

Role of salt sources in density-dependent flow

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[1] Flow equation expresses mass conservation for a fluid phase. In density-dependent problems, fluid consists of at least two components, termed salt and water here. Salt sources are usually properly accounted for when salt is dissolved in water (i.e., as a solute) but are neglected otherwise. An analysis of the effect of neglecting pure salt sources on flow regime and concentration distribution is performed. Two test cases are used to illustrate the issue. The first one is the saltwater bucket problem, which consists of adding salt to an otherwise isolated domain. The second one is the Elder problem. Discrepancies in concentrations are moderate for reasonably small salt mass fractions. However, currently available codes yield head drops in response to the addition of salt because fluid mass is kept constant while its density increases. Such results contradict basic physical principles and lead to an inversion in the flow direction.

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1. Introduction

[2] Flow and transport simulation demands the expression of mass conservation. Two equivalent approaches can be used for multicomponent problems. The compositional approach [e.g., Bear, 1972; Olivella *et al.*, 1994] considers mass conservation for each component separately. This leads to a set of n transport equations, one per component, including every component's sinks and sources. This approach is typically used for multiphase flow problems. However, for single fluid phase problems such as saltwater transport, it is more convenient to add up the equations for all components. This causes dispersion terms to cancel and results in one flow equation and $n-1$ uncoupled transport equations. This second approach is the usual one in density-dependent flow and transport and it is the focus of this work. Alternative formulations are summarized by Kolditz *et al.* [1998] and Diersch and Kolditz [2002].

[3] Flow equation represents fluid mass conservation. Therefore, it must include the sinks and sources of all components (restricted here to salt and water for simplicity) to represent a complete fluid mass balance. Yet, salt sources that do not come dissolved in water are usually ignored in the flow equation. In this work, such sources will be called pure salt sources to distinguish them from mixed salt and water sources.

[4] Pure salt sources can have either an internal origin or enter through the boundaries. Internal salt sources are associated to chemical processes. They may also be used as model simplifications. For example, salt dissolution at

the bottom of an aquifer flowing over a salt dome may be represented as an internal source in a two-dimensional model. Pure salt boundary sources occur when water flux is prescribed to be zero and either salt flux (Neumann boundary conditions) or concentration (Dirichlet boundary conditions) is prescribed at the boundary. Strictly speaking, prescribed concentration boundaries are not found in nature. However, some real boundaries can be modeled as prescribed concentration boundaries. This is the case of dissolution boundaries, which are found in aquifers flowing over salt rock, where aquifer water flux dissolves the salt rock, which creeps to fill the void.

[5] Pure salt sources (i.e., solute mass inflow together with zero water inflow) can be found in many density-dependent flow problems. For example, the dissolution of CO₂ beneath the supercritical CO₂ bubble created during CO₂ sequestration is often modeled in this fashion [Riaz *et al.*, 2006; Hassanzadeh *et al.*, 2006; Xu *et al.*, 2006].

[6] Regardless of their conceptual meaning, it is relatively frequent to adopt Dirichlet boundary conditions for transport while imposing zero flux for flow. These kind of boundary conditions is found in density-dependent code benchmarks such as the Elder [Elder, 1967], salt dome [Organization for Economic Cooperation and Development, 1988] and Horton-Rogers-Lapwood [Weatherill *et al.*, 2004] problems.

[7] Usually, pure salt sources are only included in the salt mass balance, that is, the transport equation or its boundary conditions, but not in the fluid mass balance, that is, the flow equation. This inconsistency has been pointed out in two occasions. Hassanzadeh and Leijnse [1988] acknowledge salt sources when salt rock boundaries are modeled as Dirichlet boundaries. They provide an expression for the flow boundary condition to model a dissolving cap rock in a salt dome that quantifies the amount of salt entering the system, but they do not actually solve the resulting problem. Voss and Provost [2002] mention internal pure salt sources when developing the equations implemented in the SUTRA code, but they are not included in the final formulation

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because they are assumed to be small compared with other sources.

[8] The aim of this work is to study the effect of neglecting pure salt sources in the fluid mass balance in single-phase density-dependent flow simulations. An accurate understanding of the influence of pure salt sources on density-dependent flow is pursued to determine the accuracy of problem's solutions.

