

INTERACTION OF DENSITY FLOW AND GEOCHEMICAL PROCESSES ON ISLANDS IN THE OKAVANGO DELTA, BOTSWANA

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ABSTRACT

This paper analyses the interactions of density driven flow and geochemical reactions under evapo-concentration. A multi-species hydrodynamic flow and transport simulation model (SEAWAT) is coupled to a batch reaction model (PHREEQC) to analyze density-driven flow on islands in the Okavango Delta, Botswana. Evapo-concentration on the islands leads to steadily increasing concentrations until the onset of density-driven flow against the evaporation-induced upward gradient. Lag times to the onset of density-driven flow are strongly influenced by geochemical reactions. Mineral precipitation and carbon dioxide off-gassing increase the lag time. Carbon dioxide off-gassing is enhanced in the presence of significant amounts of humic substances. Simulation results further depend sensitively on the assumed dispersivity.

1. INTRODUCTION

Salt accumulation in surface waters, soils, and groundwater is a common phenomenon in systems where the evapotranspiration rate exceeds the precipitation rate. Salt accumulation in soils is one of the most serious global environmental problems. Throughout the semi-arid regions, soil salinization threatens agricultural productivity and food security. Salt accumulation in shallow groundwater systems can be observed in many semi-arid and arid regions. A prominent example is the Okavango Delta in Botswana.

The hydrological process causing the accumulation of salts in these systems is evapotranspiration (ET). Evaporation increases the dissolved solids concentration in the residual water body, as water is removed and dissolved solids are left behind. Magnifying this effect, transpiration leads to an additional increase of total dissolved solids (TDS) concentrations, since plants selectively take up specific ions and exclude others (e.g. [Silberbush and Ben-Asher, 2001]). TDS accumulation due to evapotranspiration – which will be referred to as evapo-concentration in the remainder of this paper – can eventually lead to highly concentrated aqueous solutions in surface water bodies, soil water and shallow ground water.

As evapo-concentration proceeds, two mechanisms become increasingly important: Density-driven flow and geochemical reactions. The density of water is a function of the concentration of the various dissolved species and generally increases with increasing TDS concentration. Since most of the water is taken up at the surface, evapo-concentration leads to a hydrodynamically unstable concentration distribution with water of higher density being located on top of lower-density water. This may lead to instabilities (density fingers), which induce a vertically downward transport of salinity against the upward flow established by evapotranspiration ([Wooding, *et al.*, 1997]).

Evapo-concentration triggers a number of geochemical reactions, most importantly mineral precipitation and off-gassing of carbon dioxide. These reactions remove parts of the dissolved solids from the solution and thus slow down the process of evapo-concentration. Depending on the initial composition of the water subject to evapo-concentration, a series of different minerals will precipitate in sequence, with more soluble minerals precipitating at a later stage of evapo-concentration. In shallow groundwater settings, the system is open with respect to gas exchange with the atmosphere, and loss of carbon dioxide to the atmosphere is another process that leads to mass loss from the solution. As an additional complication, natural waters contain complexing agents in the form of humic substances ([Tipping and Hurley, 1992]).

The objective of this paper is to simulate and quantitatively analyse the geochemical evolution of shallow groundwater under evapo-concentration on islands in the Okavango Delta. Combining field data and numerical simulations the paper investigates the importance of individual processes and quantifies the interaction between variable density flow, advective-dispersive transport and geochemical reactions. In contrast to previous studies (e.g., [Zimmermann, *et al.*, 2006]) the simulations do not only consider the physically driven accumulation process within the subsurface water body under the islands but also whether geochemical reactions have a considerable effect on (i) the accumulation rate (ii) the lag-time before density-driven flow occurs and (iii) the steady-state chemical composition of the brines.

