Available online at www.sciencedirect.com
ScienceDirect
Advances in Water Resources 29 (2006) 1918–1923
Advances in Water Resources
www.elsevier.com/locate/advwatres

A note on benchmarking of numerical models for density dependent flow in porous media

B. Ataie-Ashtiani *, M.M. Aghayi

Department of Civil Engineering, Sharif University of Technology, P.O. Box 11365-9313, Tehran, Iran

Received 29 May 2005; received in revised form 26 January 2006; accepted 27 January 2006
Available online 13 March 2006

Abstract

Verification of numerical models for density dependent flow in porous media (DDFPM) by the means of appropriate benchmark problems is a very important step in developing and using these models. Recently, Infinite Horizontal Box (IHB) problem was suggested as a possible benchmark problem for verification of DDFPM codes. IHB is based on Horton–Rogers–Lapwood (HRL) problem. Suitability of this problem for the benchmarking purpose has been investigated in this paper. It is shown that the wavelength of instabilities fails to be a proper criterion to be considered for this problem. However, the threshold of instability formation has been found to be appropriate for benchmarking purpose.

Keywords: Density dependent flow; Porous media; Groundwater; Numerical model; Benchmark problem; Rayleigh number; Horton–Rogers–Lapwood problem

1. Introduction

Numerical simulation of density dependent flow in porous media (DDFPM) is a challenging issue in water resources engineering and verification of DDFPM codes by the means of appropriate benchmark problems is a very important step in developing and using these codes.

Mathematical modeling for DDFPM problems is always performed by solving two partial differential equations (PDEs) for groundwater and solute mass conservations. Since these partial differential equations are coupled together through fluid density, they must be solved simultaneously. Due to the mathematical complexities that arise in simultaneous solution of two coupled PDEs, there are very few (if any) DDFPM problems that have analytical or semi-analytical solutions and verification of DDFPM codes is often based on experimental results or comparison to numerical solutions obtained from other studies [2].

Henry's problem [5] and Elder's problem [3] are the most common problems used for benchmarking DDFPM codes. However some researchers have suggested that these problems are not sufficient for verification purpose [10,14].

There are other benchmark problems such as "salt lake" problem [13], "saltpool" problem [7,11] and "rotation of three immiscible fluids" [1] for verification of DDFPM codes. Diersch and Kolditz [2] have reviewed the existing benchmark problems for verifying DDFPM codes and the reader is referred to their work for more information.

Weatherill et al. [16] have recently presented a set of new DDFPM test cases which deal with formation of density-driven convective instabilities in porous media. The problems are based on analytical solution for a problem defined originally by Rayleigh and Strutt [12] and followed later by Horton and Rogers [6] and Lapwood [8], called Horton–Rogers–Lapwood (HRL) problem. The problem consists of an infinite layer of fluid-filled porous medium enclosed by a thermal sink at its top and a thermal source at the bottom. An initial vertical thermal gradient in the problem

* Corresponding author. Fax: +98 21 6014828.
E-mail addresses: ataie@sharif.edu (B. Ataie-Ashtiani), aghayi@mehr.sharif.edu (M.M. Aghayi).

0309-1708/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.advwatres.2006.01.009

Nomenclature

DDFPM	density dependent flow in porous media	L	layer horizontal length [L]
FHB	finite horizontal box problem	p	pressure [$ML^{-1}T^{-2}$]
FEM	finite element model	Ra	Rayleigh number [–]
HRL	Horton–Rogers–Lapwood problem	Ra_c	critical Rayleigh number [–]
IHB	infinite horizontal box problem	Ra_{c2}	second critical Rayleigh number for transient convection [–]
IIB	infinite inclined box problem	T	time [T]
PDE	partial differential equation	U_c	convective velocity [LT^{-1}]
C	solute concentration (mass fraction) [MM^{-1}]	$\beta = \rho_0^{-1}(d\rho/dC)$	coefficient of density variation (with concentration) [–]
C_{max}	maximum concentration [MM^{-1}]	ΔT	time step length [T]
C_{min}	minimum concentration [MM^{-1}]	μ_0	dynamic viscosity of the fluid [$ML^{-1}T^{-1}$]
D_0	molecular diffusion coefficient of solute in water [L^2T^{-1}]	θ	porosity [–]
g	acceleration due to gravity [LT^{-2}]	ρ_0	fluid density at reference concentration [ML^{-3}]
H	porous layer thickness [L]		
k	intrinsic permeability [L^2]		