2. Salt Sources in Single-Phase Density-Dependent Fluid Mass Balance

[9] Fluid mass balance can be written as

$$\frac{\partial(\rho\theta)}{\partial t} = -\nabla \cdot (\rho\mathbf{q}) + m_w + m_s, \quad (1)$$

where t [T] is time, ρ [ML^{-3}] is the fluid density, θ [$L^3 L^{-3}$] is the fluid content per unit volume, \mathbf{q} [$L T^{-1}$] is the volumetric fluid flux (Darcy velocity) and m_s [$ML^{-3} T^{-1}$] and m_w [$ML^{-3} T^{-1}$] are salt and water sources (sinks if negative), respectively.

[10] The salt mass balance can be written in terms of salt mass fraction ω [$M^2 M^{-3}$] as

$$\frac{\partial(\rho\theta\omega)}{\partial t} = -\nabla \cdot (\rho\mathbf{q}\omega) + \nabla \cdot (\rho\mathbf{D}\nabla\omega) + m_s, \quad (2)$$

where \mathbf{D} [$L^2 T^{-1}$] is the diffusion-dispersion tensor.

[11] Equation (2) is the divergence form of transport equation. It is also called conservative form because it expresses explicitly the salt mass balance. Groundwater modelers often prefer the advective form, which is obtained by subtracting fluid mass balance (1) multiplied by the resident salt mass fraction ω from (2), which yields

$$\rho\theta \frac{\partial\omega}{\partial t} = -\rho\mathbf{q} \cdot \nabla\omega + \nabla \cdot (\rho\mathbf{D}\nabla\omega) + (1 - \omega)m_s - m_w\omega. \quad (3)$$

2.1. Mass Balance Inconsistency Involving Internal Salt Sources

[12] Internal sources are those found within the domain. Internal pure salt sources (i.e., $m_s \neq 0$, $m_w = 0$) may be used to model chemical reactions, dissolution, precipitation or decay processes. It should be noticed that dissolution processes may be accompanied by an increase in porosity, that will in general compensate the salt source unless refilled (case of 2-D horizontal models of a continuous injection of CO_2 or a creeping salt rock). Pure salt sources may also be used as a simplified way to represent other solute inflows. Pure water internal sources (i.e., $m_s = 0$, $m_w \neq 0$) may be used to model water inflows, evaporation or dehydration of minerals (e.g., gypsum evolving to anhydrite in response to an increase in salinity). Most often, mixed sources are used ($m_s + m_w = \rho^* r$, where r [$L^3 L^{-3} T^{-1}$] is a volumetric source of fluid with density ρ^*).

[13] Model equations become inconsistent when m_s is not present in flow equation (1) whereas it is in (2). The inconsistency is more severe when the advective form of the transport equation is adopted. An incomplete flow equation is subtracted from the conservative form of the

transport equation to obtain the advective transport equation. This yields

$$\rho\theta \frac{\partial\omega}{\partial t} = -\rho\mathbf{q} \cdot \nabla\omega + \nabla \cdot (\rho\mathbf{D}\nabla\omega) + m_s - m_w\omega. \quad (4)$$

Note that the $(1 - \omega)$ factor which multiplies m_s in (3) is lost in the process.

2.2. Mass Balance Inconsistency Involving Salt Boundary Sources

[14] The flow and transport equations require appropriate boundary and initial conditions to be well posed. Regardless of the type of boundary condition adopted, a fluid flux is always established across the boundary. This flux is explicitly prescribed in the Neumann and Cauchy boundary conditions and is implicit in the Dirichlet ones. The fluid flux across the boundary can be written as

$$-\rho\mathbf{q}|_b \cdot \mathbf{n} = j_w + j_{ss}, \quad (5)$$

where \mathbf{n} is the unit vector normal to the boundary pointing outward and j_{ss} [$ML^{-2} T^{-1}$] and j_w [$ML^{-2} T^{-1}$] are salt and water fluxes, respectively. The subscript b denotes evaluation at the boundary.

[15] Similarly, the boundary salt flux for transport can be expressed as

$$(-\rho\mathbf{q}\omega + \rho\mathbf{D}\nabla\omega)|_b \cdot \mathbf{n} = j_{ss}. \quad (6)$$

The meaning of j_w and j_{ss} is problem-dependent and very much a modeler's choice.

[16] Problems arise when flow and transport boundary conditions are inconsistent. Inconsistencies appear if the salt fluxes coming from the transport boundary conditions are not considered in the fluid flux boundary conditions. To prevent these inconsistencies, all salt boundary sources from transport boundary conditions must also be boundary sources in the flow equation. That is, if j_{ss} is not null in (6) it cannot be null in (5).

