Effect of strong heterogeneity on the onset of convection in a porous medium: Importance of spatial dimensionality and geologic controls

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[1] The effect of strong heterogeneity on the onset of convection induced by a vertical density gradient in a saturated heterogeneous porous medium governed by Darcy's law is investigated. A computer package has been developed to study the applicability of an average Rayleigh number as a criterion for the onset of convection in strongly heterogeneous geologic media. The heterogeneous geologic media have been described using random spatial functions for the permeability field which are lognormally distributed and spatially correlated. Both isotropic and anisotropic correlation lengths within the geologic structure are considered. This paper presents the first 3D theoretical treatment of the conditions for the onset of convection (Rayleigh stability criteria) in strongly heterogeneous porous media. We elucidate the critical role that spatial dimensionality (2D versus 3D flow) plays in controlling convection processes and stability criteria. Our results quantitatively demonstrate for the first time that spatial dimensionality is a dominant control on the onset of convection in a strongly heterogeneous geologic medium. Unbounded Rayleigh number behavior is observed in 3D. This leads to the important new conclusion that a Rayleigh number (based on mean quantities) is unlikely to be a valid predictor for the onset of convection in 3D strongly heterogeneous porous media. Furthermore, we systematically and quantitatively demonstrate that the onset of convection in a heterogeneous geologic medium is highly sensitive to changes in the standard deviation of the lognormal permeability field, moderately sensitive to changes in the level of correlation length, and relatively insensitive to the anisotropy of correlation length.

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1. Introduction

[2] Over the last decade or two, there has been an explosion in the field of variable density flow because of worldwide concern about the future of energy and water resources and environmental pollution [*Simmons*, 2005]. Recent review articles on this topic by *Diersch and Kolditz* [2002], *Simmons et al.* [2001] and *Simmons* [2005] clearly illustrate the widespread importance, diversity and interest in applications of variable density (free convection) flow phenomena in groundwater hydrology. These include seawater intrusion, fresh-saline water interfaces and saltwater upconing in coastal aquifers, subterranean groundwater discharge, dense contaminant plume migration, DNAPL studies, density driven transport in the vadose zone, flow through salt formations in high level radioactive waste disposal sites, heat and fluid flow in geothermal systems, palaeohydrogeology of sedimentary basins, sedimentary basin mass and heat transport and diagenesis, processes beneath sabkhas and salt lakes and buoyant plume effects in applied tracer tests [*Simmons*, 2005]. Free convection has been studied for over a century but largely in theoretical and laboratory settings. The limited number of field based studies have inferred the existence of free convection and only very recently has primary evidence of free convection in a natural field setting been reported in the literature [*Van Dam et al.*, 2009]. These authors presented electrical resistivity measurements from a sabkha aquifer near Abu Dhabi, United Arab Emirates, where large density inversions exist. The geophysical images from this site provided, for the first time, compelling field evidence of fingering associated with natural free convection in groundwater.

[3] One of the most important challenges in this field of research is understanding the role that heterogeneity in geologic media plays in the onset, growth and decay of instabilities associated with free convection phenomena - flow driven by fluid density variations which occur because of changes in the solute or colloidal concentration, temperature, and pressure of the groundwater. Rayleigh numbers of the form given in (1) below have been used for nearly a

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century to predict the onset of free (natural) convection in porous media. Thermal and solute Rayleigh numbers (Ra_T and Ra_S respectively) can be defined [see, e.g., *Simmons et al.*, 2001; *Nield and Bejan*, 2006] as

$$\mathrm{Ra}_T = \frac{\alpha_T \rho_o g K \Delta T H}{\mu \kappa} \qquad \mathrm{Ra}_S = \frac{\alpha_S \rho_o g K \Delta S H}{\mu D} \tag{1}$$