domain causes a vertical density gradient that under certain conditions will produce convective instabilities in the form of symmetric square rolls (waves) in the problem domain. The HRL problem has analytically-defined values for threshold of instability formation and wavelength of instability patterns [9]. Three distinct benchmark problems are defined by Weatherill et al. [16], namely "infinite inclined box" (IIB), "finite horizontal box" (FHB) and "infinite horizontal box" (IHB). Analytical threshold of instability formation and analytical wavelength for convective instabilities have been adopted as the criteria to check the reliability of DDFPM codes [16].

The main objective of this work is to re-examine the suitability of the problem set presented in [16] for verification of DDFPM codes. Using sensitivity and convergence analyses, it will be shown here that the threshold of instability formation in IHB problem (which is the basic problem among those presented in [16]) is a proper criterion for benchmarking purpose while the wavelength of instabilities is not a good criterion for such a purpose.

2. Problem definition

Infinite horizontal box (IHB) problem is a 2D box in which a layer of denser saltwater overlays the lighter fresh water and forms a system with potential for generation of convective instabilities (Fig. 1).

Weatherill et al. [16] introduced IHB problem as a finite layer of porous medium with (length/height) ratio equal to 20. This finite layer is a 200 m × 10 m box, having two zero pressure boundary conditions at top corners (Fig. 1). Nonlinear initial conditions for solute concentration and fluid pressure are assigned to the model and a central perturbation is applied to the center of model to assist in generation of instabilities. Full definition of IHB problem can be found in [16].

Rayleigh number for solute version of the HRL problem is given by

$$Ra = \frac{U_c H}{D_0} = \frac{\rho_0 g k \beta (C_{max} - C_{min}) H}{\theta \mu_0 D_0} \quad (1)$$

where U_c is the convective velocity in the porous medium layer, D_0 is molecular diffusion coefficient of solute, ρ_0 is fluid density at reference concentration, g is the acceleration due to gravity, k is intrinsic permeability, β is the coefficient of density variation, θ is porosity of the medium, μ_0 is dynamic viscosity of the fluid and C_{max} and C_{min} are maximum and minimum concentrations of solute in the problem domain, respectively [16].

The analytically-derived critical Rayleigh number for HRL problem is $Ra_c = 4\pi^2$ [9]. For Rayleigh numbers smaller than this critical Rayleigh number, there is only diffusive flux of solute present in the porous medium layer, resulting in a series of straight horizontal concentration

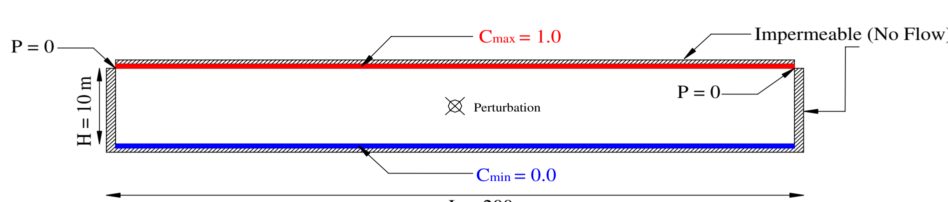

Fig. 1. Definition of IHB problem as presented by Weatherill et al. [16].

isopleths. For Rayleigh numbers greater than the critical Rayleigh number, problem conditions allow for formation of convective instabilities. In such conditions, any small perturbation in the problem domain will be amplified, resulting in strong convective fluxes in the porous medium layer. When convective fluxes occur in the problem, concentration isopleths deviate from their horizontal state and form oscillating patterns with regions of upwelling and downwelling. Convective instabilities occur in the form of square roll cells, each having an analytically-derived length of H, so the wave length for instabilities will be equal to $2H$ [9].