[17] There are situations prone to inconsistent modeling. This is the case of dissolution boundaries, usually modeled as prescribed concentration plus zero fluid flux boundaries. Concentration is prescribed because it is assumed that the boundary and the fluid are in equilibrium. The fluid flux is set to zero because the boundary is considered impervious, which requires that j_w and j_{ss} are such that the total flux through the boundary is null. This requires a binary diffusion process by which the salt influx is balanced by an outward water flux. Obviously, this contradicts the imperviousness attributed to the boundary. That is, dissolution boundaries are impervious only to water and there is an actual salt flux that cannot be overlooked.

[18] The diffusive-dispersive flux of salt established through a prescribed concentration boundary was studied by *Hassanizadeh and Leijnse* [1988], where a thorough description of dissolution boundaries and a rigorous derivation of the associated salt flux can be found. The salt flux can be obtained by subtracting (5) multiplied by ω from (6), which yields

$$j_{ss} = \frac{1}{1 - \omega} [(\rho\mathbf{D}\nabla\omega)|_b \cdot \mathbf{n} + j_w\omega]. \quad (7)$$

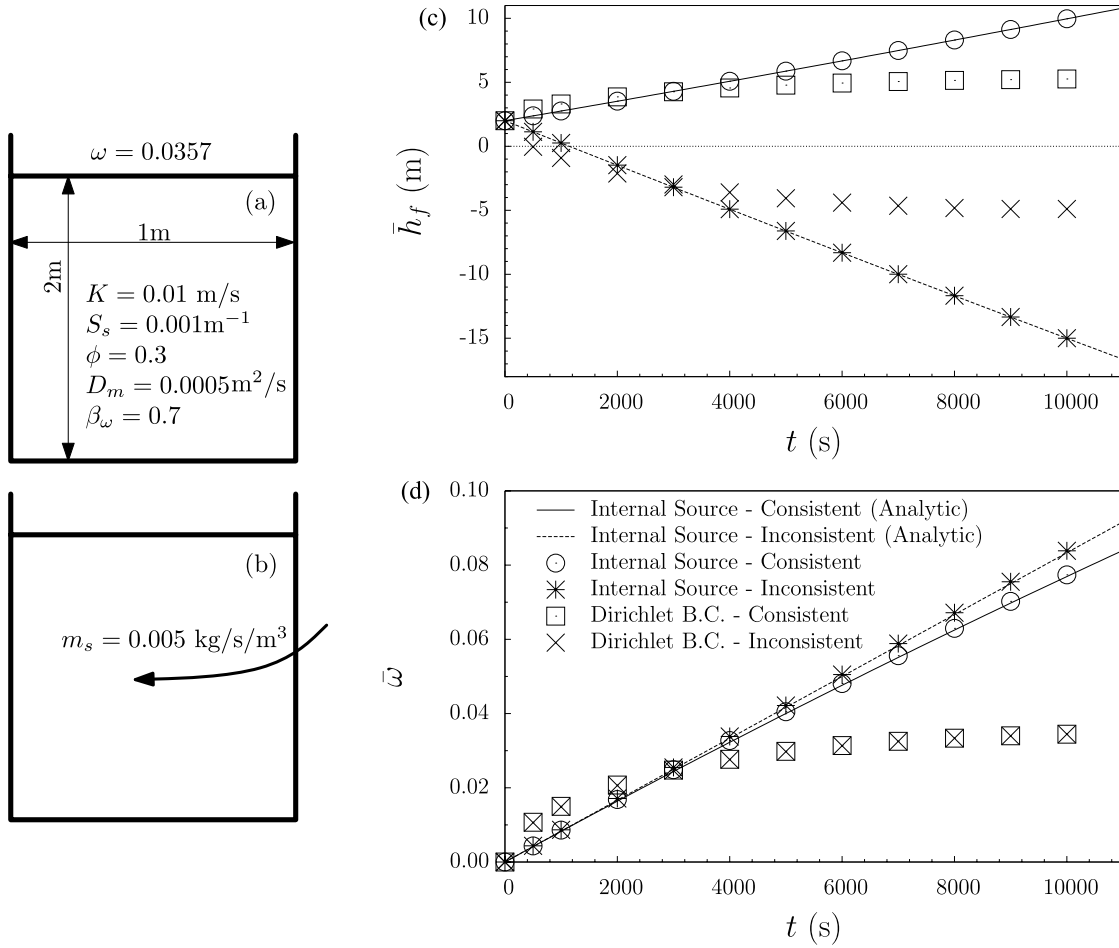


Figure 1. (left) Saltwater bucket problem setup. Salt enters the system through the top boundary. Two conceptual models for the salt sources are proposed: (a) a Dirichlet boundary condition and (b) a constant volumetric source $m_s = 0.005$ kg/s/m³. (right) Saltwater bucket (c) average equivalent freshwater head and (d) average salt mass fraction evolution. Note that solutions are significantly different in terms of head (drop instead of rise when salt sources are neglected) but are less different in terms of mass fraction.

[19] For dissolution boundaries $j_w = 0$, so that the flow and transport boundary conditions have to be written as

$$-\rho \mathbf{q}|_b \cdot \mathbf{n} = j_{ss} \quad (8)$$

$$\omega|_b = \omega^*, \quad (9)$$

where ω^* is the salt mass fraction prescribed at the boundary and j_{ss} is obtained from (7):

