measurements of different Hg and MeHg forms. Distribution of different Hg species and forms and isotopic composition in water of Lake Velenje is described in Part 1.*

Key words: *modeling, freshwater lake, transport, dispersion, hydrodynamics, mercury, methylmercury*

1. UVOD

V prvem delu članka (Kotnik et al., 2003) smo opisali Velenjsko jezero in njegove lastnosti ter uporabljene analitične metode in rezultate meritev izotopske sestave in različnih

1. INTRODUCTION

In Part 1 of the article (Kotnik et al., 2003) Lake Velenje and its properties as well as analytical methods and measurement results of isotopic composition and different Hg species zvrsti Hg v jezerski vodi, sedimentu in zraku.

Za opis tokov (cirkulacije vode) ter transporta in porazdelitve živega srebra v Velenjskem jezeru smo uporabili dve metodi: (i) s hidrodinamičnim modelom PCFLOW3D smo simulirali tokove in (ii) transport in disperzijo Hg smo izračunali s transportno-disperzijskim modulom modela PCFLOW3D.

Vse hidrodinamične simulacije v predstavljeni raziskavi so bile izvedene z modelom PCFLOW3D, izdelanim na Fakulteti za gradbeništvo in geodezijo Univerze v Ljubljani. Razvoj modela in njegova uporaba sta že opisana v številnih člankih (Rajar in Četina, 1986; Rajar, 1989; Rajar in Četina 1997; Širca *et al.*, 1999a; Širca *et al.*, 1999b; Rajar *et al.*, 2000), zato tukaj podajamo samo kratek povzetek.

PCFLOW3D je tridimenzionalen, popolnoma nelinearen model, ki izračuna tri komponente hitrosti, gladino vode in tlake. Za račun porazdelitve slanosti in temperature (in/ali poljubnega polutanta) sta v model vgrajeni transportno-disperzijski enačbi. Model je sestavljen iz hidrodinamičnega, sedimentacijskega in transportno-disperzijskega modula in je bil doslej uspešno uporabljen za reševanje praktičnih problemov v severnojadranskem priobalnem morju in slovenskih jezerih (PCFLOW3D User's Manual 1997; Rajar, 1989; 1992; Rajar in Četina, 1986; 1991; 1992b; 1997; Rajar *et al.*, 2000; Širca, 1996; Širca *et al.*, 1999a; 1999b). Tudi dodatna možnost simulacije razgradnje nekaterih vrst onesnaženja je bila uporabljena na praktičnih primerih kot npr. simulacija razlitja nafte in širjenja radioaktivnih polutantov. Dvodimenzionalna različica modela je bila razvita za simulacije hidrodinamike in živosrebrovega cikla v Tržaškem zalivu (Širca, 1996; Širca *et al.*, 1999a; 1999b).

2. OSNOVNI PODATKI ZA SIMULACIJE

Velenjsko jezero smo razdelili v 35 × 29 = 1015 celic v horizontalni ravnini, s 50-metrskimi intervali v smereh Dx in Dy. V smeri z (globina) smo območje razdelili na 19

in the water, sediment and air were discussed.

With the aim of determining water circulation, mercury transport and distribution in Lake Velenje two modeling approaches were used: (i) Water circulation calculations were performed by the hydrodynamic model PCFLOW3D and (ii) Hg transport and dispersion calculations were performed by the transport – dispersion module of PCFLOW3D.

All hydrodynamic simulations for this research have been performed by PCFLOW3D, a hydrodynamic model developed at the University of Ljubljana, Faculty of Civil and Geodetic Engineering. Since the model development and its applications are already described in several articles (Rajar and Četina, 1986; Rajar, 1989; Rajar and Četina, 1992; Širca 1996; Rajar and Četina, 1997; Širca *et al.*, 1999a; Širca *et al.*, 1999b; Rajar *et al.*, 2000), only a short summary will be presented here.

The model is 3D, fully non-linear, and computes three velocity components, water elevation and pressure. Transport-dispersion equations for salinity and heat (and/or any pollutant) are used to compute the distributions of these parameters. Up to now, the model has hydrodynamic, sediment-transport and transport-dispersion modules, which have already been used efficiently for solving some practical problems in the Northern Adriatic coastal sea and Slovenian lakes (PCFLOW3D User's Manual 1997; Rajar, 1989; 1992; Rajar & Četina, 1986; 1991; 1992b; 1997; Rajar *et al.*, 2000; Širca, 1996; Širca *et al.*, 1999a; 1999b). The simulation of fate processes for some contaminants is included, and has been used for practical applications such as oil-spill simulation and dispersion of radioactive pollutants. A two-dimensional version of the model has been developed to simulate hydrodynamics and mercury cycling in the Gulf of Trieste (Širca, 1996; Širca *et al.*, 1999a; 1999b).

2. BASIC DATA FOR THE SIMULATIONS

Lake Velenje was divided into 35 × 29 = 1015 cells in the horizontal plane, with 50 m intervals in the Dx and Dy direction. In the z-direction (depth) the field was divided into 19 slojev debeline od 1 do 5 m (debelina slojev od dna proti površini je bila: 5, 5, 5, 5, 5, 4, 3, 3, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1 in 1 m). Od površine do globine 20 m smo izbrali tanjše sloje, saj smo želeli dobiti bolj natančen prikaz toplotne stratifikacije v jezeru.

Podatke o vetru nad Velenjskim jezerom smo pridobili na Agenciji Republike Slovenije za okolje. Meritve hitrosti in smeri vetra so potekale od oktobra 1992 do septembra 1993 na vsake pol ure. V Šaleški dolini prevladujejo vetrovi iz dveh smeri: gre predvsem za vzhodne in zahodne vetrove. V simulacijah smo uporabili najpogostejše vetrove hitrosti 1 m/s z zahoda, hitrosti 2 m/s z jugovzhoda in hitrosti 4 m/s z jugovzhoda.

Poletne temperature jezera so bile merjene dvakrat (junija 1998 im avgusta 1998) v dvometrskih intervalih do globine 30 m. Povprečna poletna temperatura epilimnija je bila okoli 25 °C, medtem ko je bila v hipolimniju povprečna temperatura vode med 5 in 8 °C. Zimske temperature so bile merjene ob koncu zime 1998/1999. V simulacijah smo kot zimsko temperaturo vode po vsej globini uporabili 4,5 °C .

layers with thickness between 1 and 5 m (layer thickness from the bottom to the surface were: 5, 5, 5, 5, 5, 4, 3, 3, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1 and 1 m) down to about 55 m of depth. The smaller thickness from the surface to 20 m has been chosen to account more accurately for the thermal stratification in the lake.

The data about the wind conditions over Lake Velenje was obtained from the Environmental Agency of the Republic of Slovenia. Wind speed and direction were measured from October 1992 to September 1993 every half an hour. Easterly and westerly winds prevalently blow in the Šalek Valley. In the simulations, the most frequent winds of 1 m/s from the west, 2 m/s and 4 m/s from the southeast were used.

Summer lake temperatures were measured twice (June 1998 and August 1998) at every two meters, up to 30 m of deph. Average summer water temperature in epolimnium was approximately 25 °C, while hipolimnium water temperature was between 5 and 8 °C. Winter temperature was measured at the end of winter 1998/1999. The winter water temperature used in the simulations was 4.5 °C at all depths.

Preglednica 1. Povprečne dotočne / iztočne hitrosti za potoka Sopota in Lepena in za iztok iz Velenjskega jezera v obdobju med januarjem 1990 in decembrom 1995.
Table 1. Average flow rates for Sopota and Lepena streams and for the outflow from Lake Velenje for the period between January 1990 and December 1995.