3. Model development

In order to evaluate the suitability of IHB as a benchmark problem, SUTRA code [15] is used for modeling the problem. SUTRA (saturated–unsaturated transport) is a code for saturated–unsaturated variable-density groundwater flow with solute or energy transport. The code was originally developed for 2D problems and upgraded later by Voss and Provost [15] to account for 3D problems as well. SUTRA uses finite element approximation of governing equations for spatial discretization of model domain and fully implicit finite difference approximation for temporal discretization.

Model development was carried out according to descriptions of Weatherill et al. [16]. A 200 m × 10 m box was modeled with two zero pressure boundary conditions at upper corners (Fig. 1). Any inflowing fluid through pressure boundary conditions has concentration equal to $C = 1.0$. Initial distributions for fluid pressure and concentration were defined according to [16], i.e. a model with $Ra < Ra_c$ was constructed and executed to obtain steady state distributions for fluid pressure and concentration and this steady state solution was used as initial condition for the main model. Like Weatherill et al. [16], it was assumed that modeling results have approached steady state condition if no significant change is observed in concentration isopleths in a $T = 20$ yr period. A perturbation (as is described in [16]) was applied to the central node of the model as well (Fig. 1).

Rayleigh number of IHB problem was changed in the current study by altering the permeability of porous medium and Rayleigh numbers ranging from around Ra_c to 200 were acquired by this method.

Calculations were performed using SUTRA code with non-iterative coupling between flow and solute transport equations and Upstream FEM capability was turned off in the model. Uniform time steps were used in modeling.

Several spatial and temporal discretizations were used in the study to analyze the sensitivity of results to discretizations and perform convergence study as well. Three different meshes were used for spatial discretization, comprising a coarse mesh (200 × 10), a medium mesh (600 × 30) and a fine mesh (1000 × 50).

In order to perform sensitivity analyses for the two criteria proposed by Weatherill et al. [16] (i.e. threshold of instability formation and wavelength of instabilities), different Rayleigh numbers ($Ra = 50$, 100, 150 and 200), temporal discretizations ($\Delta T = 1.0$, 2.0, 5.0, 8.0, 10.0 15.0 and 20.0 days) and spatial discretizations (coarse, medium and fine meshes) were used in the model. Using different spatial (coarse, medium and fine meshes) and temporal ($\Delta T = 1.0$, 2.0, 5.0, 10.0, 20.0 days) discretizations, two convergence studies were also carried out for $Ra = 50$ and 150 to obtain the final solutions for the problem.

4. Modeling results

4.1. Sensitivity analysis for wavelength of instabilities

Sensitivity analyses were carried out for the model to investigate the equality of analytical and numerical wavelengths for different spatial and temporal discretizations. Table 1 shows the number of waves generated in the model domain for different time step lengths using coarse and medium meshes. For example, for $Ra = 100$ and

Table 1
Number of waves generated in the model domain for different time step lengths and different Rayleigh numbers (medium mesh, coarse mesh)

Ra	Time step length used for computations (days)						
	1	2	5	8	10	15	20
50	11, 11	10, 10	10, 10	10, 10	10, 10	10, 10	10, 10
100	14, 12	11, 12	12, 12	12, 12	12, 10	10, 10	10, 10
150	14, 14	12, 12	12, 12	12, 10	10, 10	10, 10	10, 10
200	12, 14	11, 12	11, 12	11, 10	10, 10	10, 10	10, 10

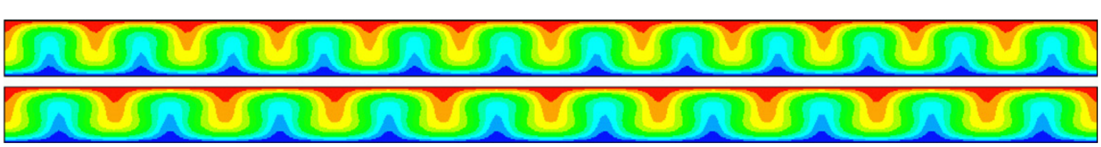

Fig. 2. Selected results for IHB problem, coarse mesh (200 × 10), $Ra = 100$: $\Delta T = 1.0$ day (top), $\Delta T = 20.0$ days (bottom).