2. MATERIALS AND METHODS

1.1 Study Sites

The Okavango Delta is a large alluvial fan situated in Northern Botswana, Southern Africa. This wetland receives its water through the Okavango River, which flows from the tropical Benguela Plateau in Southern Angola into the Kalahari basin (Figure 1). The water spreads out over approximately 6000 km² of permanent swamp and another 6000 km² of seasonal floodplains. Average water depth is less than a meter and the surface water body has a complex shape with thousands of islands and peninsulas formed by the slightly undulating topography.

Of the 300 m³/s of water entering the Delta, only about 10 m³/s proceed into the downstream Boteti River, the rest is lost to evaporation or transpiration by plants. The TDS concentration in the inflow is around 35 mg/l and increases to roughly 100 mg/l at the downstream end of the Delta. [Dincer, *et al.*, 1978] found a concurrent enrichment of the heavier stable isotopes of oxygen and hydrogen moving from the upstream to the downstream side of the Delta. [Mladenov, *et al.*, 2005] observed a similar behaviour for the dissolved organic carbon (DOC), which they attributed partly to internal DOC sources and partly to

evapo-concentration. [Bauer, *et al.*, 2006] evaluated the salt mass balance of the entire Okavango Delta and showed that the process balancing the salt budget of the Delta is accumulation along the coastline. On some of the small islands, which are surrounded by an above-ground water level, evapo-concentration leads to extremely high concentrations (20 g/l and more). Fingering instabilities were predicted by the hydrodynamic simulation models and were observed using electrical resistivity tomography.



Figure 1: The Okavango Delta in Botswana, Southern Africa. The Okavango Delta is located within the red-bordered area.

1.2 Conceptual model of groundwater flow and reactive transport

The general conceptual model of islands in the Okavango Delta is the following: Islands are slightly elevated portions of the terrain (average diameter of about 200 m) which are surrounded by permanent or seasonal floodplains (Figure 2). Due to the fact that the islands are surrounded by an above-ground water level, groundwater tables are shallow. This results in high evaporation and transpiration fluxes. Evaporation and transpiration establish a concentric flow pattern beneath the island that converges at the centre. The inflowing solutes are effectively trapped. This leads to an extreme evapo-concentration with groundwater salinity reaching seawater values in some cases.

Due to pronounced density differences between the brine and the underlying freshwater, the superficial saline lenses associated with the islands may become hydrodynamically unstable and give rise to density-driven flow as was first suggested for the Okavango by [Gieske, 1996], based on results from hydrodynamic modelling.

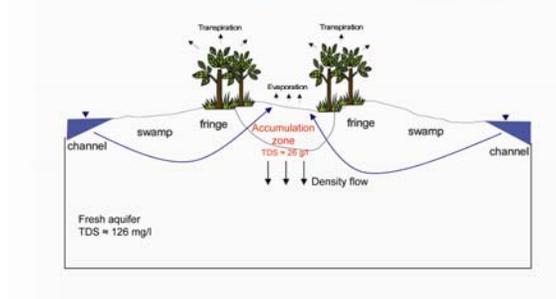


Figure 2: Conceptual island model.

1.3 Numerical modelling framework

1.3.1 Numerical models

Spatially distributed dynamic modeling of shallow groundwater systems under evapo-concentration requires the simultaneous coupled simulation of three different processes: Water flow, transport of dissolved species and geochemical reactions. MODFLOW ([Harbaugh and McDonald, 1996]) is the most widely used software package for the simulation of groundwater flow processes. MODFLOW can be combined with the MT3DMS package ([Zheng and Wang, 1999]), which simulates advective-dispersive transport processes in groundwater. In its uncoupled version, MT3DMS runs the transport simulations on the flow velocity fields provided by MODFLOW. If density-driven flow is important, MODFLOW and MT3DMS must operate in a coupled mode, since the density of the water depends on the TDS concentration. A coupled version of MODFLOW and MT3DMS was implemented in the SEAWAT package ([Guo and Langevin, 2002]). The software package PHREEQC ([Parkhurst and Appelo, 1999]) can be used to perform equilibrium speciation calculations for aqueous solutions and to simulate various equilibrium and kinetically controlled geochemical reactions. PHREEQC is a batch reactor model and was coupled to MT3DMS to enable the combined analysis of transport and reaction processes. The resulting package is called PHT3D ([Prommer, et al., 2003]). Recently, PHREEQC and SEAWAT were combined into a package (PHWAT) that simulates the coupled processes of flow, transport and reaction, taking into account the effects of variable density on the flow field ([Mao, et al., 2006]). The various software packages are applied in this paper to the example of evapo-concentration in the shallow groundwater beneath islands in the Okavango Delta.