	Celica I (smer X) *I Cell* (*X direction*))	Celica J (smer Y *J Cell* (*Y direction*)	Celica K (sloj) *K Cell* (*layer*)	U (hitrost toka v smeri X *flow speed in X direction*)	V (hitrost toka v smeri Y *flow speed in Y direction*)
Sopota	25	26	20	0	–0.00254
Lepena	34	18	20	–0.0126	0
Iztok/Outflow	5	4	20	0	–0.0151

Podatke o vtokih in iztoku vode iz jezera je priskrbela Agencija Republike Slovenije za okolje. Meritve vtokov in iztoka so potekale enkrat dnevno od januarja 1990 do decembra 1995. Povprečni pretok potoka Lepena je bil 0,127 m^3/s in potoka Sopota 0,628 m^3/s.

Inflow and outflow discharge data were provided by the Environmental Agency of the Republic of Slovenia. Inflows and outflow were daily measured from January 1990 until December 1995. The average discharge was 0.127 m^3/s for Lepena Stream, and 0.628 m^3/s

Povprečni iztok v reko Pako je bil 0,755 m^3/s. Dotoka in iztok vode so bili podani v ustreznih celicah (preglednica 1).

Pri hidrodinamičnem delu simulacij je bil časovni korak zaradi numerične stabilnosti omejen na DT = 180 s, pri čemer je bil uporabljen t.i. kriterij difuzije v vertikalni smeri za stabilnost modela:

$$DT \leq \frac{H_{\min}^2}{2N_v}$$

pri čemer je H_{min} debelina najtanjšega sloja, N$_v$ pa vertikalni kinematični koeficient turbulentne viskoznosti, izračunan po Koutitasovem modelu turbulence. Horizontalni kinematični koeficient turbulentne viskoznosti je bil ocenjen na podlagi izkušenj iz simulacij na drugih, podobnih jezerih; pri vseh simulacijah je imel vrednost 1 m^2/s.

3. HIDRODINAMIČNE SIMULACIJE

Za ugotavljanje osnovnega vzorca cirkulacije vode v jezeru v različnih razmerah smo izvedli 4 simulacije z upoštevanjem različnih smeri in hitrosti vetra ter poletno in zimsko razporeditvijo temperature po globini (preglednica 2).

for Sopota Stream. The average outflow to Paka River was 0.755 m^3/s. The two inflows and the outflow were given in isolated cells (Table 1).

In the hydrodynamic part of the simulations, the time step was limited to DT = 180 s due to numerical stability. The so-called vertical diffusion stability criterion was used:

where H_{min} represents the thickness of the thinnest layer and N_v stands for vertical kinematic coefficient of turbulent viscosity according to Koutitas turbulence model. The horizontal kinematic coefficient of turbulent viscosity was estimated from experience with other similar simulated lakes; for all simulations it was set to 1 m^2/s.

3. HYDRODYNAMIC SIMULATIONS

In order to determine the basic pattern of water circulation in the lake under different conditions, we performed four simulations with different wind directions and velocities and with summer and winter temperature distributions throughout the depth (Table 2).

Preglednica 2. Osnovni podatki, ki so bili uporabljeni pri hidrodinamičnih simulacijah.
Table 2. Some basic data used for the hydrodynamic simulations.

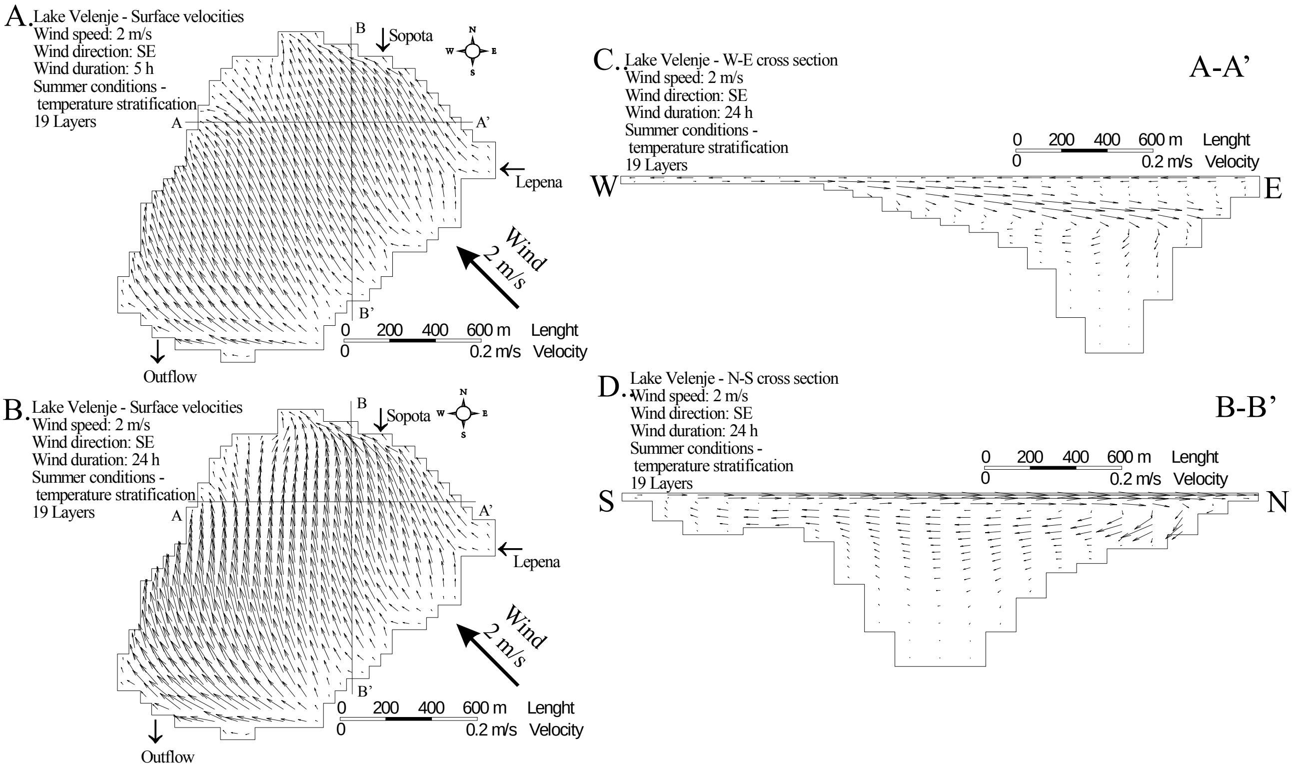
	Pretok Lepene *Lepena flow rate* (m^3/s)	Pretok Sopote *Sopota flow rate* (m^3/s)	Pretok na iztoku *Outflow flow rate* (m^3/s)	Smer vetra *Wind direction*	Hitrost vetra *Wind speed* (m/s)	Razmere *Conditions*
PRIMER1 *CASE 1*	0.628	0.127	0.755	SE	2	Poletne *Summer*
PRIMER2 *CASE 2*	0.628	0.127	0.755	W	1	Poletne *Summer*
PRIMER3 *CASE 3*	0.628	0.127	0.755	SSE	2	Zimske *Winter*
PRIMER4 *CASE 4*	0.628	0.127	0.755	W	1	Zimske *Winter*

V prvem primeru (primer 1) smo uporabili jugovzhodni veter s hitrostjo 2 m/s v poletnih temperaturnih razmerah. V drugem primeru (primer 2) smo uporabili zahodnik s hitrostjo 1 m/s v poletnih razmerah, tretji primer (primer 3) pa je bil simulacija v zimskih razmerah z jugo-jugovzhodnikom hitrosti 2 m/s. Primer 4 je bil simulacija primera 2 v zimskih razmerah. V vseh 4 primerih je simulacija trajala 24 ur. Poglavitni rezultati hidrodinamičnih simulacij so prikazani na slikah 1 in 2.