When the thermal Rayleigh number is below some critical value for a thermal system and a classic 'static' system is considered, heat transfer is primarily in the form of conduction and when it exceeds the critical value, heat transfer is primarily in the form of convection. In the case of solute transport, when the Rayleigh number is below the critical value for that system in the classic static system, solute transport is primarily in the form of diffusion. In both cases, mechanical dispersion will likely be a significant contributor once fluids are in motion (but prior to instability). The validity and appropriate use of classical Rayleigh numbers for determining the stability of a variable density flow system in realistic heterogeneous geologic systems remains an extremely important and unresolved challenge [*Simmons*, 2005; *Diersch and Kolditz*, 2002; *Nield and Simmons*, 2007]. In particular, earlier studies on the stability of variable density flows in heterogeneous geologic media by *Simmons et al.* [2001], *Prasad and Simmons* [2003] and *Schincariol et al.* [1997] have concluded that (1) an increase in the standard deviation of the lognormal permeability field results in a greater degree of instability at earlier times but promotes stability at later times, (2) an increase in the horizontal correlation length of the lognormal permeability field creates laterally extensive low permeability zones that dissipate upward and downward motion needed to maintain convection and therefore causes a reduction in the degree of instability, (3) a greater degree of heterogeneity causes greater uncertainty in predictions, and (4) traditional predictive methods such as the Rayleigh number based upon an average permeability do not generally work in their application to strongly heterogeneous geologic systems.

[4] There is an urgent need to more rigorously quantify the extent to which the classical analysis based on the concept of a Rayleigh number is valid in a heterogeneous geologic system. In particular, understanding how the validity of the Rayleigh number based on mean quantities is affected by spatial dimensionality remains an important and unresolved question in the field of free convection in porous media. Critically, all relevant previous studies have been exclusively conducted in 2D flow fields. The importance of spatial dimensionality of the flow field on the onset conditions for free convection and applicability of Rayleigh number stability criteria in 3D strongly heterogeneous geologic media has not yet been elucidated. This is clearly an extremely important matter to consider since all realistic geologic field settings are 3D in nature. In an analysis of the effect of correlation length scales, *Simmons et al.* [2001] varied both the horizontal and vertical correlation length scales but *Prasad and Simmons* [2003] and *Schincariol et al.* [1997] only varied the horizontal correlation length scale, while keeping the vertical correlation length scale fixed. A systematic analysis of the effect of correlation length anisotropy has not been conducted to date. Furthermore, these transient studies have explored both the onset as well as growth/decay of instabilities in heterogeneous geologic media. However, they have not adequately quantified the relative sensitivity to and importance of the amplitude (standard deviation of the lognormal permeability field) and structure (correlation length, anisotropy of correlation lengths) of geologic heterogeneity on the *onset conditions* for free convection in heterogeneous geologic media.

[5] Earlier work in a series of papers by *Nield and Kuznetsov* [2007a, 2007b, 2007c, 2007d, 2007e, 2008a, 2008b] and *Kuznetsov and Nield* [2008] has treated the case of weak heterogeneity and its role in the onset of convection in heterogeneous porous media. These papers assessed the applicability of an average Rayleigh number as a criterion for the onset of convection in the case where the heterogeneity is weak. By weak heterogeneity, we mean that the amount of variation of a quantity like the permeability is small in comparison with its mean value (i.e., the fractional change is of order ε where $\varepsilon \ll 1$). These authors studied the combined effects of vertical heterogeneity and horizontal heterogeneity, for a two-dimensional situation. The term *vertical heterogeneity* is used to refer to *variation in the vertical direction*. An extreme example is when one has a series of horizontal layers in which the permeability of each layer is uniform.

[6] *Nield and Simmons* [2007] proposed a rough and ready criterion for the onset of convection in a strongly heterogeneous porous medium. It is based on the classical results of *Beck* [1972]. Importantly, this criterion is not restricted to the two-dimensional situation. These results form the basis of a new computer package called the Stability Exploration Package for Strong Heterogeneity (SEPSH). This package has now successfully been applied in a sequence of papers by the authors on the onset of convection in a strongly heterogeneous porous medium [*Nield et al.*, 2009; *Kuznetsov et al.*, 2010; *Nield et al.*, 2010]. *Nield et al.* [2009] employed the SEPSH package to the various special cases of piecewise-constant, linear and quadratic variation where the variation was non-periodic and extended over the whole of the cube. *Kuznetsov et al.* [2010] applied the package to further special cases where the variation was either periodic across the cube or where the departure from mean values was confined to localized portions of the cube, with the localization being in just one dimension. At the same time the SEPSH code was extended to a stretched numerical grid system so that the resolution in one or two directions can be increased at the expense of reduced resolution in the remaining directions. *Nield et al.* [2010] considered the case in which the variation was localized in both horizontal directions and an important comment was made about the case of 3D localization leading to unbounded results for the normalized Rayleigh number. *Nield et al.* [2010] also considered a geostatistical case, modeling a much more realistic hydrogeologic situation involving a spatially correlated lognormally distributed permeability field of the type commonly used in groundwater analyses that consider geologic heterogeneity.