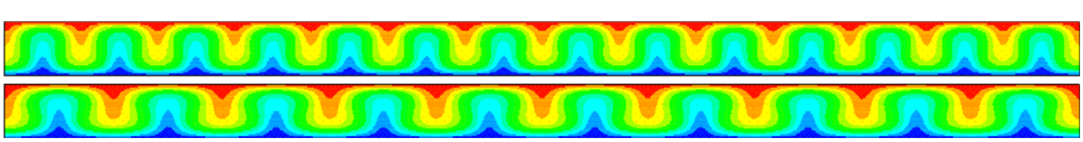

Fig. 3. Selected results for IHB problem, medium mesh (600 × 30), $Ra = 100$: $\Delta T = 1.0$ day (top), $\Delta T = 20.0$ days (bottom).

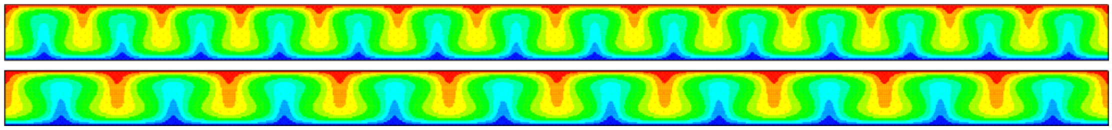

Fig. 4. Selected results for IHB problem, fine mesh (1000×50), $Ra = 150$: $\Delta T = 1.0$ day (top), $\Delta T = 20.0$ days (bottom).

$\Delta T = 1.0$ day, 14 pairs of convective cells are generated in the model with medium mesh after 20 years, while 12 pairs of convective cells are generated in the model with coarse mesh. Graphical representations of selected results are also shown in Figs. 2–4.

Table 1 shows that for long time steps, number of convective cells generated in the model domain is around 10 (similar to analytical results of HRL problem) but as ΔT decreases, more convective cells are being generated in the models, which is in contradiction with analytical results. This discrepancy becomes more evident by increasing Rayleigh number. Table 1 also shows that spatial discretization has affected the modeling results for small time step sizes, which indicates that the results may have not converged.

4.2. Convergence analysis for wavelength of instabilities

Sensitivity analyses showed that the wavelengths resulting from numerical modeling vary with spatial and temporal discretizations. This may indicate that the numerical results have not converged. In order to assure the validity of the numerical results, a convergence analysis must be performed through which the final results of the models can be determined.

Convergence analyses were performed in this study for two specific Rayleigh numbers ($Ra = 50$, 150), five different time step sizes and three different meshes. Tables 2 and 3 show the results of the convergence analysis. The tables show that numbers of convective cells generated in the model domain have converged to 11 and 14 for Rayleigh numbers 50 and 150, respectively.

Considering the results of convergence analyses, one can see that the number of convective cells generated in the model domain is not only dependent on spatial and temporal discretizations, but also dependent on Rayleigh number of the problem. While the dependency of numerical results upon spatial and temporal discretizations can be addressed to numerical errors, dependency of converged results upon Rayleigh number directly contradicts the analytical results for HRL problem.

4.3. Sensitivity analysis for threshold of instability formation

Another criterion used by Weatherill et al. [16] for benchmarking purpose was critical Rayleigh number for instability formation in the model domain. Fine and coarse meshes were used in simulations with time step sizes varying from 20.0 days to 1.0 day.

The criterion used for determining occurrence of instability in the model domain was similar to 0.5PD (maximum depth that the 50% concentration isopleth penetrates in the model) which was defined in [16] except that we used the largest concentration that occurred in the middle layer of the model as the indicator for instability formation. Fig. 5 shows that the numerically derived Ra_c is very close to the analytical Ra_c. Similar results were obtained by Weatherill et al. [16].