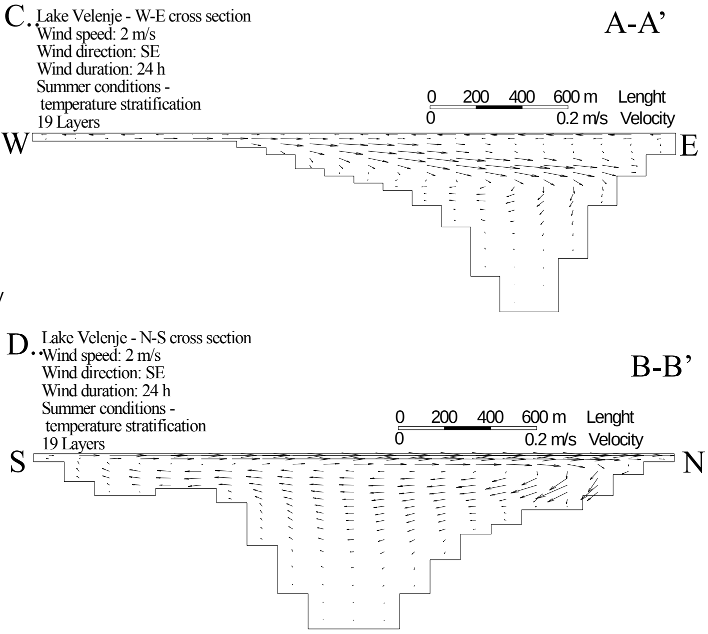
Z modeliranjem smo ugotovili, da je veter poglavitni vzrok tokov v jezeru. Ti so v veliki meri odvisni tako od hitrosti kot od smeri vetra. Simulacije z različnim trajanjem vetra kažejo, da se je hitrostno polje v prvih 12 urah pihanja vetra spreminjalo. Po 12 urah pa so se hitrost in smer gibanja vode in vetra uskladile in se niso več spreminjale. Hitrosti gibanja vode v Velenjskem jezeru so močno odvisne tudi od morfologije jezerskega dna. Hitrosti v površinskem sloju so mnogo višje v najplitvejšem delu jezera. Vtoki in iztok iz jezera pa celo pri simulacijah brez upoštevanja vpliva vetra niso pokazali skoraj nobenega vpliva na gibanje vode.

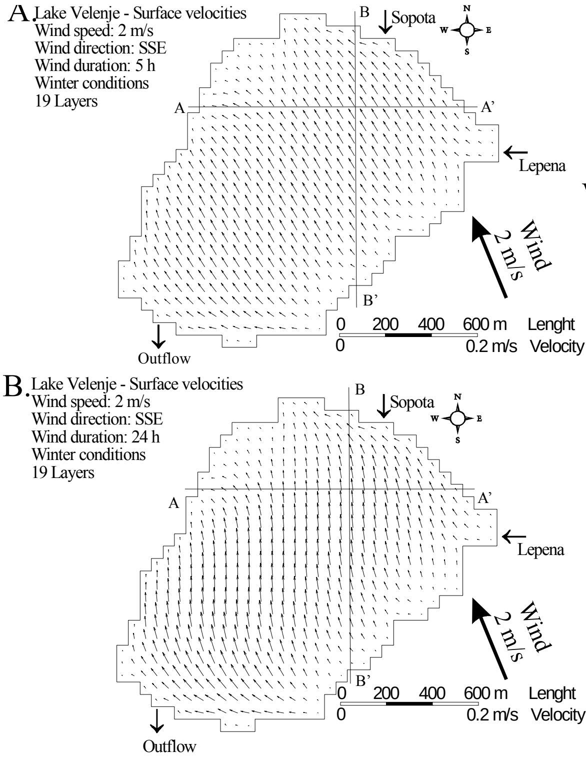
In the first case (Case 1) we used a southeasterly wind with speed of 2 m/s under summer conditions. In the second case (Case 2) a westerly wind with a speed of 1 m/s under summer conditions was used. The third case (Case 3) was a simulation under winter conditions with south-southeasterly wind of 2 m/s. Case 4 was a simulation of Case 2 under winter conditions. The simulation time was 24 hours for all four cases. The main hydrodynamic simulations results are shown on Figures 1 and 2.

Modeling revealed that the wind is the main forcing factor that causes the circulation of the lake water. Water flow in the lake is strongly dependent upon wind speed and direction. Simulations with different wind duration show that, within the first 12 hours, the wind blowing over the lake changes water velocity and direction. After a 12-hour period, wind and water velocities and directions are balanced and do not change anymore. Water velocities in Lake Velenje are also strongly dependent upon the morphology of the lake basin. Surface velocities are much higher over the shallowest parts of the basin. Even in simulations with zero wind speed, the inflows and outflow show nearly no influence on water movement.



Slika 1. Hidrodinamični rezultati v poletnih razmerah z jugovzhodnim vetrom, 2 m/s, po A.) 5 urah in B.) 24 urah simulacije v površinskem sloju in dveh prerezih Velenjskega jezera (primer 1).
Figure 1. Results of hydrodynamic under summer conditions with southeasterly wind, 2 m/s, after A.) 5 hours and B.) 24 hours of simulation in Lake Velenje surface layer and in vertical cross-sections (Case 1).





Slika 2. Hidrodinamični rezultati v zimskih razmerah z jugo-jugovzhodnim vetrom, 2 m/s, po A.) 5 urah in B.) 24 urah simulacije v površinskem sloju in dveh prerezih Velenjskega jezera (primer 3).
Figure 2. Results of hydrodynamic under winter conditions with south-southeasterly wind, 2 m/s, after A.) 5 hours and B.) 24 hours of simulation in Lake Velenje surface layer and in vertical cross-sections (Case 3).

V prečnih prerezih se pojavi gibanje vode v obliki močnejšega zgornjega in manj izraženega spodnjega vrtinca zaradi močne temperaturne stratifikacije med pomladnimi in poletnimi meseci. Ta pojav je v alpskih jezerih dobro poznan. Voda iz globljih slojev ne doseže površine jezera, zato ni neposrednega vnosa kisika v spodnje sloje, to pa v mnogih alpskih jezerih povzroča probleme s kakovostjo vode. Tudi večje hitrosti vetra ne vplivajo na kroženje vode v globljih delih jezera (nad 30 m globine).

Med zimskimi in pomladnimi meseci je voda v jezeru popolnoma premešana. Temperaturne stratifikacije ni bilo opaziti. V takih primerih lahko celo šibki vetrovi povzročijo krožno gibanje vode, ki sega od površja do dna jezera. Mešanje vode po celotni

The circulation in the vertical cross section is divided into a stronger upper vortex and less intense lower vortex due to sharp temperature stratification during the spring and summer months. This phenomenon is well known in alpine lakes. As the bottom water cannot reach the surface, there is no direct oxygenation of the bottom layers, which causes water quality problems in several lakes. Water circulation in the deepest parts of the lake (over 30 m of depth) is unaffected by higher wind speeds.

During the winter and spring months the water in the lake is well mixed. No temperature stratification was observed. In these cases even weak winds can cause a circulation vortex, which extends from the surface to the bottom. Water circulation from the surface to bottom thus causes well-globini tako povzroča dovoljšen vnos kisika tudi v globlje sloje jezera. V zelo hladnih zimah gladina jezera zamrzne. Debelina ledu je lahko do 30 cm. V takšnih pogojih veter nima vpliva na gibanje vode.

V skladu z najpogostejšimi smermi vetra lahko zaključimo, da je v površinskem sloju jezera najbolj pogosta smer toka z vzhoda proti zahodu.

