Upscaling studies of diffusion induced convection in homogeneous and heterogeneous aquifers

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Abstract

The gravitational instability of a diffusive boundary layer in porous media, or diffusion induced convection, has been studied in a number of papers in recent years [1]. This effect is important as it speeds up the dissolution of the CO₂ phase into the aquifer brine by setting up convective mixing. An empirical formula for the dissolution rate per area phase contact is given which can be used for assessing the effect of using large grid blocks in flow simulations. Simulations of diffusion induced convection in barrier type of aquifers are also considered, and it is demonstrated that standard upscaling of vertical permeability can do a fairly good job in representing the model in an anisotropic homogeneous model. For cases with low vertical communication it is seen that convective mixing is more pronounced in the heterogeneous models than in the corresponding anisotropic homogenous models, and the upscaled homogenous model under predict the dissolution rate.

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1. Introduction

Theoretical work and flow simulations of underground CO₂ storage in homogeneous aquifers show that so-called convective mixing of CO₂ in the aquifer brine is initiated after a period where only molecular diffusion is responsible for the dissolution. Such convective mixing speeds up the dissolution of CO₂ significantly, and should be considered important for assessing the long term behavior of the CO₂ in the underground. Here, simple studies of both homogenous and heterogeneous models are presented and discussed. The models considered are 2D, and the models are initialized with a gas cap on top with the aquifer below. Convective mixing results when one introduces a perturbation from the pure diffusion profile which results from CO₂ diffusing into the aquifer below the phase

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contact. The presence of the gravitational instability that triggers convective mixing is due to that aquifer brine with dissolved CO₂ has a larger mass density than brine without dissolved CO₂. Consequently, as CO₂ diffuses into the brine below the contact, a top heavy situation builds up, and eventually becomes unstable.

Figure 1 Cumulative dissolved CO₂ derived from a numerical flow simulation [2]. The dissolution of CO₂ resulting from pure diffusion is (i.e. the basic solution) is significantly less compared to the dissolution resulting from the convective mixing. The given example uses a 10m wide and 8m high aquifer having horizontal permeability of 10 Darcy and a vertical permeability of 5 Darcy. The instability is triggered by numerical round off errors.

Stability studies show that there is a typical length scale involved in the onset of convection which in general is shorter than the length scale of numerical grid blocks used in simulations of real aquifers [1]. Real aquifers are in addition heterogeneous, and to what extent results from (in general anisotropic) homogenous models are representative for much more complicated heterogeneous is still not well understood. The timing of the onset of convective mixing is independent of whether one considers the problem in 2D or 3D [1]. In general one expects convective mixing to be marginally more effective in 3D, as there is more space for convective currents in 3D models. However, fine scale 3D models require a high number of numerical grid blocks, and are not considered here. The results given in this paper are based on perturbation introduced by numerical round off errors in the finite difference flow simulations. This “weak” perturbation is sufficient to give rise to instability. However, the onset times found in the flow simulations are significantly later than predicted by stability analysis [1]. The reason for this discrepancy is at least two-fold. On one hand, stability analysis shows that even though the theoretical possibility for onset is present, the instability is weak and grows slowly in strength. In addition, the instability introduced in the given flow simulations is very weak (numerical noise), and therefore its presence is not noticed before well after the theoretical onset of instability.

It is not attempted here to give a quantitative guideline to scale change procedures for simulation of dissolution of CO₂ in aquifer brine. Plots are given to indicate the impact of changing the grid, and indicating qualitative effects of changing simulation scale. However, an empirical formula has been derived giving the dissolution rate per area phase contact after the onset of convection. Such a formula is convenient for assessing predictions of dissolution rate
in coarse scale field models. As seen below, coarse grid blocks impede the instability mechanism, making the simulation underestimate the amount of CO2 dissolving in the aquifer brine.

Also some studies of convective mixing in barrier types of aquifers are given. The simulations in heterogeneous models are compared to simulations in anisotropic homogeneous aquifers, where the vertical permeability has been averaged using the standard pressure solver. It is seen that the viscous based effective vertical permeability does a fairly good job also for the simulation of convective mixing as long as vertical communication is fairly good.

2. Homogeneous models

As discussed, the onset time for convective mixing is significantly later in numerical simulations than predicted by stability theory. In a real underground storage project one has perturbations stemming from e.g. unsymmetrical plume development, and also the presence of heterogeneities will contribute to produce perturbations away from a pure diffusion profile. The theoretical onset time should be viewed as a lower bound for this onset time, and also yet unpublished stability analysis indicate that the system goes through a relatively long period of transition from neutral stability to strong instability. The onset times given in Figure 2 predicted by the flow simulations are orders of magnitude larger than the ones predicted by stability theory. The so-called critical time giving the theoretical earliest onset of convective mixing is

\[ t_{\text{crit}} = 48.7 D \left( \frac{\phi \mu}{k \Delta \rho g} \right)^2, \]  

where \( D, \phi, \mu, \Delta \rho, g, \) and \( k \) are bulk diffusivity, porosity, brine viscosity, maximal mass density increase for fully CO2 saturated brine, acceleration of gravity, and absolute permeability respectively. One observes that the time for instability is inversely proportional with permeability. As permeability varies strongly from aquifer to aquifer (and within a given aquifer), the onset time for convective mixing will vary significantly from storage site to storage site. The factor 48.7 varies somewhat according to which method is used in the stability analysis [1]. The horizontal wave length of a perturbation which most easily gives rise to instability is given by

\[ \lambda_{\text{crit}} = \frac{2 \pi D \phi \mu}{0.057 \Delta \rho g k}. \]  