$$j_{ss} = \frac{1}{1 - \omega} \rho \mathbf{D} \nabla \omega|_b \cdot \mathbf{n}. \quad (10)$$

This mass flux is undefined when $\omega = 1$, which is frequent. However, j_{ss} can still be evaluated by computing the mass balance (2) at the boundary. This indirect measure of j_{ss} is inexact (the flux only becomes finite when $\nabla \omega = 0$) but appropriate for numerical computations.

3. Evaluation of the Effect of Salt Sources in Density-Dependent Flow Problems

[20] Two numerical experiments are carried out to illustrate the effect of pure salt sources. Numerical computations

were performed with the finite element code Trandens [Hidalgo et al., 2005], in which the flow equation is formulated using equivalent freshwater head h_f [L] and the flow storage term is approximated as

$$\frac{\partial(\rho\theta)}{\partial t} = \rho S_s \frac{\partial h_f}{\partial t} + \beta_\omega \rho \theta \frac{\partial \omega}{\partial t}, \quad (11)$$

where S_s [L⁻¹] is the specific storage coefficient and β_ω [-] is $(1/\rho) (\partial \rho / \partial \omega)$, which is taken as constant.

3.1. Saltwater Bucket Problem

[21] The saltwater bucket problem addresses the effect of salt sources in a vessel with impervious boundaries (Figure 1). The vessel is initially full of freshwater. Salt but not water enters the system through the top boundary. Two ways of representing the salt source are used. The first one considers the upper limit as a transport Dirichlet boundary (Figure 1a) and the second one as a constant rate source (Figure 1b). The two conceptual models are not equivalent, but they help in comparing the different types of sources. This benchmark is similar to the one proposed by Ackerer et al. [1999] primarily used to analyze the instabilities of numerical solutions to density-dependent flow problems.

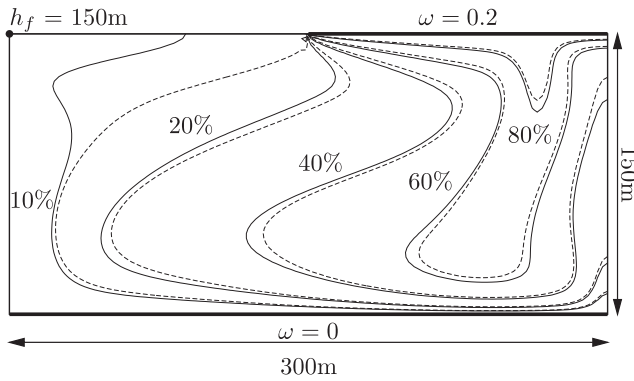


Figure 2. Definition of the Elder problem and salt mass fraction isolines (in percent of maximum mass fraction) in the 240th month (solid line, consistent solution; dashed line, inconsistent solution). Only the left half of the domain is shown.

