MODELLING WATER AND SOLUTE FLOWS AT LAND-SEA AND LAND-ATMOSPHERE INTERFACES UNDER DATA LIMITATIONS

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ABSTRACT

Water and vapour flows from land to sea and the atmosphere are important for water resources, coastal ecosystems and climate. This thesis investigates possible methods for modelling these flows under often encountered unmonitored hydrological conditions and data limitations. Two contrasting types of drainage basin and associated data limitation/availability cases are considered: the Swedish unmonitored near-coastal catchment areas Forsmark and Simpevarp, for which detailed spatial but not much temporal variability data is available; and the much larger Aral Sea Drainage Basin (ASDB), for which spatial hydrological information is limited, while there is relatively well-known temporal change occurring in the Aral Sea itself and in the land and water use of the region over the last 50 years.

The hydrologic modelling for the Forsmark and Simpevarp catchment areas showed that the relatively large focused stream flows, and the mean values and total sums of the diffuse small stream-groundwater flow fields in between the large stream flows from land to sea are largely constrained by the catchment hydrological balances and relatively robust and certain to estimate. The ASDB hydrologic modelling indicated an evapotranspiration return flow to the atmosphere from the irrigation water input on irrigated land that is much higher than previous estimates in atmospheric modelling, implying possible considerably larger than previously estimated non-local water and climate effects of the world’s irrigated areas. The more detailed groundwater-seawater dynamics modelling carried out for the coastal parts of the ASDB showed that regional topography and bathymetry largely influence coastal groundwater flows during sea level lowering, with the Aral Sea shrinkage decreasing the seawater intrusion risk into the coastal groundwater considerably more for steeper than for flatter coastal topography parts of the region.

Keywords: Submarine groundwater discharge, unmonitored flows, catchment hydrology, evapotranspiration, bathymetry, GIS, Aral Sea, nuclear waste repository sites
LIST OF PAPERS APPENDED

This thesis comprises a summary of the following appended papers:


CONTRIBUTIONS TO THE PAPERS

I have been responsible for the input data compilation, numerical modelling and model development in all the appended papers and had the lead in writing Papers III-V. Jerker Jarsjö coordinated the SKB investigations and had the lead in writing Papers I-II. The chosen investigation set-up, results interpretation and final paper formulation are in all papers the results of collaboration between co-authors.

LIST OF RELATED PAPERS THAT ARE NOT APPENDED

Conference publications
Y. Shibuo, J. Jarsjö and G. Destouni (2007), Hydrologic responses to climatic changes and irrigation expansion within the Aral Sea basin, Geophysical Research Abstracts, Vol. 9, 09963, EGU General Assembly, Vienna, Austria


Reports and manuscripts

1 INTRODUCTION

Water and associated waterborne material and energy flows at the land-sea and land-atmosphere interfaces are important in Earth and environmental sciences as well as for climate, ecosystems and human societies. Of all the water precipitated over land, about 2/3 returns to the atmosphere via evapotranspiration at the land-atmosphere interface (L'vovich and White, 1990), carrying with it also latent heat that may be of great importance for climate. Large-scale evapotranspiration and its spatial distribution on land are difficult to measure, but may be calculated from hydrological modelling that is calibrated to fit available precipitation and river runoff monitoring data (e.g., Vörösmarty et al., 2000; De Wit, 2001; Döll et al., 2003). Such calibration is possible because evapotranspiration, inland water fluxes and water flows from land to sea are interconnected in the water balances of drainage basins. Changes in water use (Boucher et al., 2004; Lobell et al., 2006; Kueppers et al., 2007) and land cover and use (Fedema et al., 2005; Foley et al., 2005; Gordon et al., 2005), as well as climate change (Milly et al., 2002, 2005), however, may change both vapour fluxes at the land-atmosphere interface and inland water flows and flow interactions at the land-sea interface.

Furthermore, continental freshwater feeds nutrients, pollutants and other substances from various sources on land to downstream inland waters (Koplin et al., 2002; Kavanaugh et al., 2003; ERMITE, 2004; Baresel and Destouni, 2005) and eventually to the sea (Jacobson et al., 2000; HELCOM, 2005) all over the world. Many coastal bays and estuaries, as well as whole seas such as the Baltic Sea, face severe eutrophication problems, caused by systematic, long-term excess nutrient transport from land to coast (e.g., Darracq et al., 2005; Griffioen, 2006). Persistent and toxic organic pollutants (POPs, such as benzene, toluene and polyaromatic or chlorinated hydrocarbons) are furthermore found in coastal seawater as well as in near-shore sediments world-wide (see, e.g., Witt, 2002). Also this coastal zone pollution may to a considerable extent originate from inland land sources at e.g. industrial areas (Jarsjö et al., 2005; Bayer-Raich et al., 2006, Kalbus et al., 2007). The possible water flow and loading of waterborne pollutants from land to sea constitute also important consideration components in the extensive work to find suitable locations for final geological repositories for high-level radioactive nuclear waste (Werner et al., 2006; Jarsjö et al., 2006).

