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The rotating movement of three immiscible fluids —a benchmark problem

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Abstract

A benchmark problem involving the rotating movement of three immiscible fluids is proposed for verifying the density-dependent flow component of groundwater flow codes. The problem consists of a two-dimensional strip in the vertical plane filled with three fluids of different densities separated by interfaces. Initially, the interfaces between the fluids make a 45° angle with the horizontal. Over time, the fluids rotate to the stable position whereby the interfaces are horizontal; all flow is caused by density differences. Two cases of the problem are presented, one resulting in a symmetric flow field and one resulting in an asymmetric flow field. An exact analytical solution for the initial flow field is presented by application of the vortex theory and complex variables. Numerical results are obtained using three variable-density groundwater flow codes (SWI, MOCDENS3D, and SEAWAT). Initial horizontal velocities of the interfaces, as simulated by the three codes, compare well with the exact solution. The three codes are used to simulate the positions of the interfaces at two times; the three codes produce nearly identical results. The agreement between the results is evidence that the specific rotational behavior predicted by the models is correct. It also shows that the proposed problem may be used to benchmark variable-density codes. It is concluded that the three models can be used to model accurately the movement of interfaces between immiscible fluids, and have little or no numerical dispersion.
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1. Introduction

The term *benchmarking* refers to the process of comparing output of groundwater models for well-defined standard problems, known as benchmark problems (Simpson and Clement, 2002). Several

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benchmark problems exist for benchmarking groundwater flow codes that include spatial and temporal variations of the density. Three of the most common benchmark problems for variable-density flow are Henry's problem (Henry, 1964; Segol, 1994), the Elder problem (Elder, 1967; Johanssen, 2002), and the HYDROCOIN saltdome problem (e.g., Herbert et al., 1988; Konikow et al., 1997). Simpson and Clement (2002) discuss the worthiness of the Henry and Elder problems for benchmarking. These and many other benchmark problems for variable-density flow are strongly influenced by hydrodynamic dispersion; the problems are significantly altered, or even become meaningless, when hydrodynamic dispersion is neglected. With the exception of the Henry problem, analytical solutions do not exist for these benchmark problems, which leaves qualitative comparison of model output as the sole method for benchmarking.

The only commonly used benchmark problems that are not dominated by hydrodynamic dispersion are problems with two immiscible fluids separated by an interface (often an interface between freshwater and saltwater). Several techniques exist for the computation of the steady-state position of the interface for the case that the heavier fluid is stagnant. These include interface solutions obtained with the hodograph method (e.g., Verruijt, 1969; Strack, 1972; Bakker, 2000), and interface solutions based on the Dupuit approximation (e.g., Strack, 1976; Van Dam and Sikkema, 1982). An exact transient solution, although based on the Dupuit approximation, exists for a rotating interface between two fluids (e.g., Wilson and Sa Da Costa, 1982). An exact solution for the initial velocity distribution of a vertical interface was given by Verruijt (1980).

In this paper, a new benchmark problem is proposed. The benchmark problem consists of the movement of three immiscible fluids of different densities; flow is caused by density differences only. The benchmark problem is intended specifically for the verification of the density-dependent flow part of groundwater flow codes, as hydrodynamic dispersion is purposely not taken into account. In addition, it may be used to assess the impact of adopted approximations (such as the Dupuit approximation). The existence and magnitude of numerical dispersion may be assessed by considering the width of the mixing zones along the interface. An exact solution is presented for the initial velocity distribution of the transient case, and the transient results of three variable density codes are compared in this paper.

2. Problem description

Consider two-dimensional confined flow in a vertical cross-section as shown in Fig. 1. A Cartesian x, y coordinate system is adopted with the y-axis pointing vertically upward. The aquifer thickness is $2b$, the length is L, and the top and bottom are horizontal; all boundaries of the aquifer are impermeable. The aquifer is filled with water of three different densities; the water with three different densities will be treated as three immiscible fluids separated from each other by interfaces. The three densities are ρ_1, ρ_2, and ρ_3 [M/L^3], with $\rho_1 < \rho_2 < \rho_3$. The difference between the smallest and largest density is of the same magnitude as the difference between the densities of freshwater and seawater, such that viscosity differences may be neglected. The freshwater hydraulic conductivity of the aquifer is homogeneous and isotropic and equal to k [L/T]. The effective porosity of the aquifer is n [−], and the aquifer and fluids are treated as incompressible. Initially, at time $t = 0$, both interfaces are straight and their centers are located at x_1 and x_2; interface 1 has a slope of b/a_1 and interface 2 has a slope of b/a_2 (see Fig. 1). Most computer programs that are able to simulate this problem require the specification of a head at one point in the aquifer; the transient evolution of the interfaces is independent of this choice.