The numerical models are based on the conceptual model presented in Figure 2. Model parameters for the different flow, transport and reaction simulations are summarized in Table 1. Four different types of simulations were performed:

- Non-reactive uncoupled flow/transport simulations using MODFLOW and MT3DMS (Code SAL). Density-driven flow is not simulated. Geochemical reactions are not simulated.
- Non-reactive coupled flow/transport simulations using SEAWAT (Code SALDENS). Density driven flow is simulated. Geochemical reactions are not simulated.
- Reactive uncoupled flow/transport simulations using MODFLOW and PHT3D (Code GC). Density driven flow is not simulated. Geochemical reactions are simulated.
- Reactive coupled flow/transport simulations using PHWAT (Code GCDENS). Density driven flow is simulated. Geochemical reactions are simulated.

TABLE 1. List of model parameters as applied for the hydrodynamic simulations. Parameter, numerical value and units are given.

Parameter	Value	Unit
Domain size (length/height)	220/100	[m]
Length of Island	100	[m]
Location of island	X=55-155	[m]
Lateral boundary conditions	Fixed head, fixed concentration	
Simulation time	2000	[years]
Horizontal K	3.9	[m/day]
Vertical K	0.224	[m/day]
Regional hydraulic gradient	0.00022	
ET-rate	0.8	[mm/day]
Porosity	0.35	
Effective molecular diffusion coefficient	10^{-9}	[m ² /s]
Longitudinal dispersivity	1	[m]
Transversal dispersivity	1	[m]

1.3.2 Geochemical reaction network

In the GC and GCDENS simulations, the following geochemical reactions were taken into account: Precipitation of calcite, dolomite, K-feldspar, Kaolinite, amorphous Silica and Trona-K. Furthermore, the shallow groundwater is assumed to be in equilibrium with a gas phase. In the gas phase, the pCO₂ is set to 3160 ppm, i.e. ten times the pCO₂ in the free atmosphere. If the pCO₂ increases above the equilibrium pCO₂, CO₂ is removed from the solution. However, CO₂ cannot be re-dissolved from the gas phase. This reflects the conditions in the shallow aquifer beneath the islands, where the bulk of the water is not in direct contact with the atmosphere but can loose CO₂ due to bubble formation.

The initial concentrations for the various species are based on typical concentrations measured in the swamp waters of the Okavango Delta. The C(4) concentration was adjusted

so that the solution is in equilibrium with a gas phase with a $p\text{CO}_2$ of 3160 ppm. The equilibrium $\text{C}(4)$ concentration was calculated in PHREEQC batch mode.

To study the effects of the presence of DOC in the initial solution, two additional simulation runs were performed. In the simulations GC+HA and GCDENS+HA, 50 mg/l of dissolved organic carbon were added to the initial solution which corresponds to the highest measured DOC concentration in the swamp waters around the surveyed islands. This high DOC concentration was chosen to clearly expose the effect the DOC has on the geochemistry under evapo-concentration. The chemical properties of the humic substances (dissociation constants, metal complexation constants etc.) are assumed to be in accordance with the model by [Tipping and Hurley, 1992]. The characterization of the humic substances based solely on literature values introduces considerable uncertainty. The simulation results for GC+HA and GCDENS+HA qualitatively indicate how the system responds to the addition of humic substances but do not accurately represent the field conditions in the Okavango Delta.