[7] The objective of this current paper is to use the Stability Exploration Package for Strong Heterogeneity (SEPSH) to study the applicability of an average Rayleigh number as a criterion for the onset of convection in realistic and strongly heterogeneous geologic porous media. The earlier SEPSH studies were largely limited to highly mathematized treatments of the heterogeneity field. Here, we continue to work with more realistic random spatial functions for

the permeability field which are lognormally distributed and spatially correlated. Both isotropic and anisotropic correlation lengths within the geologic structure are considered. A key objective of this study is to present the first 3D theoretical treatment of the Rayleigh stability criteria for the onset of convection in realistic, strongly heterogeneous porous media. This allows us to elucidate the critical role that spatial dimensionality (i.e., 2D versus 3D flow) plays in controlling convection processes and stability criteria. We also quantify the relative sensitivity to and importance of the amplitude (standard deviation of the lognormal permeability field) and structure (correlation length, anisotropy of correlation lengths) of geologic heterogeneity on the onset conditions for convection in heterogeneous geologic media.

2. Stability Exploration Package for Strong Heterogeneity (SEPSH)

2.1. Theory

[8] For the case of strong heterogeneity, *Nield and Simmons* [2007] proposed a rough and ready criterion for the onset of convection in that situation. This criterion is not restricted to the two-dimensional situation. It is based on the classical results of *Beck* [1972]. These show the variation of the critical Rayleigh number, and the preferred cellular mode, as functions of the aspect ratios $A_x = H/L_x$ and $A_y = H/L_y$ for a three-dimensional box with height H and horizontal dimensions L_x and L_y. The figures apply to a box with impermeable conducting top and bottom boundaries and impermeable insulating sidewalls, and occupied by a porous medium for which the Darcy model is applicable. Beck showed that the critical Rayleigh number for a homogeneous medium is given by

$$\mathrm{Ra} = \pi^2 \min\left(b + \frac{1}{b}\right)^2, \tag{2}$$

where

$$b = \left[(pA_x)^2 + (qA_y)^2\right]^{1/2} \tag{3}$$

and the minimum is taken over the set of nonnegative integers p and q. Beck's figures show that in the region $A_x < 1$, $A_y < 1$, the value of Ra does not exceed 40.7. Also, in the region $A_x > A_y > 1$, the critical mode is $p = 1$, $q = 0$, so that

$$\mathrm{Ra} = \pi^2\left(A_x + A_x^{-1}\right)^2. \tag{4}$$

Furthermore, when $A_x > 1$ and $A_y < 1$ the value of Ra does not exceed the value given by the expression in equation (4).

[9] Similarly, in the region $A_y > A_x > 1$, the critical mode is $p = 0$, $q = 1$, so that

$$\mathrm{Ra} = \pi^2\left(A_y + A_y^{-1}\right)^2, \tag{5}$$

and when $A_y > 1$ and $A_x < 1$ the value of Ra does not exceed the value given by the expression in equation (5).