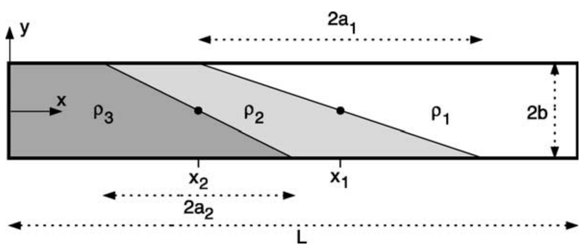

Fig. 1. Setup of problem: initial position of three fluids.

3. Exact solution for the initial flow field

An exact solution for the initial flow field is obtained for the case of an infinite strip ($L = \infty$) by application of the vortex theory of De Josselin de Jong (1958). A shear flow exists along an interface separating two fluids of different densities. The shear flow s [L/T] is defined as the difference between the tangential components of the specific discharge vector across the interface, and may be written as (e.g., Bear, 1972, p. 521)

$$s = k\frac{\rho_b - \rho_a}{\rho_a}\sin\alpha \tag{1}$$

where α is the positive angle between the tangent to the interface and the positive x-axis, and $\rho_b > \rho_a$. Along a straight interface, the shear flow is constant.

The complex specific discharge, W, is introduced as

$$W = q_x - \mathrm{i}q_y \tag{2}$$

where i is the imaginary unit, and q_x and q_y are the horizontal and vertical components of the specific discharge vector, respectively. The complex specific discharge for a constant shear flow, s, along a straight line-segment in an infinite domain may be represented by the general function F (e.g., Strack, 1989)

$$F(z,\zeta_1,\omega_1,s) = \frac{sl\mathrm{i}}{2\pi(\zeta_1-\omega_1)}\ln\frac{z-\zeta_1}{z-\omega_1} \tag{3}$$

where $z = x + \mathrm{i}y$ is the complex coordinate, ζ_1 and ω_1 are the complex coordinates of the beginning and end points of the line-segment, and l is the length of the line-segment. The flow field due to a unit shear flow along a line-segment extending from $\zeta_1 = -1 + \mathrm{i}$ to $\omega_1 = 1 - \mathrm{i}$ is shown in Fig. 2.

An expression for the flow field due to one straight interface in a horizontal confined aquifer is obtained with the method of images and is called w. Consistent imaging of one interface across both boundaries gives for w (see Fig. 3)

$$w(z,x_0,a,b,s) = F(z,\zeta_1,\omega_1,s) + \sum_{n=1}^{\infty}[F(z,\zeta_n,\zeta_{n+1},(-1)^n s) + F(z,\omega_n,\omega_{n+1},(-1)^n s)] \tag{4}$$

where ζ_1 and ω_1 are the beginning and end points of the interface, and ζ_n and ω_n are image locations of the ends of the interface (Fig. 3)

$$\zeta_n = x_0 + (-1)^n a + (2n-1)b\mathrm{i}$$
$$\omega_n = x_0 + (-1)^{1+n} a - (2n-1)b\mathrm{i} \tag{5}$$

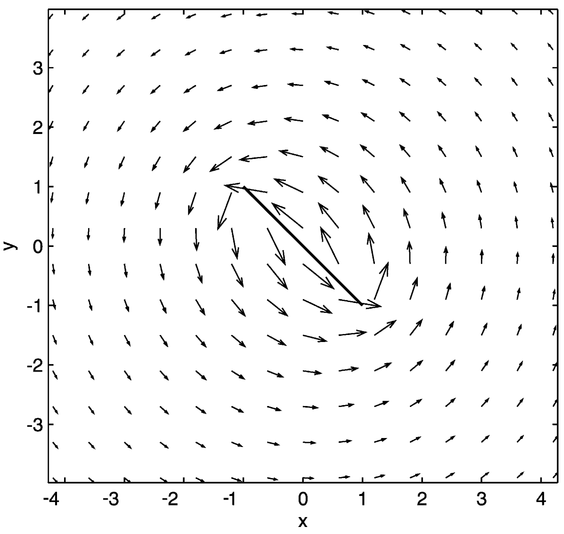

Fig. 2. Rotational flow due to a constant shear flow along a straight line-segment from $\zeta_1 = -1 + \mathrm{i}$ to $\omega_1 = 1 - \mathrm{i}$.