In all the above examples, inland sources for possible coastal zone pollution have existed and/or may potentially exist over long time periods (decades to centuries, or longer; see, e.g., Lindgren et al. (2007) for possible future long-term scenarios of nutrient loading from land to sea). These sources are further often located outside hydrologically well-monitored or well-characterised regions. For example, a recent assessment of the Swedish national monitoring of coastal nutrient loading shows that approximately 20% of the total Swedish catchment area draining into the Baltic Sea is nationally unmonitored, wherein lives a whole 55% of the Swedish population (Hannerz and Destouni, 2006). This implies that, even though Sweden is among the environmentally well-monitored areas of the world, many anthropogenic pollutant sources are located in its essentially unmonitored and most heavily populated near-coastal catchment areas.

The waterborne transport of pollutants from inland sources to the coast may follow any and, with some distribution, all of the following main hydrological pathways within and from drainage basins to the coast: the coupled groundwater-stream system, including diffuse groundwater discharge into streams and rivers, followed by stream-river discharge to the coast; only the stream pathway directly into coastal waters; only the groundwater pathway of submarine groundwater discharge (SGD) directly into coastal waters. In particular the possible magnitude of the latter, SGD pathway is often totally neglected in basin-scale nutrient
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and pollutant transport-transformation models, even though it is recently often discussed in the scientific literature (Moore, 1996; Moore and Church, 1996; Younger, 1996; Li et al., 1999; Basu, 2001; Harvey, 2002; Burnett et al., 2003; Destouni and Prieto, 2003; Smith, 2004; Prieto and Destouni, 2005; Wilson, 2005) and may be chemically and ecologically important for coastal waters (e.g., Moore, 1999; Burnett et al., 2003).

In order to realistically and accurately quantify the vapour, water and waterborne material flows from land to the atmosphere and the sea, we need to better understand and model the different pathways and distributions of inland water flows within drainage basins and along coastlines under various field conditions. Such quantification and modelling efforts, however, may currently be hampered by important hydrological data gaps, such as those implied by systematically unmonitored near-coastal catchment areas (Hannerz and Destouni, 2006). An overall aim of this thesis is to investigate and propose possible methods for modelling and quantifying water flow distributions from land to atmosphere and from land to sea under unmonitored conditions and data limitations, such as absence of the extensive time series of surface water runoff that constitute a common input data and model calibration-validation basis in hydrologic modelling. This aim is pursued by close investigation of two contrasting types of drainage basins and associated data limitation/availability cases.

The first case type includes two small Swedish unmonitored near-coastal catchment areas, the Forsmark and Simpevarp areas, for which detailed spatial data have recently become available, while there are no extended discharge time series and generally not much information on temporal flow variability available for these areas. The reason for the recent increase of fine-resolved spatial data is that, even though these catchment areas have been previously hydrologically unmonitored, at least their spatial surface characteristics, such as topography, vegetation, land use and soil texture, are now being intensively investigated as part of the Swedish site investigations for a possible geological repository of high-level radioactive nuclear waste (Werner et al., 2006). A main objective of this thesis has been to investigate how such new fine-resolved spatial data, without any available discharge time series, may be used for modelling the interconnected evapotranspiration-groundwater-surface water flows (Paper I) and quantifying the resulting land-to-sea discharge distributions (among streams and diffuse SGD) along the coastlines of these typically unmonitored near-coastal catchment areas.

The second case considered in this thesis is that of the Aral Sea Drainage Basin (ASDB), for which spatial hydrological information is quite limited, while there is relatively well-known overall temporal change occurring in the Aral Sea itself and in the land and water use of the region over the last 50 years (Björklund, 1999; Waltham and Sholji, 2001; Jarsjö and Destouni, 2004; Glantz, 2005). The second main objective of the thesis has been to investigate the possible use of such relatively well-known, long-term temporal change in the recipient coastal and marine waters (here the Aral Sea) of drainage basin discharges (here the ASDB) for modelling and quantifying the often largely unmonitored spatial-temporal distributions of evapotranspiration within the basins (Paper III) and resulting freshwater-sea water flow interactions along the coastlines that constitute the basins’ interfaces with the sea (Papers IV-V).

2 CASE AND MODEL DESCRIPTION

2.1 Forsmark and Simpevarp cases
The Forsmark and Simpevarp areas are located along the Baltic coastline in Sweden (Fig. 1). Nuclear power plants exist at both sites and during 2002 the Swedish Nuclear Fuel and Waste Management Co (SKB) started site investigations at the sites as part of the process of finding a suitable location for a deep repository for high level nuclear waste. Therefore, detailed hydrological,
hydrogeochemical and ecological investigations are now being carried out in both areas. However, hydrological runoff time series data are not available for any extended periods since the monitoring started very recently in both areas (2002).

The Forsmark area is located approximately 150 km north of Stockholm and extends 4 km inland from the coast. In this area, the land surface is characterized by mainly quaternary deposits of till that covers approximately 75% of the surface. It also contains bedrock outcrops that cover about 5% of the surface. The area is topographically flat. More than 95% of the area has a mean slope less than 5 degrees (Brydsten and Strömgren, 2004), and the highest elevation is about 50 m a.s.l. Due to post glacial isostatic rebound, there is an ongoing uplift (around 6 mm/year) of the region. Therefore, there is also a prominent shoreline displacement. The area was beneath the Baltic Sea surface around 1000 years ago, and peat growth is now rapid (see further Lindborg, 2005a, Sohlenius et al., 2004 and references therein). Lakes and wetlands are relatively common, and groundwater levels are reported to be shallow. The mean annual temperature is between 5 to 5.5 degrees and the mean annual precipitation is between 600 to 650 mm/year.