4. PREVERJANJE A MODELA IN SIMULACIJE

4.1 PREVERJANJE Z $\delta^{18}O$ IN $\delta^{2}H$

Hidrodinamični del modela je bil predhodno umerjen in preverjen v podobnih slovenskih jezerih (Rajar in Četina, 1992a; Rajar in Četina 1993 Rajar *et al.*, 1995) in v Severnem Jadranu (Rajar, 1992; Rajar in Četina, 1992b; Rajar *et al.*, 1995, Širca 1996; Širca *et al.*, 1999a; Širca *et al.*, 1999b; Rajar *et al.*, 2000). Meritve hitrosti vode v Velenjskem jezeru se niso izvajale. Približno gibanje vode v površinskem sloju smo ugotavljali s pomočjo stabilnih izotopov $\delta^{18}O$ in $\delta^{2}H$. Razmerja med vsebnostjo težjih in lažjih izotopov O in H so se uporabila kot sledila za določanje gibanja vode v Velenjskem jezeru in njegovih vtokih.

Izotopska sestava kisika v vodi je bila določena z uporabo standardnih metod, ki temeljijo na ravnotežju z referenčnim CO_2 pri 25°C v 24 h (Epstein and Mayeda, 1953), ki je potem merjeno na masnem spektrometru Varian MAT 250. Meritev izotopske sestave devterija v vodi temelji na redukciji vode na Cr pri 800 °C. Sproščen plin vodik se potem uporabi za določitev izotopske sestave devterija v vodi (Gehre et al., 1996), ki je bila izmerjena na masnem spektrometru Varian MAT 250. Kalibracija $\delta^{18}O$ in $\delta^{2}H$ vrednosti je potekala s pomočjo mednarodnih standardov VSMOW, GISP in SLAP (‰ vrednosti) analiziranih po enakem postopku kot vzorec. Natančnost meritev $\delta^{18}O$ in $\delta^{2}H$ temelječa na ponavljajočih se meritvah je bila ±0.05‰ in ±1.0‰.

Rezultati simulacij in primerjava z merjenimi vrednostmi v površinskem sloju

oxygenated bottom water. In very cold winters the lake surface can be completely frozen. The ice layer can be up to 30 cm thick. Under such conditions, the wind has no influence on water movement.

Regarding the most common wind directions, it can be concluded that the most common flow direction in the surface layer is from east to west.

4. MODEL VERIFICATION AND SIMULATIONS

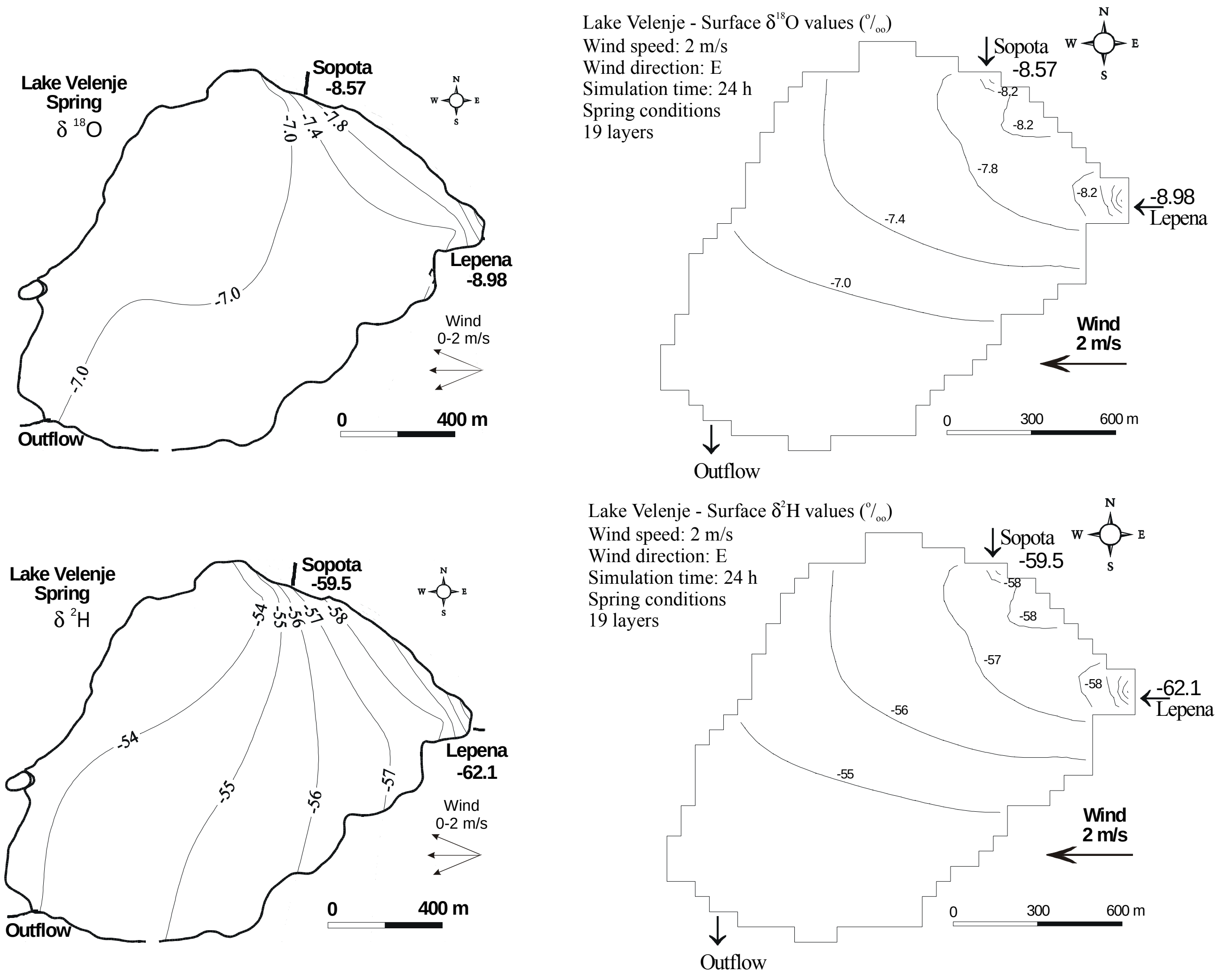
4.1 VERIFICATION BY $\delta^{18}O$ AND $\delta^{2}H$

The hydrodynamic part of the model has been previously calibrated and verified in similar Slovenian lakes (Rajar and Četina, 1992a; Rajar and Četina 1993 Rajar *et al.*, 1995) and in the Northern Adriatic Sea (Rajar, 1992; Rajar and Četina, 1992b; Rajar *et al.*, 1995, Širca 1996; Širca *et al.*, 1999a; Širca *et al.*, 1999b; Rajar *et al.*, 2000). Measurements of water velocities in Lake Velenje were not conducted. Approximate water movement in the surface layer was established by use of the stable isotopes $\delta^{18}O$ and $\delta^{2}H$. The proportions of heavier and lighter isotopes of O and H were used as tracers of water cycling in Lake Velenje and its inflows.