[22] An analytical solution for average concentration can be obtained when the salt source is modeled as a constant rate source. Volume averaging equations (1) and (2), with m_w equal to zero, leads to

$$\frac{\partial \bar{\rho}\theta}{\partial t} = \begin{cases} m_s, & \text{for the consistent case} \\ 0 & \text{for the inconsistent case} \end{cases} \quad (12)$$

$$\frac{\partial \bar{\rho}\theta\omega}{\partial t} = m_s \text{ for both cases,} \quad (13)$$

where the bar indicates volume average. Initially, $\bar{h}_f(0) = \bar{h}_{f0}$ and $\bar{\omega}(0) = 0$. Stated like this, it is evident that the inconsistent case, in which salt sources are neglected, is wrong because the only source of fluid mass is not included.

3.1.1. Analytical Solution for the Inconsistent Case

[23] In the inconsistent formulation, equation (12) implies that $\bar{\rho}\theta$ is constant and equal to the initial value $\rho_0\theta_0$. Then, (13) yields

$$\bar{\omega}(t) = \frac{m_s}{\rho_0\theta_0} t. \quad (14)$$

[24] Expanding (12) as in (11) and assuming that $\bar{\rho}(t) \approx \rho_0 e^{\beta_s \bar{\omega}(t)}$ and that $\bar{\rho}\theta\omega \approx \bar{\rho}\theta\bar{\omega}$, which are valid approximations for small values of ω , the solution for head is

$$\bar{h}_f(t) = \bar{h}_{f0} - \frac{\theta_0}{S_s} \frac{(\bar{\rho}(t) - \rho_0)}{\bar{\rho}(t)}. \quad (15)$$

Notice that this formulation causes head to drop when salt is added. In fact, head drop may be huge if storativity is small. Again, the head drop simply reflects the tendency of the fluid to shrink because its mass is held constant, while its density is increased in response to the increase in concentration.

3.1.2. Analytical Solution for the Consistent Case

[25] Equation (12) implies that $\bar{\rho}\theta$ is not constant but evolves in time as

$$\bar{\rho}\theta = \rho_0\theta_0 + m_s t. \quad (16)$$

Expanding (13) and using (16) leads to the solution for the average mass fraction

$$\bar{\omega}(t) = \frac{m_s t}{\rho_0\theta_0 + m_s t}. \quad (17)$$

The solution for head is obtained by expanding again (12) as in (11). In this case the derivative of ω is replaced by its value from (17). The resulting expression for head is

$$\bar{h}_f(t) = \bar{h}_{f0} + \frac{\theta_0}{\bar{\rho}(t)S_s} \left(\rho_0 - \bar{\rho}(t) + \frac{m_s}{\theta_0} t \right). \quad (18)$$

3.1.3. Numerical Results and Discussion

[26] The saltwater bucket problem was solved numerically for the two conceptual models described in Figure 1 using the consistent and the inconsistent formulations, which results in a total of four simulations. The simulations were carried out on a one-dimensional mesh for a time interval of 10^4 s. Results are shown in Figure 1.

[27] When salt is added, the mass, density and volume of the fluid tend to increase. Therefore, head tends to increase, as properly reproduced by the consistent formulation. However, the inconsistent formulation implies that $\bar{\rho}\theta$ is constant (recall equation (12)). As fluid mass remains constant, despite an increase in density, fluid volume tends to decrease, which causes head to fall.

[28] Despite the differences in head, salt mass fraction curves (Figure 1d) are very similar. Differences are visible only for high values of salt mass fraction ($\omega > 0.05$). Numerical and analytical solutions are virtually identical.

3.2. Elder Problem

[29] The Elder problem [Elder, 1967] is an unstable interface density-dependent problem. It consists of a 600×150 m rectangular domain with salt mass fraction prescribed at the bottom and in a 300 m long segment in the central part of the top boundary (Figure 2). All boundaries are impervious except at the two top corners, where head is prescribed. Owing to its extended use as a benchmark, it is worth examining how salt sources influence the solution to this problem. The solution to the Elder problem is known to be dependent on mesh size, temporal discretization and convergence criteria [Ackerer et al., 1999; Frolkovič and De Schepper, 2000]. Variations in those elements lead to important changes in the concentration fingering pattern, mainly in the central finger [see, e.g., Oltean and Bues, 2001; Diersch and Kolditz, 2002]. However, differences between the consistent and the inconsistent solutions should be qualitatively independent of numerical discretization because of their conceptual nature.