The Simpevarp area is located approximately 300 km south of Stockholm and extends 8 km inland from the coast, with ap-
proximately the same highest elevation as Forsmark. Most of the land surface is covered by quaternary deposits of till, but compared to the Forsmark, bedrock is more frequently exposed at higher elevations (Werner et al., 2005). Although the topography of the Simpevarp area is slightly steeper than the Forsmark area, it is relatively flat with more than 80% of the area having a mean slope of less than 5 degrees (Brydsten and Strömgren, 2005). Post glacial land uplift is less pronounced than in Forsmark (around 1 mm/year) (Lindborg, 2005b and references therein). Lakes and wetlands are also relatively common, and groundwater levels are shallow. The climate is slightly warmer than in Forsmark with an annual mean temperature of between 6 to 7 degrees. The mean annual precipitation is between 500 to 600 mm/year.

2.2 Aral Sea case
The Aral Sea is a terminal lake formed on a topographic depression in a desert area in Central Asia (Fig. 2). It is surrounded by the Ustyurt Plateau to the west and the Kyzylkum desert to the southeast. Two major rivers, Amu Darya to the south and Syr Darya to the north, are flowing into the Aral Sea. There are six countries (Afghanistan, Kazakhstan, Kyrgyzstan, Tajikistan, Turkmenistan, and Uzbekistan), who share Amu Darya, Syr Darya and their tributaries, whereas Kazakhstan and Uzbekistan are the only countries that share the Aral Sea itself. At the time when these countries were members of the former Soviet Union, a large...
scale expansion of the irrigated agriculture occurred, primarily producing cotton. Presently, the total length of the irrigation canals is estimated to be 700,000 km along the Amu Darya and Syr Darya rivers (Waltham and Sholji, 2001). As a consequence, river discharges into the Aral Sea were considerably reduced and the Aral Sea started to shrink. The Aral Sea is now reduced by 70% in its surface area and more than 90% in its volume (Micklin, 2004). It is presently split into two separate water bodies (the Small Aral to the north and the Large Aral to the south).

As a result of the sea water volume reduction, the sea salinity has increased. In former times the Aral Sea was a brackish lake, but its salinity reached and started to exceed the ocean salinity of 35 g/L already in the early 1990’s. After the sea split into two parts, the sea salinity of the Large Aral has been continuously increasing and has now reached more than 100 g/L, while the sea salinity of the Small Aral is still below 35 g/L because of fresh water inflow from Syr Darya. Furthermore, the sea volume reduction has also affected the local climate in the Aral Sea vicinity. In particular, seasonal temperature differences have increased, with higher temperatures during the summer months and lower temperatures during the winter months (Small et al., 2001). In general, observed climatic changes in the region might be due to both the considerable changes in the hydrological system within the Aral Sea basin itself and the global climate change (IPCC, 2007). From a scientific viewpoint, the large and clear changes in the hydrological balance of the Aral Sea may provide useful field data for our general understanding of large-scale, long-term cause and effect relationships, regarding surface-subsurface and freshwater-seawater flow interactions.

2.3 Modelling approaches

2.3.1 GIS-based basin-scale flow modelling

The GIS-based PCRaster-Polflow modelling approach (van Deursen, 1995; De Wit 1999; 2001) was used in the studies of both the Forsmark and Simpevarp areas and the Aral Sea drainage basin. The PCRaster modelling approach requires a discretisation of the model domain into quadratic cells. As input for the hydrological modelling module in the PCRaster-Polflow model, each grid cell was assigned properties of ground slope, slope direction, precipitation, temperature, land cover, vegetation, aquifer porosity and aquifer capacity. In the PCRaster modelling environment, the Polflow hydrologic model (De Wit 1999; 2001) first calculates a precipitation surplus $PS$ for each grid-cell as the difference between the precipitation, $P$, and actual evapotranspiration, $E_a$:

$$PS = P - E_a$$  \hspace{1cm} (1)

Different methods are used in the present thesis to estimate $E_a$, as explained more below. For any given $E_a$ quantification, the resulting total runoff of water precipitated within the cell, $R$ (mm/year) must be equal the precipitation surplus $PS$ (Equation (1)) at steady-state and may be further divided into a surface runoff and soil interflow contribution $R_s$, and a groundwater discharge contribution $R_{gw}$:

$$R = R_s + R_{gw} = PS$$  \hspace{1cm} (2)

The groundwater discharge $R_{gw}$ may locally be expressed as a certain fraction $f$ ($0 \leq f \leq 1$) of $R$ implying that $R_s$ then can be expressed as $(1-f)\cdot R$, such that equation (2) is fulfilled. The PCRaster modelling approach also allows for more detailed groundwater system quantifications. However, this thesis focuses more on total coastal discharges than on the distinction between groundwater and surface water contributions and has so far not made use of any specific model relations regarding the distribution of total flows into groundwater and surface water components within catchments.

For estimation of total water discharges, local flow directions are estimated on the basis of the digital elevation model, with each cell being associated with a unique flow direction into the neighbouring cell with the steepest slope. Then the total discharge along a coastline can be expressed as the network-routed sum of the $PS$ in each cell with cell area $A$, as:

$$\sum Q = \sum [(P - E_a) \cdot A]$$  \hspace{1cm} (3)
The cell area $A$ is uniform (10m by 10m) in the models of Forsmark and Simpevarp because the considered areas are relatively small. In the case of Aral Sea Drainage Basin, the cell areas were calculated for different latitudes, thereby accounting for effects of the earth’s curvature.