Sensitivity analysis for threshold of instability formation in the problem showed that this criterion is acceptably

Table 2
Convergence analysis results for wavelength of instabilities generated in the model domain for $Ra = 50$, numbers in the table are number of convective cells generated in the model domain

	$\Delta T = 1.0$ (day)	$\Delta T = 2.0$ (days)	$\Delta T = 5.0$ (days)	$\Delta T = 10$ (days)	$\Delta T = 20$ (days)
Coarse mesh (200×10)	11	10	10	10	10
Medium mesh (600×30)	11	10	10	10	10
Fine mesh (1000×50)	11	11	11	10	10

Table 3
Convergence analysis results for wavelength of instabilities generated in the model domain for $Ra = 150$, numbers in the table are number of convective cells generated in the model domain

	$\Delta T = 1.0$ (day)	$\Delta T = 2.0$ (days)	$\Delta T = 5.0$ (days)	$\Delta T = 10$ (days)	$\Delta T = 20$ (days)
Coarse mesh (200×10)	14	12	12	10	10
Medium mesh (600×30)	14	12	12	10	10
Fine mesh (1000×50)	14	14	12	12	10

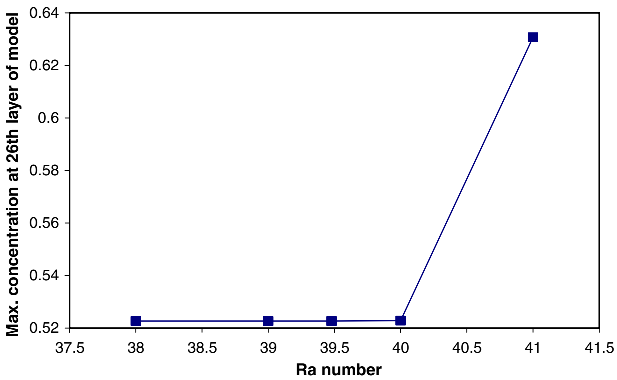

Fig. 5. Threshold of instability formation in IHB problem: fine mesh (1000×50), $\Delta T = 1.0$ day.

independent from spatial and temporal discretizations. Fig. 5 shows the numerical simulation of the criterion using fine mesh and $\Delta T = 1.0$ day. Like similar simulations performed in [16], this figure shows that numerical value of Ra_c agrees well with analytical results.

During sensitivity analysis for threshold of instability formation, it was observed that always 10 pairs of convective cells were generated in the immediate vicinity of Ra_c (i.e. Rayleigh numbers a bit larger from Ra_c). This fact indicates that for Rayleigh numbers in the immediate vicinity of Ra_c, both criteria considered for benchmarking purpose agree well with analytical results.

5. Discussion

Results of sensitivity and convergence analyses performed for wavelength of instabilities show clearly that the wavelength of instabilities in the numerical simulation of the IHB problem is sensitive to spatial and temporal discretizations. Moreover, wavelength of instabilities, predicted by numerical simulation, seems dependent on the Rayleigh number while the theory behind HRL problem predicts 10 waves in the model domain regardless of Rayleigh number.

Considering these facts, one can conclude that the wavelength of instability formation in the model domain is not a good criterion for benchmarking purpose for Rayleigh numbers much larger than Ra_c. However as it is mentioned in Section 4.3, this criterion seems to be met in the immediate vicinity of Ra_c.

Regardless of the discrepancy between analytical and numerical wavelengths of instabilities for IHB problem, it seems that this criterion is not a good benchmark criterion for IHB problem, because complete waves have to occur in the problem domain. So the number of waves (and consequently the wavelength) will be a discrete value and hence, only errors that are large enough to increase or decrease one pair of convective cells will be revealed.