[10] *Nield and Simmons* [2007] constructed a generalized Rayleigh number for a heterogeneous box in the following way. Their basic idea is that if at any stage one finds instability in any part of the enclosure at any time, then the whole system can be considered to be unstable. They started with a domain consisting of a box and considered subdomains. Each subdomain is taken to be a rectangular box, of arbitrary size and with arbitrary aspect ratios, bounded by planes $x = x_1$, $x = x_2$, $y = y_1$, $y = y_2$, $z = z_1$, $z = z_2$. They called these special rectangular subdomains "sub-boxes." We hope that the term "sub-box" is self descriptive. We note that a subset of a set is defined by mathematicians so that the whole set is one of the subsets of the whole set. For each sub-box they calculated the aspect ratios and a local Rayleigh number Ra_l based on the height of the sub-box and with other properties given by the mean value over the sub-box. In particular, the sub-box mean of the basic temperature gradient at a particular time is employed here. They then defined a geometrically adjusted Rayleigh number Ra_g defined by

$$\mathrm{Ra}_g = \begin{cases} \mathrm{Ra}_l & \text{if } A_x \le 1 \text{ and } A_y \le 1, \\ \dfrac{4\mathrm{Ra}_l}{\left(A_x + A_x^{-1}\right)^2} & \text{if } A_x > 1 \text{ and } A_x \ge A_y, \\ \dfrac{4\mathrm{Ra}_l}{\left(A_y + A_y^{-1}\right)^2} & \text{if } A_y > 1 \text{ and } A_y \ge A_x. \end{cases} \tag{6}$$

[11] Finally, they defined an overall Rayleigh number Ra_O by

$$\mathrm{Ra}_O = \max \mathrm{Ra}_g, \tag{7}$$

where the maximum is taken over all the sub-boxes and all times. They argued that one would expect that if $\mathrm{Ra}_O > 41$ (taken as a round number) then instability will occur. The criterion for instability will be met in at least one sub-box, and hence the whole system will be unstable. If $\mathrm{Ra}_O \ll 41$ then it is unlikely that instability will occur. If Ra_O is only slightly less than 41 then a closer examination of the particular situation is needed to determine whether or not instability will occur. The number 41 is obviously somewhat arbitrary. Our expectation that $\mathrm{Ra}_O > 41$ is a sufficient condition for instability is based on the fact that the impermeable conducting boundaries are the most restrictive boundaries pertaining to the Darcy model. The boundary conditions on the top and bottom of the sub-boxes are undetermined, but we can be sure our criterion is conservative. It is useful to note that specifying the value of a variable on the boundary is more restrictive than, for example, specifying the value of the derivative of that variable. In an eigenvalue problem with a given differential equation, the more restrictive the boundary conditions then the greater the eigenvalue. In Table 6.1 of *Nield and Bejan* [2006], which gives the values of the critical Rayleigh number for various boundary conditions, the largest entry for the critical Rayleigh number corresponds to the impermeable conducting boundaries.

2.2. SEPSH Package

[12] *Nield et al.* [2009] described a computer package written in FORTRAN code which they called the Stability Exploration Package for Strong Heterogeneity (SEPSH). The main program of SEPSH is designed to produce a *Rayleigh number multiplication factor* which gives the value of an effective overall Rayleigh number in terms of the

Rayleigh number based on a homogeneous domain. The reader is referred to *Nield et al.* [2009] for more details of the program. Following the approach first outlined by *Nield and Simmons* [2007] and briefly recounted in Section 2.1, SEPSH considers a big box with impermeable conducting top and bottom boundaries and insulating sidewalls which is divided into small boxes by horizontal and vertical planes. It also utilizes the subdomain approach described in Section 2.1. The input into the main program consists of a parameter defined in terms of three factors that are allowed to vary as a result of the heterogeneity (permeability K, thermal conductivity k, and applied vertical temperature gradient β) and which are then normalized in terms of their mean values. Spatial coordinates are taken relative to the height of the original box, and the subscript s refers to a sub-box. Its height is $z_B - z_A$ and its aspect ratios (height to horizontal dimension) are

$$A_{sx} = (z_B - z_A)/(x_B - x_A) \text{ and } A_{sy} = (z_B - z_A)/(y_B - y_A). \quad (8)$$

[13] The normalized Rayleigh number relative to the Rayleigh number based on mean quantities with the mean taken over the whole box, for a sub-box, based on the height of the sub-box and with other properties given their mean values over the sub-box, is given by

$$\mathrm{Ra}_{Ns} = \frac{\beta_s K_s (z_B - z_A)}{k_s}, \quad (9)$$

where K_s, k_s, and β_s are the means of K_r, k_r, and β_r taken over the sub-box.