Regarding estimation of the $E_a$ terms in equation (1), different methods were used in the Swedish and the Aral Sea case studies. For the Swedish studies, two independent estimation methods were used following the original Polflow model (De Wit 1999; 2001). In the first method by Turc (1954), $E_a$ is assumed to be a relatively simple function of precipitation and potential evapotranspiration, which is estimated based on annual mean temperature according to Langbein (1949). In the other method by Wendland (1992), $E_a$ is related empirically but explicitly to different soil and vegetation conditions (Table 1 in Paper I). However, the Wendland method could not be used in the Aral Sea case, because it was empirically calibrated for ambient conditions in Germany, which differ considerably from Aral Sea region soil, climate and hydrological conditions. Instead, another $E_a$ method according to Thornthwaite (1948) was applied in the Aral Sea case, based on monthly number of daylight hours and monthly temperature. More details about the $E_a$ calculations in the Aral Sea case are given in the Supplementary Information to Paper III.

2.3.2 Detailed modelling of fresh groundwater-seawater interactions

Detailed numerical simulations of fresh groundwater-seawater interactions (Fig. 3) at the most near-coastal parts of the ASDB are necessary in order to investigate the combined effect on surrounding coastal aquifers of the shrinking Aral Sea and the increasing salinity in the reduced sea volume. Catchment-scale hydrological models do not commonly account for density driven flows, which may be considerable in near-coastal areas.

For detailed numerical modelling of coastal aquifers, the U.S. Geological Survey SUTRA code (Voss, 1984) was chosen as a general and flexible modelling platform (Paper IV) and used for a series of numerical experiments (Paper V). SUTRA simulates density-dependent flows under combined unsaturated-saturated conditions and allows users to customize imposed time dependent boundary conditions in the block-structured source code. In the present thesis, a subprogram code in SUTRA was slightly customized for handling of the dynamic boundary condition imposed by the Aral Sea water body changing its lateral and vertical extents. This was done by updating the boundary

![Figure 3. Schematic image of the coastal transition zone between fresh groundwater and saline seawater, with submarine groundwater discharge (SGD) and saltwater intrusion (SWI).](image)
matrix in accordance with information on the receding Aral Sea shoreline. Boundary nodes which were initially representing the sea bottom, and hence were assigned certain hydrostatic pressures and salt contents (water entering the seabed), were removed from the boundary matrix if they were left behind the receding shoreline. Hydrostatic pressures and salt contents were then imposed only to the updated boundary matrix. The structure of the code modification is listed in Appendix A in Paper V.

3 THE GIS-BASED PCRASTER-POLFLOW MODELLING APPROACH APPLICATION TO THE FORSMARK AREA (PAPER I)

Paper I outlines and explains the GIS-based catchment-scale hydrologic modelling approach PCRaster-POLFLOW, which was originally developed by Van Deursen (1995; PCRaster) and De Wit (1999, 2001; Polflow) and later used, further adapted and applied to many different basin-scale model studies (De Wit, 2001; Jarsjö et al., 2006; Darracq et al., 2005; Darracq and Destouni, 2005; Lindgren et al., 2007). Paper I in particular shows the specific application of this modelling approach to the unmonitored Forsmark catchment area. Data from the available Swedish Nuclear Fuel and Waste Management Co (SKB) database was used as input for the model application to the Forsmark catchment area. The SKB data base includes detailed spatial data for the Forsmark as well as for the Simpevarp (which is also considered in this thesis, Paper II) catchment areas, because these locations are being investigated as part of the process to find a suitable location for a deep repository for spent nuclear fuel.

Rhén et al. (2003) report a methodology for the development of hydrogeological site descriptive models within the SKB repository site investigation programme. This report identified the need to develop site-specific models of the surface water hydrology that are consistent with groundwater models of the same area. In general, realistic site-specific hydrological models require consistency between surface water and groundwater flows, implying a need for some degree of subsurface and surface water coupling in the process representations of the model. Overall objectives in the development of such coupled models are to obtain water mass balances that are consistent with observations of precipitation, evapotranspiration and water discharges, on local and catchment scales, and model representations of groundwater recharge and discharge zones that are realistic. Open research questions remain regarding, e.g., the necessary level of detail in the model representation of physical processes that underlie surface water-groundwater exchanges. However, it is clear that trustworthy models of surface water hydrology are necessary for site-specific understanding of both the potential biosphere effects of pollutant-carrying groundwater flows and the interactive effects of surface hydrology with these groundwater flows, which motivates the specific objective of Paper I to develop a GIS-based coupled groundwater-surface water model of the Forsmark catchment area hydrology on the basis of available geographic, hydrological and hydrogeological data in SKB’s database, using the PCRaster-POLFLOW tool kit.

Results in Paper I show that the PCRaster-POLFLOW model produces water flow results that, without using any site-specific model calibration, agree well with the available independently measured, area-averaged runoff data. In addition, Paper I reports results for four planned hydrological stations within the Forsmark catchment, thus allowing for future direct comparisons with streamflow monitoring. Paper I shows further also that, and how, the PCRaster-POLFLOW model in its present state may be used for predicting average seasonal streamflow.