Other criterion (i.e. threshold Rayleigh number for instability formation) seems to be a proper criterion for benchmarking purpose because it is not dependent on spatial or temporal discretizations of the modeling domain. Moreover unlike the former criterion, the threshold of instability formation in the model has a continuous nature which makes it a proper criterion for benchmarking purpose from this viewpoint as well.

It seems that the steady state solution of the IHB problem is very sensitive to numerical errors (including truncation and round off errors). So even when steady state solutions of the IHB problem converge to a specific solution (like the two cases studied here in convergence analyses), still it cannot be assured that this stationary solution is unique. Such a phenomenon is observed in some other numerical problems which were based on formation of convective instabilities in porous media [4].

6. Summary and conclusions

The suitability of infinite horizontal box (IHB) problem that is presented as a benchmark problem for DDFPM numerical models was investigated in the present paper. Two benchmark criteria have been defined by Weatherill et al. [16] for this problem: critical Rayleigh number for instability formation in the problem domain and wavelength for convective patterns created in the problem domain when instability occurs.

Sensitivity and convergence analyses were carried out for IHB problem using different spatial and temporal discretizations for the modeling domain. It was found that wavelength of convective patterns is highly dependent on Rayleigh number and discretizations used for simulation, but threshold for instability formation in the model is considerably independent from discretization of the model domain and hence, can be a good criterion for benchmarking purpose.

References

[1] Bakker M, Oude Essink GHP, Langevin CD. The rotating movement of three immiscible fluids – a benchmark problem. J Hydrol 2004;287:270–8.
[2] Diersch H-JG, Kolditz O. Variable-density flow and transport in porous media: approaches and challenges. Adv Water Resour 2002;25:899–944.
[3] Elder JW. Steady free convection in a porous medium heated from below. J Fluid Mech 1967;27(1):29–48.
[4] Frolkovic P, Schepper HD. Numerical modelling of convection dominated transport coupled with density driven flow in porous media. Adv Water Resour 2001;24:63–72.
[5] Henry HR. Effects of dispersion on salt encroachment in coastal aquifers. USGS Water supply paper 1613-C, Sea Water in Coastal Aquifers; 1964. p. C70–84.
[6] Horton CW, Rogers Jr FT. Convection currents in a porous medium. J Appl Phys 1945;16:367–70.
[7] Johannsen K, Kinzelbach W, Oswald S, Wittum G. The saltpool benchmark problem – numerical simulation of saltwater upconing in a porous medium. Adv Water Resour 2002;25:335–48.
[8] Lapwood ER. Convection of a fluid in a porous medium. Proc Cambridge Philos Soc 1948;44:508–21.
[9] Nield DA, Bejan A. Convection in porous media. 2nd ed. New York: Springer-Verlag; 1999.

[10] Oldenburg CM, Pruess K. Dispersive transport dynamics in a strongly coupled groundwater–brine flow system. Water Resour Res 1995;31(2):289–302.

[11] Oswald SE, Kinzelbach W. Three-dimensional physical benchmark experiments to test variable-density flow models. J Hydrol 2004;290: 22–42.

[12] Rayleigh Lord, Strutt JW. On convection currents in a horizontal layer of fluid when the higher temperature is on the under side. Philos Mag 1916;6(32):529–46.

[13] Simmons CT, Narayan KA, Wooding RA. On a test case for density-dependent groundwater flow and solute transport models: the salt lake problem. Water Resour Res 1999;35(12):3607–20.

[14] Simpson MJ, Clement TP. Theoretical analysis of the worthiness of Henry and Elder problems as benchmarks of density-dependent groundwater flow models. Adv Water Resour 2003;26: 17–31.

[15] Voss CI, Provost AM. SUTRA – A model for saturated–unsaturated variable-density ground-water flow with solute or energy transport. US Geological Survey Water-Resources Investigations Report, 02-4231; 2002, p. 250.

[16] Weatherill D, Simmons CT, Voss CI, Robinson NI. Testing density-dependent groundwater models: two-dimensional steady state unstable convection in infinite, finite and inclined porous layers. Adv Water Resour 2004;27:547–62.