[30] Simulations were carried out using a fine mesh of triangular elements. Because of the symmetry, only half of the domain was simulated. The simulations span 240 months. Two simulations were performed. They are identical to the original problem except that the value of ω the imposed at the boundary is 0.2 (rescaling β_ω to maintain density contrast), because the typical value of 1.0 is absurd (it implies that the fluid consists solely of salt). The first simulation uses the traditional formulation (neglecting salt sources in the flow equation). The second simulation acknowledges salt sources.

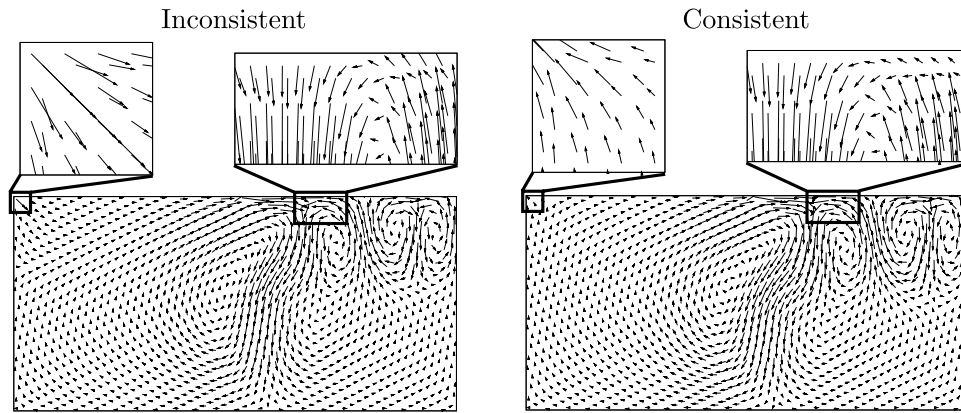


Figure 3. Darcy velocities for the Elder problem in the 36th month including (consistent) and not considering (inconsistent) salt sources in the flow boundary condition at the region where concentration is prescribed. The vertical component of velocity has been exaggerated 10 times in the inset of this region. Only the left half of the domain is shown.

[31] Results of the simulations (Figure 2) show that concentration contours change little when salt sources are considered. This reflects that the influence of salt sources on concentration is small for moderate values of the salt mass fraction.

[32] The main difference between consistent and inconsistent solutions is found in the velocity field (Figure 3). Velocities never cross the boundaries in the traditional problem solution, but point toward the Dirichlet ones in the adjacent elements (displayed in Figure 3) to compensate the downward diffusion with an upward advection. This is consistent with the impervious boundary condition set for the flow equation. When salt sources are acknowledged, velocities are tilted downward to become parallel to the no flow boundaries. This reflects the direction of salt flux at prescribed concentration boundaries, which occurs mostly by diffusion.

[33] The behavior of flow across the prescribed head corner (Figure 3) node is illustrative. Freshwater enters the system through this point in the inconsistent solution. By contrast, water leaves the system when salt sources are acknowledged. Salt mass entering the system causes the fluid volume and, hence, head to increase, thus pushing fluid out of the system. The inversion in the flux direction explains the difference in the 10% line in Figure 2.

4. Conclusions

[34] Pure salt sources are not common in density-dependent flow problems. Yet, when present, their effect may be qualitatively important. Salt influxes cause both fluid density and volume to increase. Therefore, they cause head to rise and fluid to flow away from the source. The opposite occurs when salt sources are accounted for in the transport but not in the flow equation. The obvious conclusion is that salt sources, when present, should also be acknowledged in the flow equation.

[35] Neglecting the influence of pure salt sources on fluid mass balance can lead to erroneous solutions. This is especially important when Dirichlet boundaries for transport and impervious (i.e., no water flux) boundaries for flow are combined inconsistently. Discrepancies in concentrations are significant only when prescribed mass fraction is

close to one. However, solutions are wrong for flow, at least from a qualitative point of view. The fluid mass balance will not close. Moreover, the head drop caused by the salt influx needs to be offset by a water influx, which causes an inversion in flux direction at prescribed head or mixed boundary condition nodes.

[36] Two final disclaimers should be made. First, the inconsistency discussed here does not occur if the compositional approach is used. Second, the problem can be fixed even in density-dependent flow codes that do not handle pure salt sources. It is sufficient (1) to add a water source term of magnitude equal to the salt source term to the flow equation and (2) to multiply the salt source term in the transport equation by $(1-\omega)$, if the advective form is used. If the pure salt source term is not known a priori, it can be evaluated from a preliminary inconsistent run because the effect on concentration is small.

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