Furthermore, Paper I shows and quantifies clearly the interconnection of basin-scale evapotranspiration and coastal discharges (Fig. 12, Paper I), which is controlled by the basin-wide water balance. A Paper I result of main importance for the general context of the whole thesis is then that different ways to model evapotranspiration from the basin...
to the atmosphere (Ea-methods (i) and (ii) in Paper I) yielded the same relative flows, i.e., the same relative spatial distribution of total flow among the different main coastal outlets (and their associated sub-catchments) of the whole catchment area (Fig. 4). Hence, the difference between the evapotranspiration modelling methods concerns mainly their absolute mean, or total, coastal discharge estimates, with hardly any difference being exhibited in the resulting relative spatial distribution of this total/mean outflow. This important result is investigated further in Paper II, considering in addition to the main stream outlets to the sea also the possible diffuse discharges from smaller streams and SGD along both the Forsmark and Simpevarp area coastlines.

4. Spatial distribution of unmonitored inland water fluxes to the sea (Paper II)

In Paper II, the GIS-based hydrological model investigation that was initiated in Paper I was extended to include also the unmonitored coastal Simpevarp catchment area and focused on the spatial distribution of coastal discharges to the Baltic Sea from both the Simpevarp and Forsmark catchment areas. The total main stream discharges and potential diffuse discharges from smaller streams and SGD along the unmonitored coastlines of these catchment areas were modelled with the PCRaster-Polflow approach based on two different evapotranspiration (Ea) model estimates: (i) Turc (1954); and (ii) Wendland (1992). Specifically, method (i) estimates Ea as a simple function of climatic data, whereas method (ii) estimates Ea based on local land surface characteristics. This implies that method (ii) reflects the greater spatial variability exhibited by the detailed land surface distribution within the catchment areas, in comparison with the relatively less variable temperature distribution that governs method (i).

The relatively high resolution (10m x 10m) of available topographic information in these catchment cases allowed us to construct detailed topography-driven flow networks and model their discharges along the

Figure 4. Relative flow distribution \( Qi/Q_{tot} \) of total flow \( Q_{tot} \) (see sum of Figure 7 in Paper I) among the different main coastal outlets in the Forsmark catchment area (numbered in Fig. 1), for Ea-method (i) (dark colour) and Ea-method (ii) (light colour).
coastlines of the two catchment areas. Based on the modelled flow networks and their discharges, it was found that, for both catchment areas and associated coastlines, about 80% of their total coastal discharge occurs through focused stream runoff and remaining about 20% as diffuse coastal discharges, which may occur as SGD, small transient streams or both at different points in time (Fig. 5).

It is here interesting to note that the around 80:20 ratio of focused main stream to diffuse smaller stream-SGD discharges found for both the Forsmark and the Simpevarp areas is consistent with the monitored main river to unmonitored diffuse near-coastal catchment area ratios found by Hannerz and Destouni (2006) for the whole of Sweden (80:20 ratio) and the whole Baltic Sea Drainage Basin (86:14 ratio), despite all the differences in both catchment area characteristics and scales between all these coastal catchments.

It was found that the spatial distribution of local precipitation surplus (Equation (1), equalling the locally created runoff according to Equation (2)) can be largely influenced by small-scale variability in evapotranspiration, as governed by local vegetation, soil texture and land-use details. However, even for the relatively small Forsmark and Simpevarp catchments, the focused surface water discharges were essentially unaffected by the spatial variability and uncertainty in local ET estimates, because local differences were averaged out along the length of the flow paths. By contrast, local flux values within the diffuse small stream-SGD flow fields are more affected by the spatial variability of local ET estimates due to generally shorter flow paths. This implies that spatial modelling uncertainties are the largest for the relatively small local flux values within the

Figure 5. Discharges from land to sea along the total coastline of the Forsmark and Simpevarp catchment areas (Fig. 1).
diffuse discharge fields, for which observation through direct measurement is not easy or practically possible.

5 Hydrological Responses to Climate Change and Irrigation in the Aral Sea Drainage Basin (Paper III)

The GIS-based PCRaster-Polflow modelling approach that was used and applied to the small Swedish Forsmark and Simpevarp catchment areas in Papers I-II was in Paper III further applied to the much larger Aral Sea Drainage Basin (ASDB) in Central Asia. In the ASDB study, the land-use based Ea estimate method was not applicable because it had been obtained from empirical calibration to considerably different ambient conditions in Germany. Therefore, another Ea estimate method was used in Paper III for the ASDB case, based on average monthly number of daylight hours and temperature, according to Thornthwaite (1948).

The main aim of Paper III was to quantify relative and combined effects of regional irrigation and climatic change on evapotranspiration (ET) in the ASDB, as an integral part of the overall water balance of the basin. The ET quantification was here possible with reasonable certainty because other main hydrological changes in this basin (precipitation and river discharge into and shrinkage of the Aral Sea) are measurable, large and essentially known (Jarsjö and Destouni, 2004), while more uncertain hydrological changes of SGD into the Aral Sea are relatively small (Paper IV).

The results of Paper III indicated important effects of freshwater diversions and irrigation on regional water resources and climate. The water diversions to irrigation areas in primarily the southeastern part of the ASDB appear to have considerably increased evapotranspiration. This may have contributed to the fact that the temperature increases in this part are smaller than in other parts of the basin. The precipitation increase in this part of the basin may also be related to the local ET increase due to irrigation (Fig. 6). In total, the net water flux from the atmosphere to the surface of the ASDB (precipitation minus evapotranspiration) appears to have decreased by 60% (from about 66 km$^3$/year to about 26 km$^3$/year; Table 1 in Paper III), primarily due to the irrigation. This indicates that the irrigation in the ASDB may also have non-local water resource and climate effects.