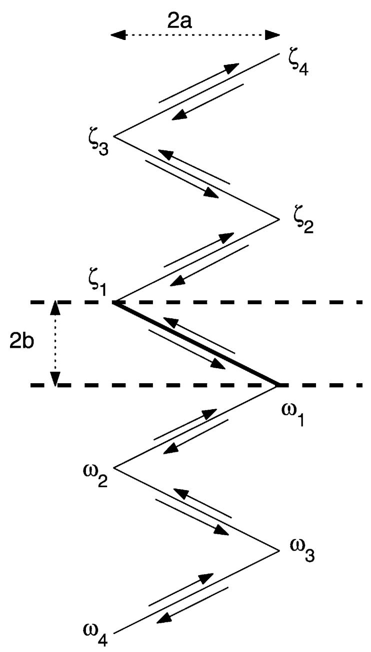

Fig. 3. Consistent imaging of an interface between ζ_1 and ω_1; dashed lines are top and bottom of the aquifer.

Although in theory an infinite number of images is needed, in practice the effect of a line-segment vanishes at a distance of several times l away from the segment (Fig. 2). The specific discharge contains a singularity at the intersections of an interface with the top and bottom of the aquifer (at ζ_1 and ω_1). This means that in reality, there cannot be a non-zero angle between the interface and the horizontal top and bottom of the aquifer; near the top and bottom of the aquifer, the interface will curve until it is horizontal. Evaluation of the specific discharge vector near the singularity shows that the effect of the singularity is very local and does not affect the solution significantly (i.e. the simplified mathematical model is a reasonable representation of reality).

The initial flow field of the problem shown in Fig. 1, which has two interfaces, may now be obtained through superposition as

$$W(z) = w(z, x_1, a_1, b, s_1) + w(z, x_2, a_2, b, s_2) \quad (6)$$

where s_1 and s_2 are computed with Eq. (1). Once the specific discharge is known, the horizontal velocity v_h of an interface with a slope $-b/a$ may be computed as the sum of the horizontal velocity of the water minus the vertical velocity of the water divided by the slope.

$$v_h = v_x + v_y a/b \quad (7)$$

where $v_x = q_x/n$ and $v_y = q_y/n$ are the x and y components of the velocity along the interface; v_x and v_y should be evaluated on the same side of the interface (i.e., either both just left or just right of the interface).

4. Computer programs used for comparison

Results of three computer programs are compared in the subsequent sections of this paper. Each program makes use of a modified version of the finite-difference code MODFLOW (McDonald and Harbaugh, 1988; Harbaugh and McDonald, 1996; Harbaugh et al., 2000) to compute the freshwater head at the center of each cell. A brief description of each program is given in what follows; short descriptions and examples of all three programs may also be found in Langevin et al. (2003).

4.1. SWI package for MODFLOW

The Sea Water Intrusion (SWI) package is intended for the modeling of regional seawater intrusion with MODFLOW2000 (Bakker and Schaars, 2002). The formulation used in the SWI package is based on the Dupuit approximation, meaning that the vertical resistance to flow is neglected within an aquifer, and the pressure distribution within an aquifer is hydrostatic. The advantage of using the Dupuit approximation to model multi-aquifer systems is that each aquifer can be represented with one layer of cells. Variable-density flow may be simulated as stratified flow (which is used here) or as continuously varying density flow, in which case the positions of isosurfaces of the density within an aquifer are tracked. The basic principle behind the formulation is to solve, during each timestep, for the freshwater-head by considering continuity of flow in the entire aquifer, and to solve for the elevations of the interfaces by considering continuity of flow below each interface. A simple algorithm is employed to keep track of the movement of the tip and toe of each interface. The SWI package requires one additional input file to simulate seawater intrusion with an existing MODFLOW model. Details of the formulation are given in Bakker (2003).