[14] A geometrically adjusted Rayleigh number Ra_{Nsg} is defined by

$$\mathrm{Ra}_{Nsg} = \begin{cases} \mathrm{Ra}_{Ns} & \text{if } A_{sx} \le 1 \text{ and } A_{sy} \le 1, \\ \dfrac{4\mathrm{Ra}_{Ns}}{\left(A_{sx} + A_{sx}^{-1}\right)^2} & \text{if } A_{sx} > 1 \text{ and } A_{sx} \ge A_{sy}, \\ \dfrac{4\mathrm{Ra}_{Ns}}{\left(A_{sy} + A_{sy}^{-1}\right)^2} & \text{if } A_{sy} > 1 \text{ and } A_{sy} \ge A_{sx}. \end{cases} \quad (10)$$

An overall normalized Rayleigh number Ra_{NO} is then defined by

$$\mathrm{Ra}_{NO} = \max \mathrm{Ra}_{Nsg}, \quad (11)$$

where the maximum is taken over all the sub-boxes, including that sub-box which is identical with the whole of the original box. Then Ra_{NO} is the required Rayleigh number multiplication factor. Note is taken of which sub-box (or sub-boxes) gives the maximum. This gives an indication of the favored mode of instability i.e., the one that is most unstable and hence is likely to be observed in practice. In our first paper [*Nield et al.*, 2009] we presented results in terms of variation of the permeability K and variation of the thermal conductivity k treated as separate quantities, with the assumption that the applied temperature gradient β was homogeneous. In our later papers we compressed the computations by working in terms of what we called the *potential convectivity* defined as

$$\widetilde{K} = K\beta/k. \quad (12)$$

For practical purposes, variation of $\widetilde{K}$ can be considered as variation of K with no variation of either k or β. In the present paper we continue to work in terms of $\widetilde{K}$.

2.3. Geostatistical Application of SEPSH

[15] The approach used here builds upon that used previously by *Nield et al.* [2010] who considered a geostatistical application of SEPSH involving a spatially correlated lognormally distributed permeability field. In this stochastic approach, a statistical model was adopted whereby input parameters such as hydraulic conductivity are considered to be random spatial functions with an associated probability density function for the entire flow domain. Numerous studies have used this approach in groundwater flow and solute transport modeling and they are now commonplace in groundwater hydrology [e.g., *Dagan*, 1994, 1990, 1989; *Freeze*, 1975; *Gelhar*, 1993, 1986; *Gelhar and Axness*, 1983; *Smith and Freeze*, 1979; *Smith and Schwartz*, 1981, 1980]. Accordingly, we consider a stochastic case, modeling a fairly realistic hydrologic situation involving a correlated lognormal field. We use the Sequential Gaussian Simulation (SGSIM) package that is part of the GSLIB library [*Deutsch and Journel*, 1992] to generate spatially correlated random permeability (or potential convectivity) fields that can then, after an appropriate transformation, be used as input to SEPSH. In the previous and current paper, thirty Monte Carlo simulations were run for each set of input variables giving a confidence interval of $\pm 0.36\sigma$ at a confidence level of 95%, where σ is the appropriate standard deviation [*Kreyszig*, 1988]. Since SGSIM works in terms of standard normal distributions with mean of zero and standard deviation of unity, the lognormal permeability field used as input to SEPSH is determined using the transformation

$$\tilde{K}_{SEPSH} = \exp\left(\sigma \tilde{K}_{SGSIM}\right). \quad (13)$$

where σ is the standard deviation of the new normal distribution that is used to generate the lognormal permeability field. The standard deviation σ is modified as a key input in SEPSH. To represent increasing levels of heterogeneity that mirror the behavior of natural geologic media, permeability fields with standard deviation of the lognormal permeability field with values 0.1, 0.3, 1 and 3 were used. Previous studies have reported on the range of permeability variance encountered in field-scale geologic media. For example, a variance value of $\sigma^2 = 0.26$ was reported for the Cape Cod site [*LeBlanc et al.*, 1991] and a variance value of $\sigma^2 = 4.5$ was reported for the significantly more heterogeneous aquifer at the MADE site [*Barlebo et al.*, 2004].