Non-local climatic effects of irrigated areas have previously been estimated by atmospheric modelling assuming an added ET return flow to the atmosphere of about 40% of the irrigation water input (Boucher et al.,

Figure 6. a) The spatial distribution of temperature change within the Aral Sea Drainage Basin (ASDB; Fig. 2) between the temporal (50 years) average condition before 1950 and in the recent 20 years (1983-2002). b) Modelled changes in the ASDB evapotranspiration (ET$^a$) from its average pre-1950 condition to the recent 20 years condition, after both irrigation and climate changes.
This assumption yields considerably smaller estimates of ET from the irrigated areas of the world (Seckler et al., 1998; Döll and Siebert, 2000; Boucher et al., 2004) than both earlier and later hydrological ET assessments (Shiklomanov and Markova, 1987, as quoted by Milly and Dunne (1994) and Boucher et al., 2004; Gordon et al., 2005). The results in Paper III support the higher ET estimates, by indicating a 96-98% return flow from the applied irrigation water in the ASDB. This implies possible considerably larger than previously estimated non-local water and climate effects of the world’s irrigated areas.

6 MODELLING GROUNDWATER – SEAWATER INTERACTIONS IN THE ARAL SEA REGION (PAPER IV)

Submarine groundwater discharge (SGD) from coastal aquifers into the sea may in some cases be considerable even in comparison with stream and river discharges (Moore, 1996). At the same time, coastal aquifers and their freshwater resources are generally vulnerable to salt water intrusion (SWI), with many cases of SWI being reported in coastal areas and islands all over the world (e.g., Koussis et al., 2002).

Understanding of the near-coastal transition zone of groundwater-seawater flow interactions is important, particularly in the immediate vicinity of the shrinking Aral Sea. Due to the dramatic shrinkage of the Aral Sea, the region has experienced severe environmental deterioration by the salinization and accumulated chemical contaminants, causing a shortage of clean fresh water. Groundwater remains then one of few options for a potentially safe fresh water supply, and it is important to understand and quantify the changes that may have been caused in the surrounding fresh groundwater system by the dramatically shrinking Aral Sea. On the one hand, the Aral Sea level lowering, in itself, implies decreased SWI risk and, on the other hand, increasing salt content and density of the seawater should imply an increased potential for SWI.

In order to understand the net effect on coastal aquifers of the changing levels of and conditions in the Aral Sea, relatively detailed quantifications of density-driven flow in the near-coastal transition zones is necessary. Even though the GIS-based basin-scale hydrologic modelling approach used in Paper III provides independent quantifications of landside freshwater flows towards the sea, it cannot resolve the detailed and changing groundwater-seawater flow interactions during the Aral Sea shrinkage.

The objectives of Paper IV were to set up a conceptual and numerical modelling platform for simulating these groundwater-seawater flow interactions and investigate the usefulness of the approach quantifying different coastal flow components under the dynamic sea boundary conditions created by the continuously receding shoreline and increasing seawater salinity of the Aral Sea. The main investigated flow components are shown schematically in Fig. 7.

Results show that the generally quite small flow changes over the simulation period, during which the sea surface level and shoreline positions change considerably, are explained by the fact that the regional hydraulic gradient remains approximately the same, despite the sea surface lowering, because of the flat coastal topography and bathymetry of this region. This result is consistent with independent quantifications by Jarsjö and Destouni (2004), who however did not account for density driven fresh water-seawater flow interactions.

Regarding the seaside boundary flows investigated in Paper IV, the model results showed that, apart from an initial period, discharge into the sea occurred only through the seaside boundary B (Fig. 7), while recharge occurred both through the landside boundary and the seaside boundary A. Furthermore, the SGD flow component (QSGD in Fig. 7) exhibited an initial decrease followed by a small yet steady increase, and the inland boundary freshwater flow (QFWI in Fig. 7) increased throughout the transient simulation. In general, the modelling set-up and first model investigations in Paper IV provided a basic under-
standing of groundwater-seawater flow component interactions, which was used and further extended in Paper V.

7 BATHYMETRY-TOPOGRAPHY EFFECTS ON SALTWATER-FRESH GROUNDWATER INTERACTIONS AROUND THE SHRINKING ARAL SEA (PAPER V)

Paper V made use of the basic conceptual model and modelling platform for density-driven groundwater-seawater flow interactions that was developed in Paper IV in order to further investigate the effects of regional topography and bathymetry differences around the coast of the shrinking Aral Sea on the coastal groundwater system and the vulnerability of that system to seawater intrusion. Previous investigations had already indicated possible important bathymetry-topography effects, however without considering density-driven flow effects (Jarsjö and Destouni, 2004).

Based on available hydrogeological information, in conjunction with the mapped topography of the Aral Sea vicinity, Paper V considered two different topographical-bathymetrical cases for the coastal regions: flat bathymetry, which is representative for a large part of the south-eastern Aral; and steep bathymetry, which is representative of the north-western part of the sea. In addition, for each model scenario, two possible boundary conditions of constant head and constant flow for the landside boundary were considered. Regarding the coastal aquifer vulnerability to seawater intrusion, hypothetical pumping simulations were performed in order to investigate in which cases the water quality may deteriorate due to groundwater pumping. In these simulations, scenarios with and without the sea shrinkage were considered in order to understand the Aral Sea shrinkage effects on the seawater intrusion vulnerability.

