GeoStudio Example File

Verification – Solute convection in a cube

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Introduction

Convection is one of the major means of solute transfer in engineering and earth science problems. It occurs as pore fluid moves within the soil due to external forces (such as pressure) or internal forces (such as gravity). These latter forces act upon fluid density variations brought on by non-uniform temperature fields and/or non-uniform concentration of fluid components. In the case of a non-uniform concentration field, the fluid closest to the solute sink becomes less dense and rises due to a decrease in concentration. This movement alters the flow regime, which affects the fluid density, and thereby creates a coupled system. The manner in which this buoyancy-driven flow occurs depends on the boundary conditions and the geometry (or shape) of the domain.

The objective of this example is to verify the solute transfer formulation against a widely used benchmark for solutal convection in a brine-saturated porous cube. In this problem, a constant concentration differential is applied between the horizontal walls of an otherwise impervious cube. The exercise lends credibility to the use of the software in multi-dimensional problems involving solutal convection.

Numerical Simulation

The purpose of the example is to model solutal convection in a brine-saturated porous cube with impervious vertical walls and impervious and isosolutal horizontal walls. The brine is initially hydrostatic and the initial concentration is representative of a slightly disturbed diffusive state. At some point, a constant concentration differential is applied between the horizontal walls. The brine closest to the lower low-concentration wall rises as its density decreases. This gives rise to convective motion as the top-heavy fluid column becomes unstable. Other than density, fluid properties are assumed to remain constant. The domain is discretized in a structured mesh of 80×80×80 hexahedral elements and an exponential time stepping scheme is used in the transient analyses. The analyses are deemed to have reached steady-state conditions when the differences between the solute fluxes at the upper and lower walls is less than 2%.

The solutal Rayleigh-Darcy dimensionless number characterizes the flow regime within the cubic enclosure:

$$
\begin{aligned}
Ra_{D,C} &\equiv Ra_C Da \frac{D_d}{D_d^{'}} \\
&\equiv Gr_C Sc Da \frac{D_d}{D_d^{'}} \\
&= \frac{g\beta_{c,o_f} H^4 \Delta C / H^{\mu_{f_o}} / \rho_{f_o}}{\left(\mu_{f_o} / \rho_{f_o} \right)^2} \frac{\mu_{f_o}/\rho_{f_o}}{D_d} \frac{k \frac{\mu_{f_o}}{\rho_{f_o} g}}{H^2} \frac{D_d}{D_d^{*} n}
\end{aligned}
\qquad \text{Equation 1}
$$

where Ra_C, Da are the solutal Rayleigh and Darcy dimensionless numbers, respectively; D_d is the molecular diffusion coefficient of the dilute solution (brine); $D_d^{'}$ is the effective diffusion coefficient;

Gr_C is the solutal Grashof dimensionless number; Sc is the Schmidt dimensionless number; g is the gravity constant; $\beta_{c,o_f} = \frac{1}{\rho_{f_o}}(\partial \rho_f / \partial C)_{P,T}$ is the reference volumetric solutal expansion coefficient of the fluid (brine) at constant pressure and temperature; H is the reference dimension, which is taken equal to the height of the cube; ΔC is the concentration differential; μ_{f_o} is the reference dynamic viscosity of the fluid (brine); ρ_{f_o} is the reference density of the fluid (brine); k is the conductivity of the porous media; D_d^* is the bulk diffusion coefficient; n is the porosity. In order to obtain results at various solutal Rayleigh-Darcy numbers, the transient analyses are set up with different values of conductivity and constant diffusive material properties, such that:

$$k = \frac{\left(\mu_{f_o}/\rho_{f_o}\right)^2 \quad D_d \quad H^2 \; D_d^* n}{g\beta_{c,o_f} H^4 \Delta C / H \mu_{f_o}/\rho_{f_o} \frac{\mu_{f_o}}{\rho_{f_o} g} \quad D_d} Ra_{D,C}$$