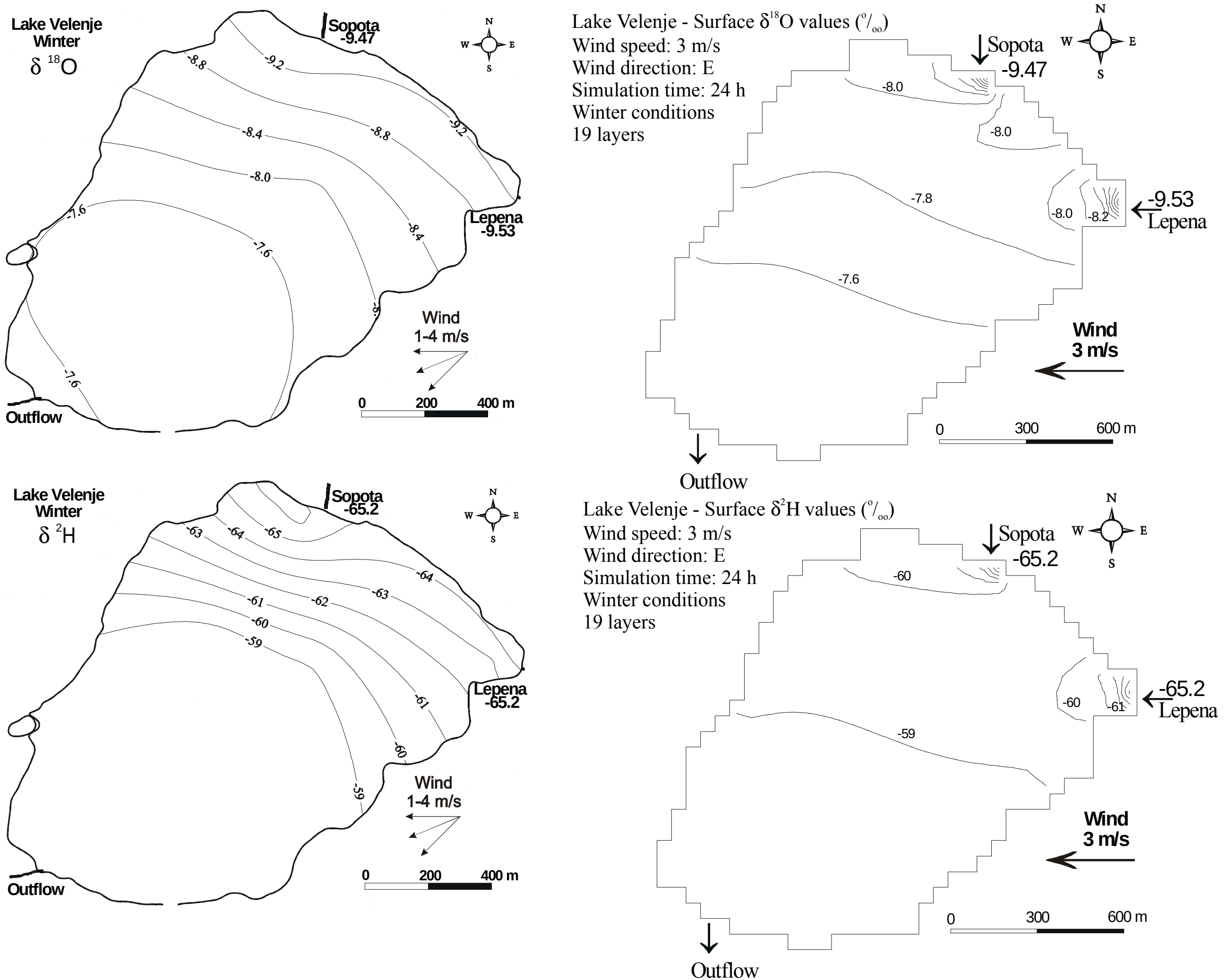
The isotopic composition of oxygen in water was determined using the standard method based upon equilibration with referenced CO_2 at 25°C for 24 h (Epstein and Mayeda, 1953), which was then measured on a Varian MAT 250 mass spectrometer. Reduction of water on Cr at 800 °C to produce hydrogen gas is used to determine the isotopic composition of deuterium in water (Gehre et al., 1996). The hydrogen gas was then measured on a Varian MAT 250 mass spectrometer. The calibration of the $\delta^{18}O$ and $\delta^{2}H$ values analysed with respect to the international standards was carried out by analysing VSMOW, GISP and SLAP (‰ values) with the same procedures. The precision of the analyses of $\delta^{18}O$ and $\delta^{2}H$ based upon replicate measurements was ±0.05‰, and ±1.0‰, respectively.

Velenjskega jezera so prikazani na slikah 3 in 4.

Simulation results and comparison to measured values in surface layer of Lake Velenje are shown in Figure 3 and Figure 4.



Slika 3. Izmerjene vrednosti $\delta^{18}O$ in $\delta^{2}H$ (v ‰) in primerjava s simuliranimi vrednostmi v površinskem sloju Velenjskega jezera (pomlad 1998).
Figure 3. Measured $\delta^{18}O$ *and* $\delta^{2}H$ *values (in ‰) and comparison to simulated values in the surface layer of Lake Velenje (spring 1998).*



Slika 4. Izmerjene vrednosti δ^{18}O in δ^{2}H (v ‰) in primerjava s simuliranimi vrednostmi v površinskem sloju Velenjskega jezera (zima 1999).

Figure 4. Measured δ^{18}O and δ^{2}H values (in ‰) and comparison to simulated values in the surface layer of Lake Velenje (winter 1999).

Kroženje in mešanje vode, ki vteka v jezero je odvisno od hitrosti vetra in vtočnih hitrosti. Voda, ki vteka v jezero, ima na dotoku nižje vrednosti δ^{18}O (pomlad: –8,57 do –8,98 $^{o}/_{oo}$; zima: –9,4 do –9,35 $^{o}/_{oo}$) in δ^{2}H (pomlad: –59,5 do –62 $^{o}/_{oo}$; zima: –65,2 $^{o}/_{oo}$) kot jezerska voda. V jezeru se te vrednosti višajo v odvisnosti od količine dotekajoče vode, stopnje mešanja z jezersko vodo in izhlapevanja. Razvidno je, da je porazdelitev vtekajoče vode po jezeru odvisna predvsem od hitrosti vetra in vtočnih hitrosti. Pozimi, ko je bil veter močnejši kot spomladi, je dotekajoča voda po površini jezera segla veliko dlje kot spomladi. Dejanska smer gibanja vode je podobna rezultatom simulacij. Tako vrednosti δ^{18}O kot δ^{2}H so pokazale enak gradient

Water cycling and the distribution of inflow water depend upon wind speed and inflow velocity. The inflows have lower δ^{18}O (spring: –8.57 to –8.98 $^{o}/_{oo}$; winter: –9.4 to –9.35 $^{o}/_{oo}$) and δ^{2}H (spring: –59.5 to –62 $^{o}/_{oo}$; winter: –65.2 $^{o}/_{oo}$) values than the lake water. In the lake, these values are changing toward higher values depending upon the inflow water discharge, its degree of mixing with the lake water, and evaporation. As can be seen, inflow water is distributed from the inflows to the lake depending primarily on wind speed and inflow velocity. In winter, when the wind was stronger than in the spring, the inflow water flows out over the lake surface much further into the lake than in the spring. The true direction of the water movement is similar to the simulated movement. Both the δ^{18}O and koncentracij. Na obeh slikah (sliki 1 in 2) sta prikazani hitrostni polji v površinskem sloju jezera. Simulacijo smo izvedli z uporabo podobnega vetra, ki je pihal nad jezerom na dan, ko smo opravljali meritve.

Omeniti je treba, da je to preverjanje zgolj kvalitativno, posredno in zelo približno. To je bil le poskus korelacije hitrostnih polj v površinskem sloju vode s porazdelitvijo različnih izotopov istega elementa. Meritve izotopov so lahko zelo uporabne pri sledenju gibanja vode. Za boljše rezultate pa bi bilo treba izvesti mnogo več meritev in simulacij (Wachniew in Rozanski, 1998).

4.2 MODELIRANJE TRANSPORTA ŽIVEGA SREBRA IN PRIMERJAVA Z MERITVAMI

Model PCFLOW3D vključuje tudi tako imenovani “modul za račun transporta” (transportno-disperzijski modul), imenovan tudi “modul za račun transporta in pretvorb snovi”, s katerim lahko simuliramo transport in disperzijo določenih masnih količin (npr. kontaminanta). Modeliranje masnega transporta v celoti temelji na poznavanju gibanja vode, ki je rezultat hidrodinamičnega modula in dodatnega koeficienta disperzije (Nihuol *et al.,* 1992). Ker koncentracija določenega kontaminanta v večini primerov bistveno ne vpliva na gostoto vode in kroženje vode, je hidrodinamični modul (HD) ponavadi neodvisen od transportno-disperzijskega modula (MT).