4.2. MOCDENS3D

MOC3D (Konikow et al., 1996) was adapted for density differences by Oude Essink (1998) to model the movement of fresh, brackish and saline groundwater in porous media in three dimensions. In this new version of MOC3D, called MOCDENS3D, buoyancy terms are introduced in the vertical effective velocities to account for density effects. The equation of density-dependent groundwater flow is solved by the MODFLOW module. Solute transport is modeled by the method of characteristics (MOC) module. The particle-tracking method is used to solve advective solute-transport, and the finite-difference method is used for hydrodynamic dispersive transport; an equation of state couples groundwater flow and solute transport. The horizontal sizes of the elements should be uniform, whereas the timestep to recalculate the groundwater flow equation must be determined manually. Numerical dispersion and oscillations are limited as the MOC is applied. MOCDENS3D has been applied recently to model the effect of sea level rise, land subsidence, and human activities in several, three-dimensional regional groundwater systems in the Netherlands (e.g., Oude Essink, 2001).

4.3. SEAWAT

The SEAWAT program (Guo and Langevin, 2002) is a combination of MODFLOW and MT3DMS (Zheng and Wang, 1999) designed to simulate three-dimensional, variable-density, groundwater flow and solute-transport. The program was developed by modifying MODFLOW subroutines to solve a variable-density form of the groundwater flow equation and by combining MODFLOW and MT3DMS into a single program. SEAWAT reads and writes standard MODFLOW and MT3DMS input and output files, allowing most of the existing pre- and post-processors to facilitate application of the program to a wide range of practical problems. One advantage of SEAWAT is that because it uses MT3DMS to represent solute-transport, the program contains several methods for solving the transport equation including the MOC, a third-order total-variation-diminishing (TVD) scheme, and an implicit finite-difference method. An example of a SEAWAT application to estimate submarine groundwater discharge is presented in Langevin (2001).

5. Comparisons

Two comparisons will be presented. For each case, the initial horizontal velocity of one of the interfaces will be compared to the exact solution. There is no exact solution for the transient evolution of the interfaces, so that the results of the three programs will be compared to each other. The aquifer parameters and initial geometry of the two comparisons are identical and are given in Table 1. Initially, the two interfaces are parallel. The first comparison is the symmetric case where the density of the middle fluid is the average of the other two fluids. The symmetric case is useful for benchmarking, because non-symmetric model results will indicate a problem with the code. For the second comparison, the density of the middle fluid is closer to the density of the lighter fluid and the flow field is asymmetric. The densities used in the comparisons are given in Table 2. The discretization used in the three models is the same for both comparisons and is given in Table 3.

Each program requires the specification of some program-specific parameters. For the SWI model, the maximum slope of the interfaces is specified as 0.5, and the tip and toe tracking parameters are specified according to the guidelines given in the user's manual. The SWI package uses only one cell in the vertical. For MOCDENS3D, each cell initially contains 16 particles. The solute timestep is computed automatically (Konikow et al., 1996) and the Courant number (the fractional cell distance allowed for advection) is specified as 0.5. For SEAWAT, the TVD option was used to solve the solute-transport equation. The TVD option, which is intended for sharp density contrasts, runs faster than the MOC option, but it also results in more numerical dispersion. SEAWAT uses a variable timestep based on stability criteria of the transport solution method; the Courant number was specified as 0.25. For both MOCDENS3D and SEAWAT, dispersion was excluded from the simulations by setting dispersivity and molecular diffusion to zero.

Table 1
Aquifer and geometry data of comparisons

L	300 m	a_1	40 m
b	20 m	a_2	40 m
k	2 m/d	x_1	170 m
n	0.2	x_2	130 m

Table 2
Densities used in comparisons

	Symmetric case	Asymmetric case
ρ_1 (kg/m^3)	1000	1000
ρ_2 (kg/m^3)	1012.5	1005
ρ_3 (kg/m^3)	1025	1025

Table 3
Discretization

Model	Δx (m)	Δy (m)	Number of cells	Δt (d)
SWI	5	40	60	4
MOCDENS3D	1	0.5	24,000	10
SEAWAT	1	0.5	24,000	13.8[a]

[a] Average for asymmetric case.