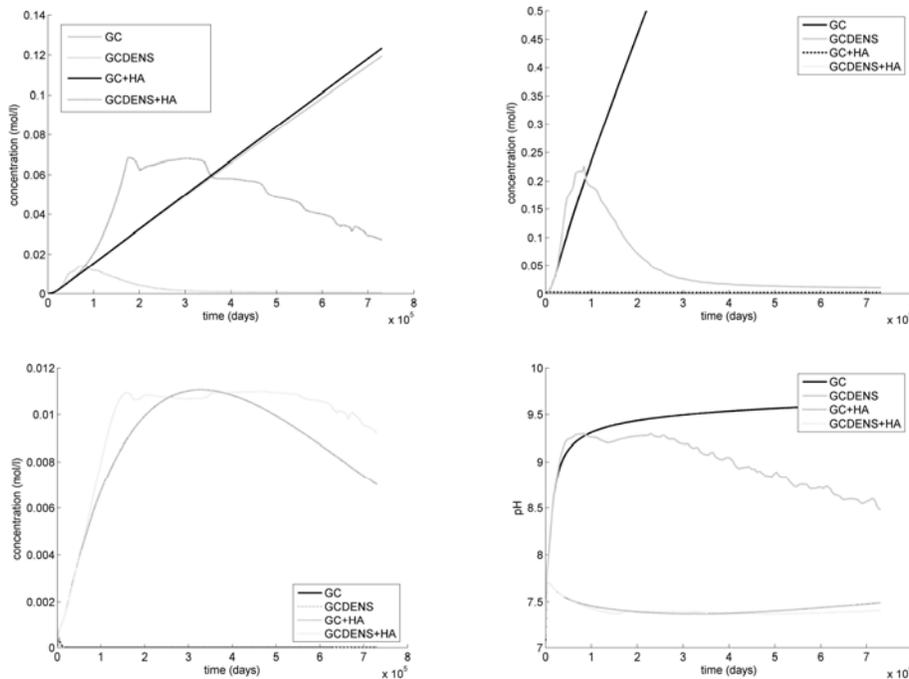


Figure 3: Concentrations (mol/l) as a function of time at $x=124.75$ m and $y=0.25$ m. Upper left: $\text{Cl}_{(aq)}$, Upper right: Alkalinity, Lower left: $\text{Ca}_{(aq)}$, Lower right: pH.

3. RESULTS

Modelling results in general, and particularly the time until the onset of density-driven flow, sensitively depend on the amount of humic substances present in the initial solution prescribed at the domain boundaries. Comparing the results of the six different simulation runs (SAL, SALDENS, GC, GCDENS, GC+HA and GCDENS+HA) allows identifying the effects of the various individual processes and coupling mechanisms.

Figure 3 shows the concentrations of four selected conservative and reactive species in the superficial groundwater on the island as a function of time. Chloride behaves conservatively. In the GC and GC+HA simulations, chloride is continuously accumulated and the

concentration increases almost linearly with time. In the GCDENS simulation, the chloride concentration is stabilized by density-driven flow, at the onset of this process after around 200 years. In the GCDENS+HA simulation, the onset of density-driven flow is delayed by up to about 500 years and the maximum chloride concentrations simulated on the island are therefore much higher than in the GCDENS run (0.07 mol/l versus 0.02 mol/l). Total inorganic carbon (C(4)) behaves almost conservatively in the GC simulation. In the GCDENS simulation, the concentration is stabilized by density-driven flow. In the simulations with humic substances, almost no carbon accumulation occurs. The concentration stays at its initial level. This is due to the buffering of the pH value by the dissolved humic substances. The pH stays almost constant, and since the solution is in equilibrium with a gas phase of fixed pCO₂, carbon is lost to the gas phase. Calcium is stabilized at very low concentration levels by calcite and dolomite precipitation in the simulations without humic substances. In the simulations with humic substances, the complexing agents hold the calcium ions in solution and calcium behaves almost conservatively. In the GCDENS+HA simulation, density-driven flow eventually stabilizes the total calcium concentration. The evolution of the pH value is markedly different in the simulations with and without humic substances. Without humic substances, the pH increases on the island, until it is stabilized by density-driven flow. This is due to increasing bicarbonate and carbonate ion concentrations needed to balance the increasing metal cation concentrations. In the simulations with humic substances, the humic substance anions partly balance the cation charge, carbon is lost to the gas phase and the pH stays almost constant.