[16] SGSIM uses a spherical variogram to generate correlated random spatial fields. Besides σ, the key input variables are τ_x and τ_y, the relative correlation lengths in the x, y directions, and we express these as fractions of the corresponding domain lengths. In our previous paper [*Nield et al.*, 2010], with one exception, we considered just the case where the domain lengths in the x- and y- directions were equal, and considered the case of isotropic correlation lengths (where $\tau_x = \tau_y = \tau$) only. Relative correlation length values were set to values of $\tau = 0.05$, 0.2, 0.3 and 0.5. This ensured that an appropriate number of correlation lengths fitted within the SEPSH domain and that the correlation

Table 1. Values of the Mean of Ra_{NO} for Various SGSIM Input Values of σ, for $\tau = 0.30$, for Various Sample Sizes N_s With the Monte Carlo Procedure, and With Grid Number $N = 49$, for the 3D Case[a]

	2D Exact	$N_s = 10^5$	$N_s = 10^6$	$N_s = 10^7$
$\sigma = 0.1$	1.000 (0.001)	0.927 (0.021)	0.963 (0.011)	0.981 (0.008)
$\sigma = 0.3$	1.003 (0.005)	0.932 (0.021)	0.960 (0.014)	0.979 (0.007)
$\sigma = 1.0$	1.066 (0.099)	0.939 (0.031)	0.972 (0.018)	0.989 (0.159)
$\sigma = 1.5$	1.436 (0.436)	1.132 (0.532)	1.394 (0.619)	1.597 (0.711)
$\sigma = 2.0$	2.169 (0.934)	2.568 (1.66)	3.406 (2.54)	4.098 (2.46)
$\sigma = 2.5$	3.181 (1.500)	5.001 (3.42)	7.245 (6.24)	8.827 (5.07)
$\sigma = 3.0$	4.402 (2.104)	9.510 (7.43)	11.64 (7.98)	16.20 (11.56)

[a]A comparison with the 2D exact case obtained with a grid number N = 101 is made. Standard deviation is given in parentheses.

length itself was sufficiently discretized to resolve it (we employed N = 101 i.e., 101 × 101 SEPSH data points).

2.4. Monte Carlo Extension to SEPSH

[17] The basic SEPSH code and approach described in Section 2.3 forms the basis for the work conducted in the present study. In the present paper we extend the investigation to the case of correlation length anisotropy, and to the case where the aspect ratio A, defined as the ratio of the domain length in the x-direction to that in the y-direction (in the 2D case the domain length in the y-direction is the height of the box or layer), has values other than unity. In an investigation of the present type one obviously needs good spatial resolution but is severely restricted by feasible computer time. Computations were performed on the North Carolina State University IBM Blade Center computer facility that had 866 3.0 GHz dual-core Xeon processors; each processor had 2GB memory per core. One job ran on a single Xeon node of an IBM Center Linux Cluster. Although we could access more memory, we did not need it. The challenge in the current work was the large number of operations associated with the SEPSH code scanning through a very large number of sub-boxes. Memory was far less of an issue. It is important to note that once SEPSH was done performing a calculation with a sub-box, it did not need to keep any information about this sub-box except to compare Ra for this sub-box with the Ra that was accumulated to this point associated the most unstable configuration. Therefore the memory requirements were not that great and we were more restricted by the run times for our simulations than we were by memory. It is interesting to note that the run times are therefore largely controlled by the number of sub-boxes employed by the SEPSH routine. For both the 2D and 3D meshes (101 × 101 and 21 × 21 × 21 for the exact cases, respectively), it can be shown that the number of sub-boxes are both approximately 10^8. This explains why the run times for the 2D and 3D problems were comparable. In order to generate credible statistical information we used 30 realizations for each case. We limited our maximum computational time to about 7 days for all 30 realizations, which gave us a single data point. Parametric analysis was accomplished by simultaneously running multiple jobs at different nodes. For the 3D problem we were able to use N = 21 (i.e., 21 SEPSH data points in each of the three dimensions). For the 2D problem we were able to use N = 101 (i.e., 101 SEPSH data points in each of the two dimensions).