For the conceptual model cross-section representing the steep bathymetry of the north-western Aral Sea, the submarine groundwater discharge (SGD) increased considerably in response to the dynamic groundwater conditions caused by a 21 meter sea level lowering over 40 years. Throughout the main part of the considered 40-year simulation period, the salinity of the SGD was lower than the initial (pre-1960) salinity of the Aral Sea, reflecting the presence of a considerable fresh groundwater component. For the cross-section representing the flat bathymetry of the south-eastern Aral Sea, including the irrigated Amu Darya delta, the SGD exhibited an initial decrease

Figure 7. Schematic illustration of different groundwater-seawater flow components through the different boundaries of the conceptual model land-sea cross section in the Aral Sea case: QA, the inflow at the seaside sediment boundary A; QB, the net flow at the seaside sediment-water boundary B; QSGD, the discharge into the sea at the seaside sediment-water boundary B; QFWI, the fresh groundwater inflow at the upstream landside boundary; and QNET, the net sum of flows through all system boundaries. The seaside sediment inflow, QA, is given from a hydrostatic pressure boundary condition in Paper IV, whereas a no-flow boundary condition is assigned in Paper V.
as the sea started to shrink, and an analysis of trends (considering a 4 year simulation period) revealed that the subsequent increase in SGD was considerably lower than in the steep bathymetry case. In addition, the groundwater discharging into the Aral Sea from this bathymetry case became saline already within the considered 4-year simulation period, without any considerable fresh water component. All these model results were independent of the choice of inland water boundary condition.

The hypothetical groundwater pumping simulation results for the post-1960 shrinkage of the Aral Sea implied that pumping wells in the coastal aquifers would generally be less affected by salt water intrusion (SWI) from the sea itself, in comparison with the pre-1960 conditions (Fig. 8). While the flat bathymetry results showed a remaining risk for SWI in, e.g., the south-eastern Aral, the steep bathymetry model results imply an increased potential for fresh groundwater pumping in mainly the north-western regions, with decreased risk of SWI.

Figure 8. Salinity transitions in the modelled coastal aquifers of the Aral Sea case, resulting from groundwater pumping scenario simulations with a steady sea level (steady SL; solid lines, relevant for the pre-1960 conditions) and a decreasing sea level (transient SL; dashed lines, relevant for the period 1960-64), as would be observed approximately 500 metres downstream of the hypothetical pumping wells for the: (a) flat bathymetry case, and (b) steep bathymetry case.
8 DISCUSSION

The GIS-based PCRaster-POLFLOW approach used here for the basin-scale hydrologic modelling in Papers I-III has previously been applied to relatively large and well-monitored drainage basins, such as Rhine, Elbe and Norrström (De Wit 1999, 2001; Darracq et al., 2005; Darracq and Destouni, 2005; Lindgren et al., 2007). The present thesis shows that and how the same modelling approach can also be used for quantifying land-to-atmosphere and land-to-sea water flows and flow distributions in the much smaller unmonitored Forsmark and Simpevarp catchment areas, using relatively fine resolved catchment surface data, as well as in the large Aral Sea drainage basin, with limited spatial data, but with relatively good information on large long-term temporal change. Paper I identifies also possible fruitful ways of further developing this modelling approach with respect to the generally important evapotranspiration modelling and to the coupled modelling of groundwater-surface water interactions and reactive solute transport in catchments.

With regard to the close connection, through the basin-scale hydrological balance, between the land-to-atmosphere and land-to-sea flows of vapour and water from a drainage basin, Paper II shows that the spatial distribution of local precipitation surplus (PS in Equation (1), quantifying precipitation minus evapotranspiration and equalling the locally created runoff (Equation (2))) may be largely influenced by small-scale variability in evapotranspiration, which is in turn governed by local vegetation, soil texture and land-use details. However, even for the relatively small areas of the Forsmark and Simpevarp catchments, the relatively large focused stream discharges from land to sea were essentially unaffected by the spatial variability and uncertainty in local PS, because local PS differences were averaged out along the length of the main water flow paths. In contrast, local flux values within the diffuse smaller stream and groundwater flow fields from land to sea are generally characterised by shorter flow paths and are therefore more affected by the spatial variability of local PS.

This implies that spatial flow modelling uncertainties may be relatively large for local flux values within diffuse small stream and SGD flow fields; in particular for the latter, SGD field, the full flux variability range can also not be readily and fully observed through direct measurement. Nevertheless, the results in Paper II indicate that the magnitude of mean values and total sums of SGD along some considerable coastline length may be considerably more certain and robust than the local flux values, because the former are heavily constrained by the catchment-scale hydrological balance. A particular result with potential greater generality is the around 80:20 ratio of focused large stream to diffuse small stream-SGD flow from land to sea, which was found for both the Forsmark and the Simpevarp areas. This ratio is consistent with the monitored large river to unmonitored near-coastal diffuse flow catchment area found for both the whole of Sweden and the whole Baltic Sea Drainage Basin (Hannerz and Destouni, 2006) and should be worthy of further investigation in other coastal areas of different scales.