Equation 2

where μ_{f_o} = 1.028×10^{-3} N s/m^2, ρ_{f_o} = 1008.793 kg/m^3, g = 9.807 m/s^2, β_{c,o_f} = 6.7937×10^{-4} m^3/kg, H = 1 m, ΔC = 1 kg/m^3, D_d = 1.408×10^{-9} m^2/s, D_d^* = 9.920×10^{-10} m^2/s, and n = 0.35. The influence of the flow regime is measured with the mean solutal Nusselt dimensionless number $\bar{N}u_C$, which is defined as the ratio of convective to diffusive mass transfer normal to the upper boundary:

$$\bar{N}u_C = -\frac{\frac{1}{B}\left(\int_{x=0}^{B} \frac{\partial C}{\partial y} dx\right)_{y=H}}{\Delta C/H}$$

Equation 3

where B is the width of the enclosure.

Results and Discussion

Numerical studies have shown that various steady-state convective flow structures (or patterns) can occur in a cubic enclosure. Figure 1 shows the most prevalent structures that occur at low solutal Rayleigh-Darcy numbers. The first of these structures, referred to as S2, consists of a single two-dimensional roll oriented along the *z*-direction. This structure appears as the diffusive state undergoes a bifurcation, or loss of stability, when the solutal Rayleigh-Darcy number reaches $4\pi^2$. At this point, the brine rejects solute to the lower wall and rises as it reaches the vertical wall. It then travels along the upper wall, increases in density, and descends along the other vertical wall. The second structure, referred to as S3, is slightly more complex and unstable at Rayleigh-Darcy numbers smaller than 50 (Sezai, 2005). The brine at the top surface of the cube moves away from the low concentration upwelling plumes and inwards into the high concentration plummeting flow. The low concentration upwelling plumes (and high concentration plummeting flow) are at diagonally opposite corners of the cube. As pointed out by Straus and Shubert (1979), the upwelling plumes are narrow and the plummeting flows cover a broad portion of the cross-sectional area in the lower portions of the cube. The third structure, referred to as S4, consists in two counter-rotating, two-dimensional rolls, oriented along the *z*-direction. As pointed out by Sezai (2005), this structure only prevails at Rayleigh-Darcy numbers larger than 130 and smaller than 290.

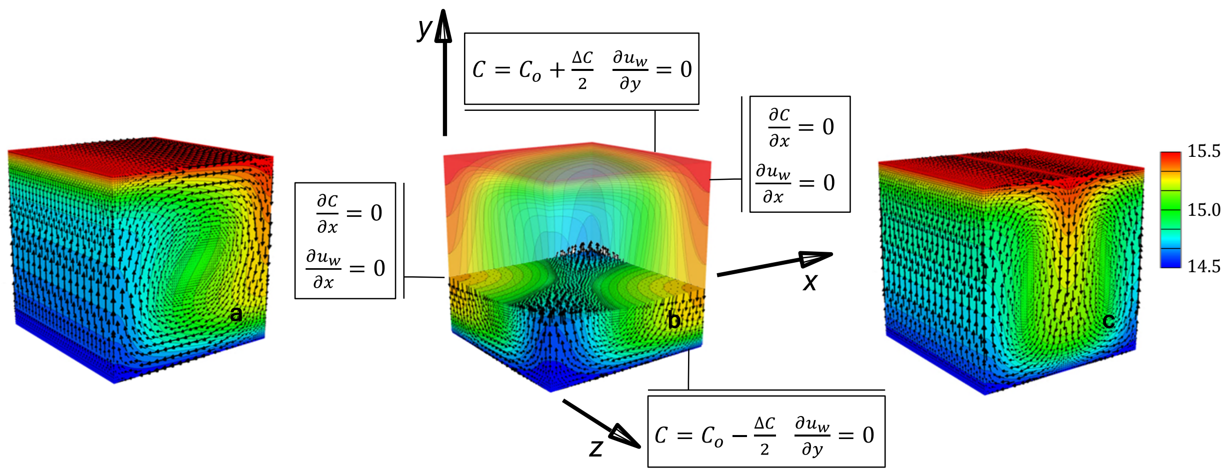

Figure 1. Concentration contour plot, vectors and boundary conditions, $Ra_{D,C}$ = 150. (a) Structure S2, (b) Structure S3, (c) Structure S4.