5.1. Symmetric case

The exact solution of the initial velocity field for the symmetric case, computed with Eq. (6), is shown in Fig. 4(a) (only the center part of the flow field from $x = 65$ to 235 is shown). Notice that there is a stagnation point at the center of the aquifer, and that the velocity becomes very small within a short distance of the extent of the interfaces. Even though the exact solution is for an infinitely long strip ($L = \infty$), the velocities at $x = 0$ and 300 have become so small (in Fig. 4(a) they are almost zero at $x = 70$ and 230) that from a practical standpoint, the solution may be treated as the exact solution for this case. The initial horizontal velocity of the interfaces, computed with Eq. (7), is shown graphically in Fig. 4(b). It may be seen from Fig. 4(b), that the initial velocity of the toe of the left interface is larger than the velocity of the toe of the right interface. As a result, the toe of the left interface will approach the toe of the right interface over time, provided that the length L of the strip is long enough. The reverse happens at the top of the aquifer, where the velocity of the tip of the right interface is larger than the velocity of the tip of the left interface. As a result, the two interfaces will not remain parallel, but the tips and toes will move closer together. The behavior described above may be observed from Fig. 5, where the horizontal velocity v_h of the left interface is plotted along the horizontal axis and the vertical position of the interface along the vertical axis; the bottom of the left interface does indeed move quicker to the right than the top of the left interface moves to the left.

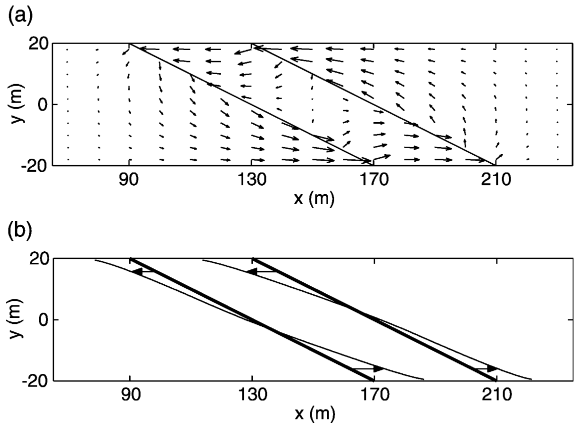

Fig. 4. Exact solution symmetric case (a) initial velocity field, (b) locus of end points of initial horizontal velocity of interfaces with bold lines representing the initial interface positions.

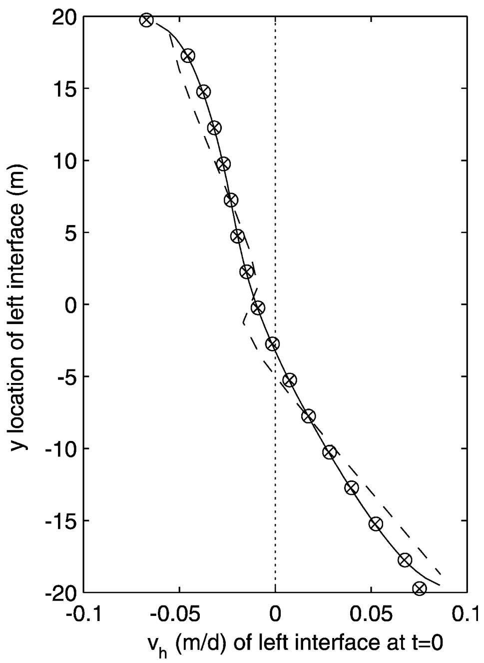

Fig. 5. Initial horizontal velocity versus vertical position of left interface, exact (solid), SWI (dash), MOCDENS3D (circle), SEAWAT (cross).

The exact solution of the initial horizontal velocity of the left interface is compared to the results of the three models in Fig. 5. The solid line is the exact solution, the dashed line is the SWI solution, the circles represent points of the MOCDENS3D solution, and the crosses represent the SEAWAT solution. It is noted that the latter two solutions are represented by markers rather than lines because they are so close to the exact solution that plotting lines would make them virtually indistinguishable. The SWI results deviate slightly more from the exact solution.