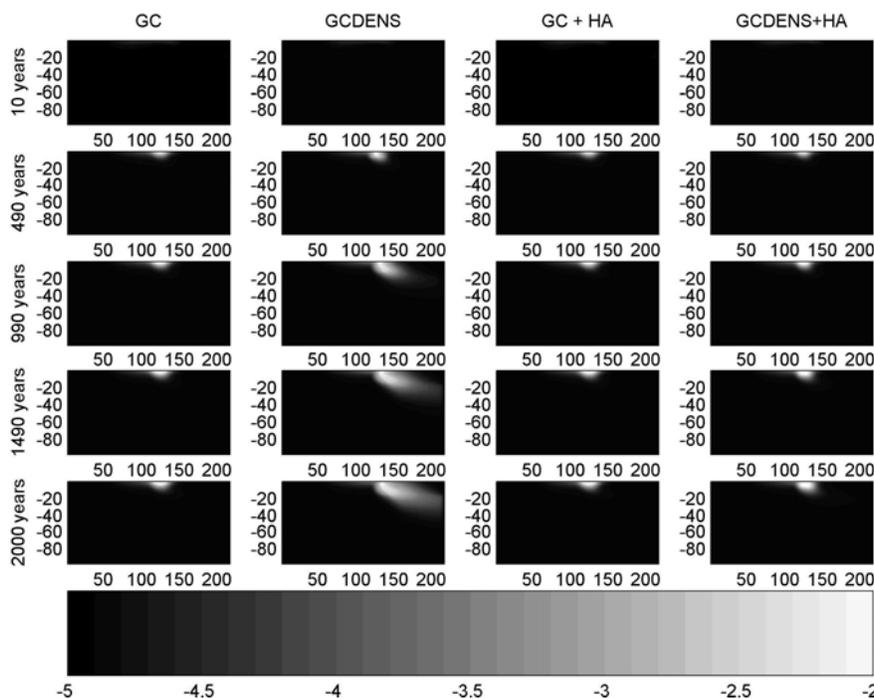


Figure 4: Comparison of the spatial patterns of chloride concentrations (mol/l, decadic logarithm) for the five different simulation types at four different time steps.

Figure 4 shows the spatial patterns of chloride concentrations in a vertical cross section of the island. The GC and GC+HA simulations show the ongoing accumulation below the island and the diffusive/dispersive mixing. Both GCDENS and GCDENS+HA show indications of

density-driven flow, however, the onset of density-driven flow is much delayed in the GCDENS+HA simulation as compared to the GCDENS simulation. Due to the regional hydraulic gradient acting across the entire domain, the density finger is advected horizontally.

4. CONCLUSIONS

Density-driven flow establishes vertically downward directed solute transport against an evapotranspiration-induced upward hydraulic gradient on islands in the Okavango Delta. The influence of geochemical reactions on this process is a general slow down and an increased period of time to the onset of density-driven flow. All simulations show, however, that eventually, density-driven flow stabilizes dissolved solids concentrations on the islands. Mineral precipitation and off-gassing are important mass loss mechanisms that increase the time until the onset of density-driven flow and change the chemical composition of the shallow groundwater at the onset of density-driven flow. Whereas the chemical processes control the duration of the accumulation phase and the chemical composition of the shallow groundwater, the direction of the salinity plume primarily depends on the regional flow field.

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