Again the numerical factor may vary somewhat. From fine scale simulations one finds that this wave length agrees well with the width of the instable fingers when convective mixing is initiated. In Figure 4 the predicted wave length is one tenth of the model width. This number agrees very well with the number of fingers appearing in this example. The finest scale simulation has 100 by 100 grid blocks, meaning that each finger is resolved with approximately 10 grid blocks, which then clearly is sufficient. The case in the next plot in Figure 4 has 50 by 50 grid blocks, and one sees that one starts loosing fingers, even though the critical wave length is resolved with approximately 5 grid blocks. The last two plots in Figure 4 show the cases 25 by 50 grid blocks (horizontal by vertical) and 25 by 25 grid blocks. This resolution is clearly too coarse for accurate simulations of onset of convective mixing. Figure 3 shows cumulative dissolution of CO2 per area phase contact for a case which is 1280m wide. One observes that the simulation with grid blocks 80m wide, which can be typical for field scale simulations, predicts much lower dissolution of CO2 than predicted using significantly smaller grid blocks. This effect is manifest in both the dissolution rate and in the time for onset of convective mixing.

After onset of convection, the physics of the problem is nonlinear, and an explicit expression for dissolution rate is probably very difficult to obtain. However, one observes that the simulations predict more or less a constant dissolution rate in the period after convective mixing is initiated. Later, when the effect of a limited aquifer is felt, the dissolution rate will of course decrease again. For the constant rate period the following formula for the flux of CO2 is suggested from numerical simulations

\[ J = KD \left( \Delta c_f \phi \right)^2 \frac{\Delta \rho g k}{\mu}, \]  

where \( c_f \) is the fraction of injected CO2.
where $\Delta \rho$ is the mass density difference corresponding to the concentration difference $\Delta c_0$. The constant $K$ has been estimated to $1.5 \cdot 10^6$ ms/kg. Formula (3) then gives the rate of dissolution per area phase contact, and can be used to assess predictions of the dissolution in simulations with large grid blocks. The issue of artificially increasing the dissolution rate in coarse scale simulations, and obtaining a reasonable onset time for convective mixing is challenging. Increasing $\Delta \rho$ will give earlier onset time and stronger instability, and might be appropriate. However, such requires a separate study and is not considered here.

Figure 2 Example of times for instability predicted by stability analysis compared to numerical flow simulations. The high values for permeability are for practical simulation purposes (early onset of instability).

Figure 3 Dissolution of CO$_2$ per area phase contact for different grid block sizes. The examples are of a 1280m wide and 100m deep aquifer. For very large grid blocks the dissolution rate is comparable to pure diffusion.
3. Heterogeneous models

A series of simulations of convective mixing in heterogeneous aquifers has been performed. A barrier type of geometry is considered as illustrated in Figure 5. The models are 10m wide and 8m deep, and have an isotropic background permeability of 1800mD. The critical wave length (see formula (2)), or the characteristic width for the fingers are in the order of a meter. The models use 200 by 200 grid blocks, i.e. the fingers are well resolved by the numerical grid. The effective vertical permeability of the model has also been estimated by simulating single phase flow in the vertical direction. When the effective vertical permeability is larger than one fifth of the background permeability, the corresponding homogeneous anisotropic model seems to predict more or less the dissolution rate as the heterogeneous model. Therefore it seems that the viscous based upscaling of permeability seems sufficient for representing the physics for modest values of the horizontal to vertical permeability ratio. However, when effective vertical permeability is significantly smaller than the background permeability, the corresponding homogeneous simulations predict less dissolution than the heterogeneous. The reason for this discrepancy is that in the heterogeneous models the unstable fingers develop in the homogeneous background permeability, even though the characteristic width of the fingers can less than the typical distance between the impermeable layers. In the very anisotropic homogeneous models the onset of convective mixing is impeded by the low vertical permeability, and any onset of convection will be much later than in the corresponding heterogeneous model.
The diffusivity in the barriers in Figure 5 have been set to 0.1 of the diffusivity in the high permeable background. Estimated effective vertical permeability is 365mD for the regular barrier geometry, and 100mD for the irregular geometry on the right.

One observes from Figure 7 that the upscaled homogenous model predicts fairly well the dissolution rate for the regular barrier geometry. For this case the permeability ratio is approximately 5, and convective mixing is initiated more or less simultaneous for the heterogeneous and homogenous cases. Also the effect of varying shale diffusivity is measurable. For both cases one observes that no diffusivity in the shale lead to less dissolution. For the regular geometry one has maximal dissolution when the shale diffusivity is set to 70% of the background (sand) diffusivity. This effect is not seen in Figure 8 where maximal shale diffusivity gives maximal dissolution.
Figure 7 Dissolution of CO$_2$ per area for the regular barrier geometry for varying shale diffusivities. The dissolution of the homogenous case is also shown. The upscaled homogenous model predicts fairly well.

One observes for the irregular geometry in Figure 8 with a permeability ratio of 18 that no convective mixing starts for the upscaled homogeneous case, since the dissolution curve follows the same curve as for a pure diffusion process. Thus, viscous based upscaling of vertical permeability is not representative for the physics of diffusion-convection at high permeability ratios.

Figure 8 Dissolution of CO$_2$ per area for the irregular barrier geometry for varying shale diffusivities. The dissolution of the homogenous case is also shown. Now the permeability ratio for the homogenous model is 18, and no onset of convection is observed for the homogenous model. Its dissolution rate is the same as for pure diffusion.
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