Also the hydrological modelling application to the ASDB in Paper III yielded robust and potentially important results on the effects of freshwater diversions and irrigation on regional water resources and climate. Specifically, and regardless of chosen evapotranspiration quantification within the used GIS-based PCRaster-Polflow modelling approach, the major water diversion and irrigation schemes in this region after the 1950s appear to have considerably increased evapotranspiration and decreased net water flux (precipitation minus evapotranspiration) from the atmosphere to the surface of the ASDB. Increased evapotranspiration cools the irrigated areas, and the decrease of net atmospheric water influx to the ASDB may also yield non-local effects outside the basin. Such effects have previously been estimated by atmospheric modelling (e.g., Boucher et al., 2004), assuming a return flow by evapotranspiration to the atmosphere of
about 40% of the irrigation water input. Our results indicate higher return flows, of nearly 100% of the applied irrigation water in the ASDB. This may imply considerably larger than previously estimated non-local water and climate effects of the world’s irrigated areas and is therefore also a result worthy of further investigation.

The results in Paper III show also that the drastic reduction of river discharges into the Aral Sea and the associated dramatic sea level lowering of more than 20 m since 1960 are indeed caused by the large-scale water diversion and irrigation schemes, rather than by climate change in the ASDB. Papers IV-V in the thesis show further how the large Aral Sea level change has in turn affected the dynamics of submarine groundwater discharge (SGD) and the vulnerability of coastal groundwater to saltwater intrusion (SWI), and that a detailed near-coastal modelling approach (here the U.S. Geological Survey SUTRA code; Voss, 1984) is needed for quantifying such groundwater-seawater flow interaction effects. The results show in particular that regional topography and bathymetry may largely influence SGD and SWI transients during extended periods of sea level change.

Furthermore, with particular regard to different Aral Sea region conditions, the flat topography in the southeastern Aral Sea part with the irrigated Amu Darya delta imply that SGD drops as the sea starts to shrink because the shoreline displacement prevents seawater inflow to the aquifer and subsequent return flow to the sea. In this flat bathymetry case, the groundwater discharging into the Aral Sea becomes as saline as the seawater that remains for long time below the dried seabed as the sea shrinks. In the steep bathymetry case of the essentially uninhabited northwestern Aral Sea region, however, the SGD increases and its salinity is smaller than the seawater salinity due to a considerable freshwater component. The paper V result of decreased SWI risk due to the Aral Sea shrinkage is also practically important and worthy of further regional investigation, considering the potential for groundwater pumping to provide a well-needed increase of freshwater supply in the region.

9 CONCLUSIONS

Several open research questions still remain regarding the quantitative coupling of inland surface water and groundwater flows, and the associated flows of vapour and water at the land-atmosphere and land-sea interfaces of whole drainage basins. Nevertheless the results of this thesis indicate that, in absence of the extensive runoff time series that constitute a common input data and calibration-validation basis in hydrologic modelling, the GIS-based PCRaster-POLFLOW hydrologic modelling approach is capable of providing useful temporal average flow and flow trend quantifications across a range of different basin scales. Furthermore, the thesis shows the need for more detailed dynamic groundwater modelling in order to understand and quantify the development of fresh groundwater-seawater flow interactions in coastal aquifers under periods of large sea level change, and exemplifies a useful such modelling approach by use and site-specific adaptation of the U.S. Geological Survey SUTRA code.

Main methodological contributions of this thesis include: i) the application of topographic-surface data-based modelling to unmonitored catchment area delineation and hydrologic quantification, and the use of this modelling for interpretation and quantification of unmonitored coastal discharge distributions; ii) the comparative use of different possible evapotranspiration quantifications in basin-scale hydrologic modelling in order to investigate the effect of this uncertain flux quantification on other hydrological flows and identify robust hydrological results; and iii) the handling of dynamic boundary conditions of long-term sea level change, by use and adaptation of the SUTRA code. These methodological contributions facilitated in turn a series of different site-specific results and conclusions, of which some main conclusions of potential more general significance and interest for future studies are summarized here.
The Forsmark and Simpevarp hydrologic modelling showed that the relatively large focused stream flows and the mean values and total sums of diffuse discharges from small streams and SGD along some considerable coastline length are largely constrained by catchment-scale hydrological balances and considerably more robust and certain to estimate than the spatially variable and relatively small local fluxes within the diffuse flow fields. An interesting result for possible future studies is also the consistent 80:20 ratio of the catchment area of large stream flows relative to that of diffuse small stream and SGD flows, which was found for both the Forsmark and the Simpevarp catchments and which is also consistent with the ratio of monitored large river to unmonitored diffuse near-coastal flow catchment area found earlier for the whole of Sweden and the whole Baltic Sea Drainage Basin. This consistency should be worthy of further investigation in other coastal catchment areas of different scales.

The ASDB hydrologic modelling showed an evapotranspiration return flow from applied irrigation water input that is much higher than previous estimates in atmospheric modelling. This result implies possible considerably larger than previously estimated non-local water and climate effects of the world’s irrigated areas and should also be investigated further.

The more detailed coastal groundwater-seawater dynamics modelling for the coastal parts of the ASDB showed that regional topography and bathymetry may largely influence SGD and SWI transients during large sea level lowering. Such sea shrinkage may further considerably decrease the SWI risk in coastal aquifers, and considerably more so for steeper than for flatter coastal topography. Both these results and the modelling method used and further developed for arriving at them may be important also for other coastal aquifers around seas or lakes that undergo long-term level or salinity changes, such as the Great Salt Lake and the Mono Lake in USA, Lake Chad in Africa or the Dead Sea in the Middle East.

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