Figure 2a shows the concentration profile at the center of the cubic enclosure in the presence of an S2 structure at solutal Rayleigh-Darcy numbers of 50, 100, 150, and 180. The concentration profile is close to linear at smaller solutal Rayleigh-Darcy numbers, when diffusion is predominant, and sigmoidal (or S-shaped) at larger solutal Rayleigh-Darcy numbers, when convection prevails. At these larger solutal Rayleigh-Darcy numbers, the interior of the cube approaches isosolutal conditions and the concentration gradients are largest in the boundary layers at the top and bottom of the cube, where sodium chloride is transferred from the porous media to the boundary or vice versa. Figure 2b shows the mean Nusselt number of the steady-state S2 structure at various solutal Rayleigh-Darcy numbers. As expected, the model captures the onset of steady-state convection that occurs as the solutal Rayleigh-Darcy number reaches $4\pi^2$. The numerical results are also shown to be in very close agreement with those obtained by Shubert and Straus (1979). The difference between the two sets of results translates into an average percent difference of approximately 1%. It should be noted that these results are in perfect agreement with those found in a square enclosure in which the vertical walls are impervious and rigid barriers to solute transfer, and thus numerically equivalent to the solutal equivalent of the Horton-Rogers-Lapwood problem.

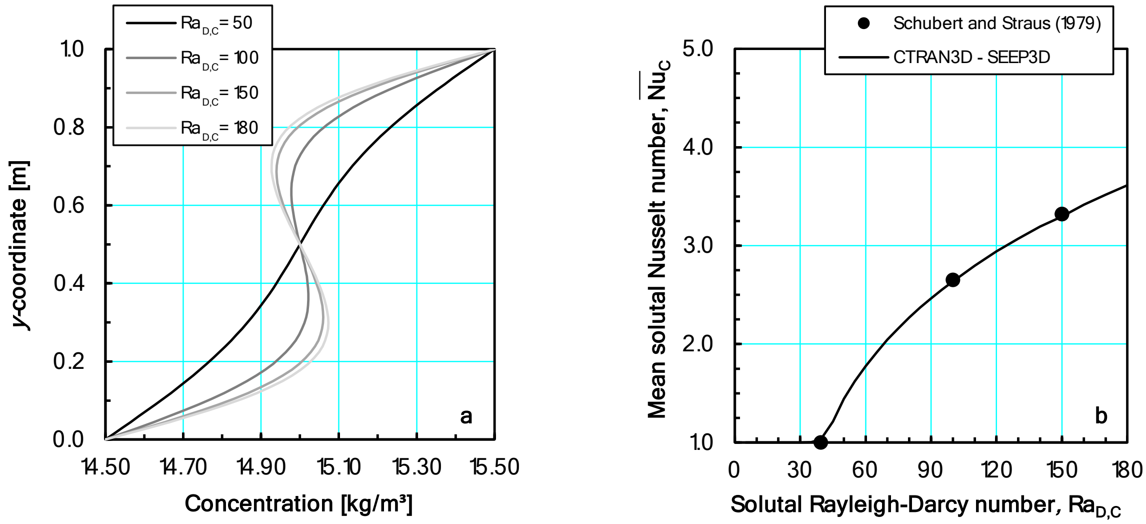

Figure 2. Results of the benchmark problem with an S2 structure. (a) Concentration profile at the center of the cube. (b) Relationship between the mean solutal Nusselt number and the solutal Rayleigh-Darcy number.

Summary and Conclusions

The objective of this example was to demonstrate the ability of coupled CTRAN3D and SEEP3D analyses to solve multi-dimensional problems involving solutal convection. The capabilities of the software were assessed using a widely used benchmark for convection in a cube. The results were shown to capture the onset of steady-state convection that occurs as the solutal Rayleigh-Darcy number reaches $4\pi^2$. The results were also shown to be in very close agreement with those of a reference numerical analysis.

References

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