[18] In earlier work [*Nield et al.*, 2010] we modified our 3D code for SEPSH to fit a 2D problem in which the flow is constrained to that plane, recognizing that this meant that we were restricting the range of modes for stability analysis and were therefore not finding the global minimum Rayleigh number. Accordingly we ran SGSIM with matching 2D data. In the present paper we have extended the feasible size of N by developing an alternative code which employs a Monte Carlo approach in which only a sample of the sub-boxes is examined at the optimization stage. This provides an approximation to rather than an exact estimate of the Rayleigh number multiplier but from a computational perspective was the only feasible way of proceeding.

3. Results and Discussion

3.1. Spatial Dimensionality: 2D Versus 3D Isotropic Correlation Length

[19] First we tested the accuracy of our new Monte Carlo procedure for the 3D case with isotropy of correlation lengths with the grid number N increased from 21 to 49. The results are presented in Table 1. The results presented throughout this paper are tabulated in precise data tables rather than figures. We are necessarily interested in the precision of the Ra_{NO} values and this requires precise data tables in order to make the necessary quantitative comparisons. A problem with most previous studies has been that the results have not been tabulated, but rather presented in graphical form without supporting data tables. This has made objective quantitative assessments difficult, especially where there are often very small differences in values of important instability diagnostic variables. We found the practical limit on the sample size N_s, the number of sub-boxes considered for the optimization, based upon the computational matters described earlier was 10^7. For comparison, the total number of sub-boxes involved in the 3D case is $[N(N-1)/2]^3$, and when $N = 49$ this has the value 1.6×10^9. We conclude that when σ is not greater than 1.0 the Monte Carlo procedure gives a reasonably accurate value for Ra_{NO}. In fact, since this value is close to 1.0, this means that a Rayleigh number based on average values is then a good predictor for the onset of instability. When σ has a value 2.0 or larger it is clear that the Ra_{NO} value (both mean and standard deviation) is significantly larger. However, it is not immediately obvious that the Monte Carlo procedure gives accurate answers in this case. While we can see a definite trend that the Ra_{NO} value increases as σ increases, we do not know whether the answer has converged to an exact solution. Furthermore, there may not be an exact solution since *Nield et al.* [2010] found that in the case of localized 3D heterogeneity the value of Ra_{NO} becomes unbounded. It is therefore difficult to distinguish unbounded behavior from possible non-convergence using the Monte Carlo procedure. While we have not conclusively demonstrated unbounded behavior in this study for larger values of σ, we have demonstrated that it is plausible by inference from the earlier unbounded results of *Nield et al.* [2010] for the case of localized 3D heterogeneity. This matter is described in further detail below. Irrespective of this convergence issue, the heterogeneous fields, on average, are clearly destabilizing as evidenced by the increasing mean Ra_{NO} as σ increases. Whether the system is unstable will

depend on the value of the Rayleigh number based on mean quantities and how it compares to the critical Rayleigh number of approximately Ra = 40. In addition to this generally destabilizing behavior, there is also a greater range of behavior encountered with increasing standard deviation of the lognormal permeability field as evidenced by increasing standard deviation in Ra_{NO}. Furthermore, it is immediately clear from the present results that spatial dimensionality is a critical control on the onset of convection in heterogeneous porous media. In contrast to their 2D counterparts, the 3D heterogeneous geologic systems have much larger mean Ra_{NO} values (and hence more widespread instability overall on average) as well as much larger standard deviation in Ra_{NO} values (suggesting that there is also a greater range in observed behavior). These results suggest that, for identical geostatistical properties, 3D heterogeneous geologic systems are inherently more unstable than their 2D counterparts. This conclusion holds irrespective of whether or not the results are bounded or unbounded.