The positions of the two interfaces at 2000 and 10,000 days are shown in Fig. 6; the solid line is the SWI model, the dashed line is MOCDENS3D, and the dash-dotted line is SEAWAT. As the latter two models compute a density at the center of each cell, the lines represent contours of the density for $(\rho_1 + \rho_2)/2$ and $(\rho_2 + \rho_3)/2$; the zone over which the density varies between ρ_1 and ρ_2, and between ρ_2 and

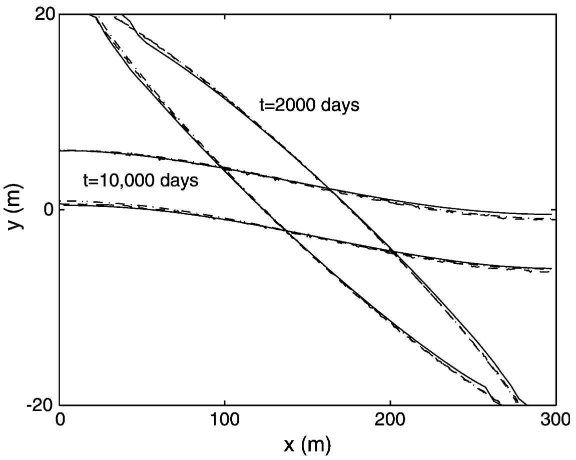

Fig. 6. Evolution of interfaces symmetric case, SWI (solid), MOCDENS3D (dash), SEAWAT (dash-dot); vertical scale exaggerated.

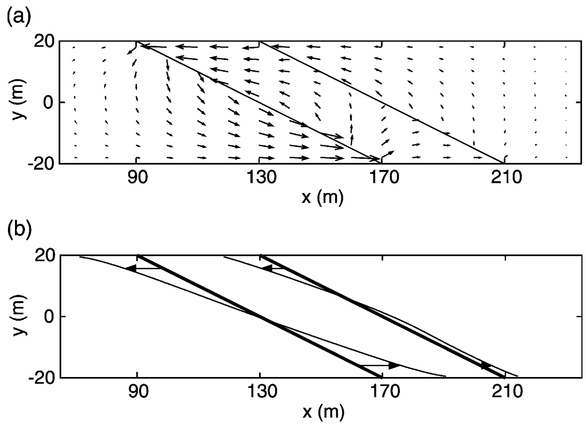

Fig. 7. Exact solution asymmetric case (a) initial velocity field, (b) locus of end points of initial horizontal velocity of interfaces with bold lines representing the initial interface positions.

ρ_3 are generally less than a couple of cell widths. At $t = 2000$ days, the interfaces move closer together at the top and bottom of the aquifer, as may be seen from Fig. 6. At $t = 10,000$ days, the interfaces are nearly horizontal and are moving slowly to equilibrium. The results of all three models are quite similar. The SWI package seems to result in a slightly quicker rotation of the fluids; this difference is small but may be a result of adopting the Dupuit approximation. MOCDENS3D and SEAWAT were also run with larger cell sizes (a smaller number of cells). This resulted in a slightly slower rotation of the interfaces than the run with smaller cell sizes (for SEAWAT), and also resulted in a more substantial deviation from the exact solution for the initial horizontal velocity of the interfaces, because the velocities are computed at the boundaries of cells. The codes were further verified by noting that the simulated interface positions were symmetrical with respect to the center of the strip.

5.2. Asymmetric case

The exact solution of the initial flow field for the asymmetric case is shown in Fig. 7(a). The effect of the left interface is now dominant, because the difference in density between fluids 2 and 3 is much larger than between fluids 1 and 2. The initial horizontal velocity of the interfaces is shown graphically in Fig. 7(b). Along both the top and bottom of the aquifer, the left interface moves much faster than the right interface. Fluid 2 is so much lighter than fluid 3 that the tendency of fluid 2 to flow to the top is greater than the tendency to rotate. As a result, the horizontal distance between the two interfaces will become larger at the top of the aquifer and (much) smaller at the bottom of the aquifer.

The exact solution of the initial horizontal velocity v_h of the right interface is compared to the results of the three models in Fig. 8. The solid line is the exact solution, the dashed line is the SWI solution; the MOCDENS3D and SEAWAT results are represented by markers (circles and crosses, respectively) to distinguish them visually from the exact solution. The top of the right interface moves much quicker to the left than the bottom moves to the right, as expected.