Simulacije transporta različnih zvrsti živega srebra so odvisne od istih vhodnih podatkov kot hidrodinamične simulacije, obravnavane v prejšnjem delu. Podatki o vetru in temperatura jezerske vode, uporabljeni v simulacijah, so bili približno enaki kot veter in temperatura, izmerjena v dneh, ko smo izvajali meritve.

V teh simulacijah so bile različne zvrsti živega srebra obravnavane kot konzervativni polutanti in niso vplivale druga na drugo. Sedimentacija in resuspendiranje ter vnos iz ozračja in v ozračje niso bili upoštevani.

S temi simulacijami smo želeli potrditi

δ^2H values gave the same gradient of concentration. On both figures (Fig. 1 and Fig. 2) the velocity fields in the water surface layer are shown. The simulation was performed using wind conditions similar to those found over the lake on the day when the samples were collected.

It should be noted that this verification is only qualitative, indirect and very approximate. This was a trial to correlate water velocity fields to the distribution of different isotopes of the same element. Isotope measurements can be very useful for water movement tracing. For more detailed results many more measurements and simulations should be done (Wachniew and Rozanski, 1998).

4.2 MODELING OF MERCURY TRANSPORT AND COMPARISON TO MEASUREMENTS

The model PCFLOW3D has included within it a so-called “mass-transport module”, also known as the transport and fate module, which simulates transport and dispersion of the relevant quantity (i.e. of a contaminant). Mass transport modeling depends entirely upon the hydrodynamic circulation obtained by the hydrodynamic module and additionally upon dispersion coefficients (Nihuol *et al.*, 1992). As the concentration of a particular contaminant in most cases does not significantly influence water density and its circulation, the hydrodynamic module is usually independent of the mass-transport module.

Mercury species transport simulations are based upon the same input data as the hydrodynamic simulations in the previous section. Wind conditions and lake water temperature used for the simulations were approximately the same as measured wind and temperature on the day when the samples were collected.

In these simulations, different mercury species are conservative pollutants and do not interact with each other. There is no sedimentation or resuspension, and neither input from the atmosphere nor evasion to the atmosphere.

pravilno delovanje modela. Dokazovati bi morale, da bi bile nadaljnje simulacije cirkulacije vode zanesljive vsaj do določene mere natančnosti. Ugotoviti smo želeli tudi, kakšen vpliv imajo na transport živega srebra v jezeru vtoki in različne hitrosti in smeri vetra.

Simulirali smo dva primera transporta živega srebra (primer A in primer B). V obeh simulacijah smo se z modelom skušali čim bolj približati dejanskemu stanju. Pretočne hitrosti na vtoku so bile v obeh primerih iste in so bile enake kot pri hidrodinamičnih simulacijah. Pretoki Sopote in Lepene so bili merjeni med januarjem 1990 in decembrom 1995.

V primeru A smo izvedli simulacijo vnosa živega srebra z vtoki v jezero ter njegovo razporeditev v spomladanskih razmerah. Upoštevali smo vzhodni veter s hitrostjo 2 m/s, kar je bil najboljši približek izmerjenim podatkom. Začetne koncentracije različnih oblik Hg in MeHg v jezeru prikazujemo v preglednici 3.

V drugem primeru (primer B) smo simulirali zimske razmere. V tem primeru je bil veter močnejši kot pri prvi simulaciji (vzhodni veter s hitrostjo 3 m/s). Začetne koncentracije Hg v jezeru in vtokih so prikazane v preglednici 4.

With these simulations we wished to validate the model. This verification should be a proof, that further simulations of water circulation are reliable, at least to a certain degree of accuracy. We also wished to establish the influence of the inflows and of different wind speeds and directions on mercury transport in the lake.

Two cases (Case A and Case B) of mercury transport were simulated. In both simulations we tried to accommodate the model to the real situation as much as possible. Inflow flow rates were the same in both cases, and were also similar in the hydrodynamic simulations. Flow rates of Sopota and Lepena Streams were measured in January 1990 and December 1995.

In Case A, a simulation of mercury input from inflows and its distribution under spring conditions were performed. An easterly wind with a speed of 2 m/s was used, which was nearest to the measured data. Initial concentration of different Hg and MeHg forms in the lake and inflow water were shown in Table 3.

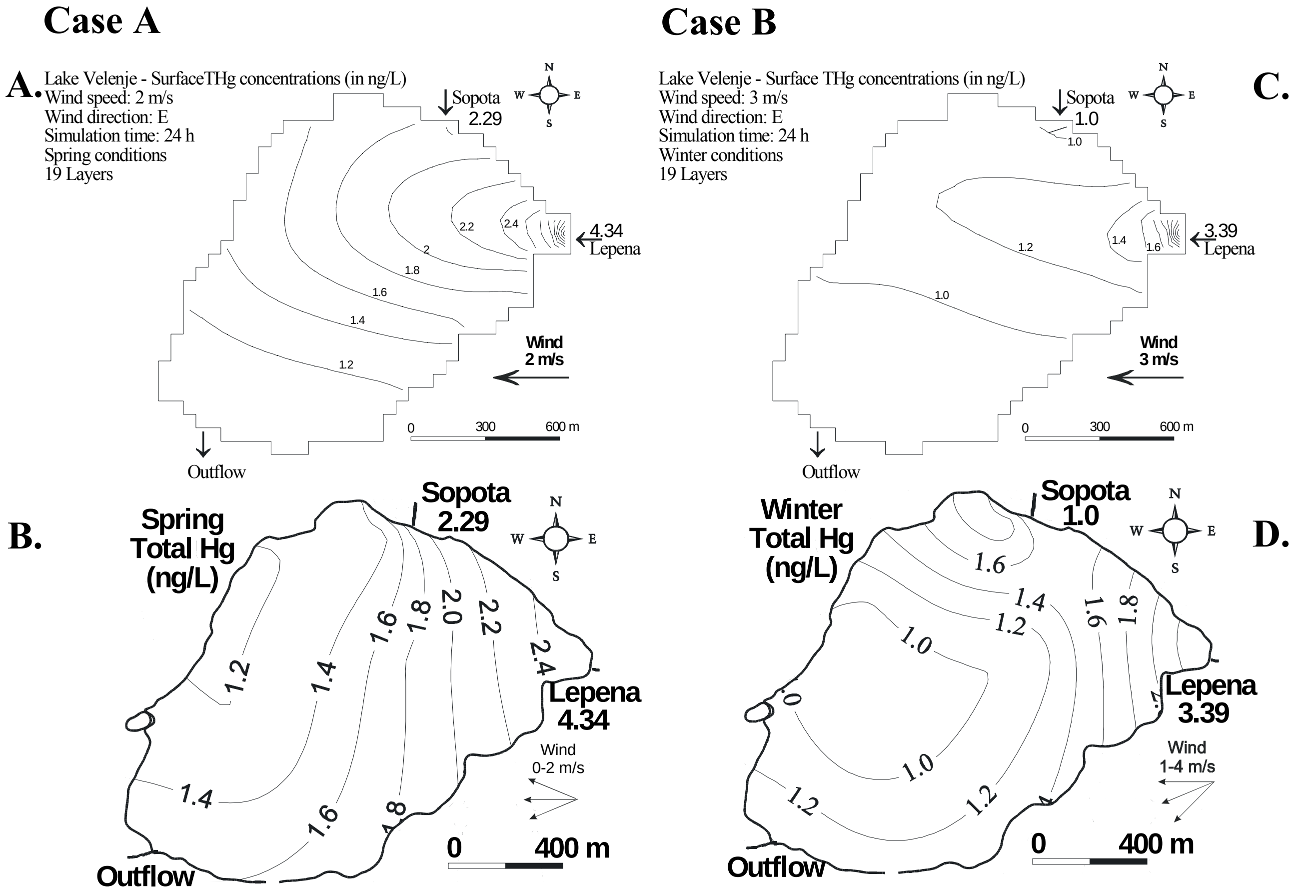
The second case (Case B) was a simulation under winter conditions. In this case, wind was stronger than in the previous simulation (easterly wind with a speed of 3 m/s). Initial Hg concentrations in the lake and inflows were as follows in Table 4.