The positions of the interfaces at 2000 and 20,000 days are shown in Fig. 9; the solid line is the SWI model, the dashed line is MOCDENS3D, and the dash-dotted line is SEAWAT. During rotation, the two interfaces move so close together at the bottom of the aquifer that an interface between fluids 1 and 3 develops, as can be seen at $t = 2000$ days. Over time, this interface disappears slowly ($t = 20,000$ days); it takes much longer for the interfaces to rotate to the horizontal positions. Again, the results of the three models are similar, although not as similar as for the symmetric case. The SWI and MOCDENS3D results

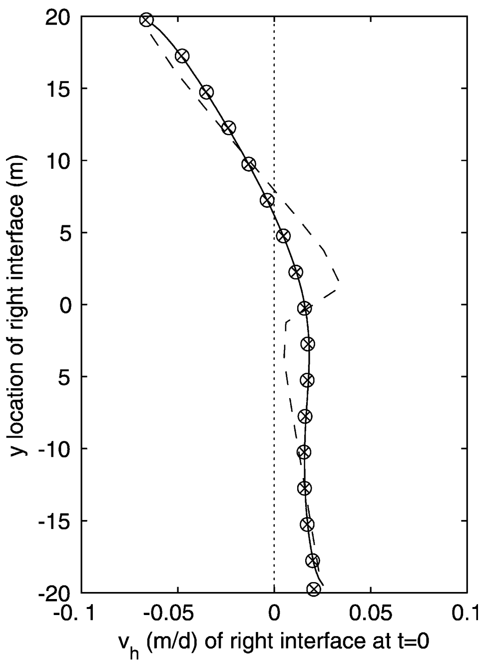

Fig. 8. Initial horizontal velocity of right interface, exact (solid), SWI (dash), MOCDENS3D (circle), SEAWAT (cross).

are very close at $t = 20,000$ days. SEAWAT produces a less distinct interface between fluids 1 and 3 at the right side of the model, but the differences are small. As compared with the symmetric case, the asymmetric case appears to be more challenging in terms of numerical dispersion.

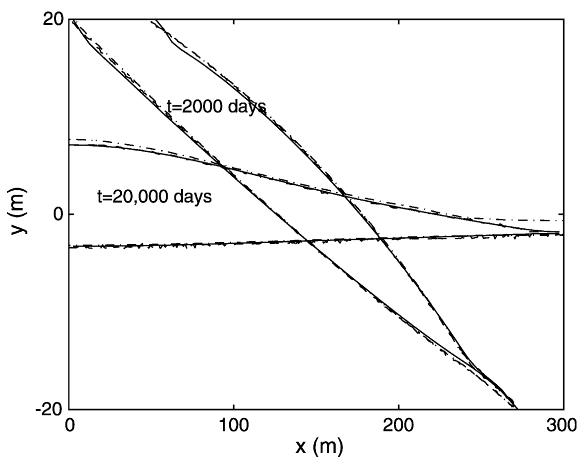

Fig. 9. Evolution of interfaces asymmetric case, SWI (solid), MOCDENS3D (dash), SEAWAT (dash-dot); vertical scale exaggerated.

6. Discussion and conclusions

A benchmark problem for the verification of the density-dependent part of groundwater flow codes was proposed. The problem consists of the rotation of three immiscible fluids with different densities; the fluids are separated from each other by interfaces. An exact solution was presented for the initial flow field of initially straight interfaces in a horizontal aquifer. Results of the three programs SWI, MOCDENS3D, and SEAWAT were compared; all three programs use modified versions of MODFLOW to compute the distribution of the freshwater head. The SWI model is based on the consecutive application of continuity of flow, whereas the MOCDENS3D and SEAWAT models solve the combined flow and transport equations. MOCDENS3D and SEAWAT produced initial horizontal velocities of the interfaces that were almost indistinguishable from the exact solution, but a coarser discretization gave somewhat larger deviations; the SWI results of the initial horizontal velocity distribution showed a small difference from the exact solution, probably as a result of the Dupuit approximation. The transient results of all three models were similar at both times considered. The SWI model results did not deviate much from the other two models, even though the SWI package is based on the Dupuit approximation and uses substantially less cells; the SWI package has no numerical dispersion. Results of the MOCDENS3D and SEAWAT models showed that these models do not have much numerical dispersion, as they can accurately simulate the movement of interfaces between immiscible fluids. The similarity of the results of all three models at all times confirms the general behavior of the three rotating fluids, which was shown in Figs. 6 and 9. The benchmarking of the three programs is an independent confirmation of the accuracy of implementation of the density-dependent flow part of each program.

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