Preglednica 3. Hitrost in smer vetra, pretok in različne oblike živega srebra pri simulaciji primera A.
Table 3. Wind speed and direction, flow rates, and different mercury forms used for the simulation of Case A.

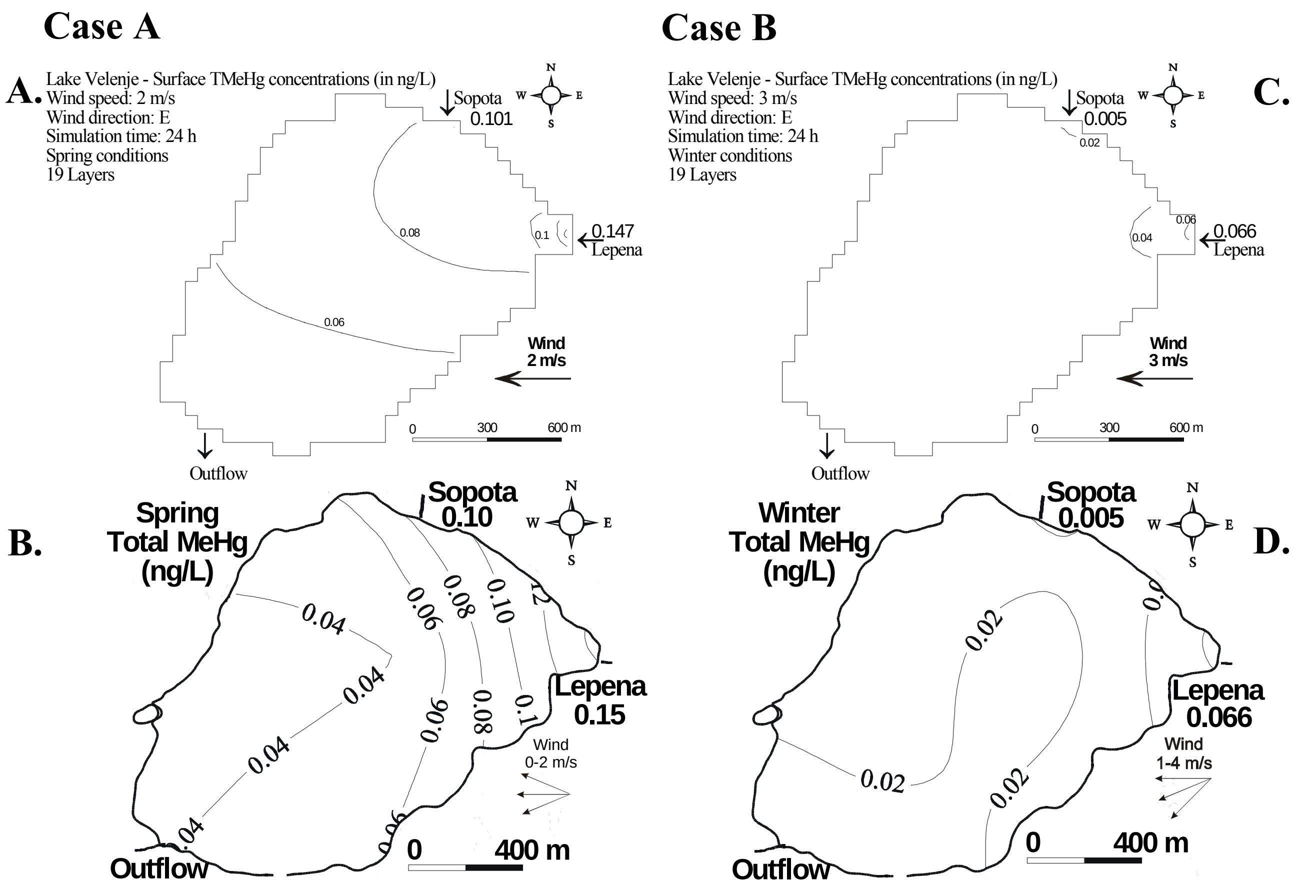
	Hitrost vetra *Wind speed* (m/s)	Pretok/ *Flow rate* (m^3/s)	THg (ng/l)	DHg (ng/l)	PHg (ng/l)	TMeHg (ng/l)	DMeHg (ng/l)	PMeHg (ng/l)
Sopota	2 m/s, E	0.127	2.29	0.64	1.66	0.101	0.052	0.049
Lepena		0.628	4.34	1.07	3.27	0.147	0.027	0.120
Začetna koncentracija v jezeru *Initial concentration in the lake*			1.24	0.56	0.68	0.619	0.024	0.026

Preglednica 4. Hitrost in smer vetra, pretok in različne oblike živega srebra pri simulaciji primera B.
Table 4. *Wind speed and direction, flow rates and different mercury forms used for the simulation of Case B.*

	Hitrost vetra/ *Wind Speed* (m/s)	Pretok/ *Flow rate* (m^3/s)	THg (ng/l)	DHg (ng/l)	PHg (ng/l)	TMeHg (ng/l)	DMeHg (ng/l)	PMeHg (ng/l)
Sopota	3 m/s, E	0.127	1.00	0.42	0.59	0.005	0.004	0.0001
Lepena		0.628	3.39	1.11	2.27	0.066	0.009	0.056
Začetna koncentracija v jezeru *Initial concentration in the lake*			0.97	0.73	0.25	0.0253	0.0145	0.0133



Slika 5. Rezultati simulacije transporta celokupnega živega srebra in njegova porazdelitev (A., C.) v Velenjskem jezeru v pomladanskih (primer A) in zimskih (primer B) razmerah in primerjava z izmerjenimi vrednostmi (C., D.) (koncentracije so v ng/l).
Figure 5. *Simulation results for total mercury transport and distribution (A., C.) in Lake Velenje under spring (Case A) and winter (Case B) conditions and comparison to measured values (C., D.)(concentrations are in ng/l).*



Slika 6. Rezultati simulacije transporta celokupnega metil-živega srebra in porazdelitev (A., C.) v Velenjskem jezeru v pomladanskih (primer A) in zimskih (primer B) razmerah in primerjava z izmerjenimi vrednostmi (B., D.) (koncentracije so v ng/l).
Figure 6. Simulation results for total methylmercury transport and distribution (A., C.) in Lake Velenje under spring (Case A) and winter (Case B) conditions and comparison to measured values (B., D.) (concentrations are in ng/l).

Rezultati primera A kažejo, da gibanje vode v površinskem sloju jezera poteka pretežno z vzhoda proti zahodu. Simulirane razporeditve THg (slika 5), DHg in PHg so približno primerljive z meritvami. Živo srebro v teh treh oblikah vstopa v jezero z Lepeno in se razporedi po površini jezera z gibanjem vode.

Rezultati simulacije za različne oblike MeHg (slika 6) se bistveno razlikujejo od izmerjenih vrednosti drugih oblik Hg. To lahko obrazložimo z dejstvom, da je verjetno znaten delež Hg v jezeru metiliran in da razporeditev MeHg v različnih oblikah ni odvisna samo od gibanja vode, temveč tudi od kemijskih in bioloških lastnosti jezera. Biološki in kemični vplivi v modelu niso upoštevani, kar je verjetno vzrok razlikam, ki so se pojavile med rezultati simulacij in

The simulation for Case A shows that water movement in the lake surface is mainly from east to west. The simulated distributions of THg (Figure 5), DHg and PHg are approximately comparable to the measurements. All three forms entered the lake mostly via Lepena Stream and are distributed across the surface of the lake by water movement.

The simulation results for the various MeHg (Figure 6) forms are much more different from the measured values than are the other Hg forms. This difference can be explained by the fact that probably a significant part of Hg is methylated in the lake, and that distribution of MeHg forms depends not only on water movement, but also on chemistry and biology of the lake. Biological and chemical interactions are not included in the model and this is probably the reason for meritvami.

Pri simulaciji zimskih razmer (primer B) so koncentracije in razporeditev Hg na površju zgolj grobo primerljive z izmerjenimi vrednostmi. V obeh primerih (za THg, DHg in PHg) simulacije in meritve kažejo, da je glavni vir Hg v jezeru potok Lepena. Živo srebro je večinoma vezano na delce. Izračunane koncentracije in porazdelitev Hg na površini jezera so odvisne od smeri vetra in hitrosti nad površjem in posledičnega gibanja vode v jezeru. Živo srebro je imelo v Lepeni začetno koncentracijo 3,39 ng/l za THg, 1,11 ng/l za DHg in 2,27 ng/l za PHg. Koncentracije so se zniževale v smeri od vzhoda proti zahodu, tako pri simulacijah kot pri meritvah vseh treh oblik Hg.

Simulirane in izmerjene vrednosti različnih zvrsti MeHg so v grobem primerljive. Glavna razlika je, da meritve kažejo višje koncentracije vseh izmerjenih oblik MeHg na zahodni strani jezera poleg deponije, simulacije pa kažejo ravno obratno sliko; višje koncentracije so bile na vzhodni strani jezera poleg vtokov, predvsem poleg Lepene. V simulacijah so se koncentracije MeHg na površini jezera zniževale od vzhoda proti zahodu. Koncentracije v sredini jezera pa so v istem velikostnem razredu za vse tri zvrsti MeHg, tako v izračunanih kot v izmerjenih rezultatih.

5. ZAKLJUČKI

Kot je bilo pričakovati, rezultati simulacij kažejo, da lahko rezultati modela brez nadaljnjih izboljšav pokažejo zgolj osnovne značilnosti transporta in disperzije živega srebra v Velenjskem jezeru. Poglavitne vzroke razlik med simuliranimi in izmerjenimi rezultati lahko povzamemo:

- Vhodni podatki o vetru, ki smo jih uporabili pri simulaciji hidrodinamične cirkulacije, niso bili dovolj natančni, saj sta se hitrost in smer vetra v času meritev spreminjala, hitrost vetra pa tudi ni enakomerna nad celim jezerom.
- V simulacijah nismo upoštevali procesov pretvorb živega srebra, čeprav nekateri od njih niso zanemarljivi (npr. izhlapevanje,

the differences between the simulated and measured results.

In the simulation of winter conditions (Case B) concentrations and surface Hg distributions are very roughly comparable to the measured values. In both cases (for THg, DHg and PHg), the simulations and measurements show that the main source of Hg in the lake is Lepena Stream. Mercury was mostly bound to particulate matter. The simulated concentrations and Hg distribution in the lake surface depend upon wind direction and speed over the lake surface, and accordingly on water movement in the lake. Mercury is distributed from Lepena Stream with an initial concentration of 3.39 ng/l for THg, 1.11 ng/l for DHg and 2.27 ng/l for PHg. The concentrations are decreasing in the direction from east to west in both the simulations and measurements for all three Hg forms.

The simulated and measured values for MeHg species are roughly comparable. The main difference is that the measurements show higher concentrations of all measured MeHg forms on the western side of the lake near to the landfill, while the simulations show the opposite situation; higher concentrations were on the eastern side of the lake near the inflows, particularly near Lepena Stream. In the simulations, MeHg concentrations in the lake surface decrease from east to west. Concentrations in the middle of the lake are in the same range for all three MeHg species, both in the simulations and measured results.

5. CONCLUSIONS

As expected, the simulation results show that the model without further upgrade can give only the very basic features of the transport – dispersion phenomena of mercury in Lake Velenje. The main causes of the differences between the simulated and measured results can be summarized as follows:

- The wind input data used to simulate HD circulation were not quite accurate, as the wind speed and direction were changing during the time of measurement and partly also spatially over the lake surface.
- The processes of mercury transformation were not taken into account in the simulations, but some of them are not negligible in reality (e.g. evaporation,

usedanje, metilacija, redukcija).

- Pri simulacijah niso bili upoštevani nekateri drugi pomembnejši pojavi, (to so sedimentacija/resuspenzija, adsorbcija/desorpcija).

Zaključimo lahko, da so bile poglavitne značilnosti hidrodinamične cirkulacije uspešno simulirane, medtem ko moramo rezultate simulacije transporta in disperzije različnih oblik živega srebra obravnavati z zadržkom.

Z modeliranjem smo pokazali, da je veter glavni vzrok gibanja jezerske vode. Tokovi v jezeru so močno odvisni od hitrosti in smeri vetra. Simulacije z različnim trajanjem vetra kažejo, da se v prvih 12 urah hitrostno polje zaradi vpliva vetra spreminja. Po 12 urah pa so se hitrost in smer gibanja vode in vetra uskladile in se niso več spreminjale. Hitrostno polje v Velenjskem jezeru je močno odvisno tudi od morfologije jezerskega dna. Hitrosti v površinskem sloju so bistveno višje v plitvejših delih jezera. V prečnih prerezih se pojavi gibanje vode v obliki močnejšega zgornjega in manj izraženega spodnjega vrtinca zaradi močne temperaturne stratifikacije med pomladnimi in poletnimi meseci. Ta pojav je v alpskih jezerih dobro poznan. Voda iz globljih slojev ne doseže površine jezera, zato ni neposrednega vnosa kisika v spodnje sloje, to pa v mnogih alpskih jezerih povzroča probleme s kakovostjo vode. Tudi večje hitrosti vetra ne vplivajo na kroženje vode v globljih delih jezera (nad 30 m globine).

Tudi vtoki vode nimajo večjega vpliva na kroženje vode, saj je pretok na vtoku premajhen. Tudi pri simulacijah brez upoštevanja vetra vtoki in iztoki nimajo skoraj nikakršnega vpliva na gibanje vode.

V skladu z najpogostejšimi smermi vetra lahko zaključimo, da je v površinskem sloju jezera najbolj pogosta smer toka z vzhoda proti zahodu.

ZAHVALA

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sedimentation, methylation, reduction, etc.).

- Some phenomena significant to the simulated events (i.e. sedimentation/resuspension, adsorption/desorption), were not taken into account in the simulations.

We can conclude that the main features of the HD circulation are simulated, while the results of the simulation of transport – dispersion of the different mercury forms must be regarded with caution.

Modeling revealed that the wind is the main forcing factor that causes the circulation of the lake water. Water flow in the lake is strongly dependent upon wind speed and direction. Simulations with different wind duration show that, within the first 12 hours, the wind blowing over the lake changes the water velocities and direction. After a 12-hour period, wind and water velocities and directions are balanced and do not change anymore. Water velocities in Lake Velenje are also strongly dependent upon the morphology of the lake basin. Surface velocities are much higher over the shallowest parts of the basin. The circulation in the vertical cross section is divided into a stronger upper vortex and less intense lower vortex due to strong temperature stratification during the spring and summer months. This phenomenon is well known in alpine lakes. As the bottom water cannot reach the surface, there is no direct oxygenation of the bottom layers, which cause water quality problems in several lakes. Water circulation in the deepest parts of the lake (over 30 m of depth) is unaffected by higher wind speeds.

The inflows also do not have much influence on water cycling because the inflow discharge is too small. Even in simulations with zero wind speed, the inflows and outflow show nearly no influence on water movement.

Regarding the most common wind directions, it can be concluded that the most common flow direction in the surface layer is from east to west.

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