[20] By way of comparison, it is interesting to remark briefly on how spatial dimensionality controls the onset of natural free convection in homogeneous situations. The results of *Beck* [1972] [see, e.g., *Nield and Bejan*, 2006, Figures 6.22 and 6.23] clearly show that convection is expected to occur more easily in 3D, since three dimensional systems allow a wider range of disturbance modes. Two dimensions provide additional constraints and reduce the inherent "flow freedom." Thus, even in a purely homogeneous system and all other things being equal, one would expect a three dimensional system to be inherently more unstable than a two dimensional counterpart.

[21] It is important to further explore how spatial dimensionality controls the onset conditions for free convection. We now consider the earlier papers by *Nield et al.* [2009], *Kuznetsov et al.* [2010] and *Nield et al.* [2010] and note from the outset that the present results for spatial dimensionality follow as both a logical progression and consequence from earlier results. These early papers considered "tower blocks" where the variation of $\widetilde{K}$ was localized in one direction, both horizontal directions, and in all three directions. One can think of the degree of localization as being related to the width of the tower block. In particular, as the tower narrows the degree of localization increases. *Nield et al.* [2010] considered a deterministic distribution with either 2D localization in the horizontal plane or 3D localization. With the 2D localization they obtained values of the Rayleigh number multiplier with magnitudes up to 10, significantly higher than we had obtained with 1D localization. For comparison, for the case of 1D tower variation reported by *Kuznetsov et al.* [2010], the increase in the values of Rayleigh number multiplier was found to be limited to about 30%. With 3D localization the Rayleigh number multiplier can be arbitrarily large and is unbounded [*Nield et al.*, 2010]. These unbounded results for the 3D case were obtained through the SEPSH analysis but are also expected. For the 3D case, *Nield et al.* [2010] considered the situation where $\widetilde{K}$ is large within a small cube of side length δ and very small everywhere outside it. If $\widetilde{K}$ has a mean value of unity averaged over the original cube (side length 1) then $\widetilde{K}$ can be as large as $1/\delta^3$ within the small cube. From its definition, the Rayleigh number is proportional to the product of $\widetilde{K}$ and the square of the characteristic length scale. Hence the Rayleigh number based on the dimension of the small cube can have magnitude of order $1/\delta$, and obviously this is unbounded as δ tends to zero. Now let us consider the same argument in 2D. Now, for the 2D case, this involves a small square of side length δ and hence an area δ^2, within which $\widetilde{K}$ can be as large as something of order $1/\delta^2$ but no larger. Thus Ra can be no larger than a number of order $1/\delta^2$ times δ^2, the product of which is a finite number. This clearly provides a finite upper bound on the Rayleigh number. However, whether the bound on the Rayleigh number multiplier is something of order 10, or order 100, or order 1000 is not determined by this argument. The critical finding is that 2D results are always expected to be bounded with some finite upper limit but that 3D results may be arbitrarily large and unbounded.

[22] In the case of the geostatistical fields considered in the present study, it is clear that as σ increases, the degree of localization of free convection is also expected to increase. The increasing permeability contrasts progressively lead to a transition from "layer scale" (or large scale) convection which occurs throughout the entire system to "local" convection confined mainly to a few high permeability zones in the domain. When σ is less than unity the heterogeneity is relatively weak and the situation does not differ very much from the standard Horton-Rogers-Lapwood problem [*Nield and Bejan*, 2006]. For large values of σ, if convection occurs it will be concentrated within a small sub-region where the permeability is relatively high. This localization was also reported in the 2D geostatistical fields considered by *Nield et al.* [2010] who noted that in the cases for which Ra_{NO} was close to unity the optimum sub-box was the whole cube. In the cases where Ra_{NO} was large the optimum sub-box was small. The same behavior is expected in both 2D and 3D cases. It is for this reason that the findings from the present 3D geostatistical study may be directly related to the results of the highly mathematized "localized" results from the earlier studies. It is also the basis upon which, by inference from the earlier unbounded results of *Nield et al.* [2010] for the case of localized 3D heterogeneity, we contend that unbounded behavior is entirely plausible for larger values of σ in more realistic heterogeneous porous media.

[23] An integrated evaluation of the key findings from the previous papers [*Nield et al.*, 2009; *Kuznetsov et al.*, 2010; *Nield et al.*, 2010] as well of those from the present study shows that spatial dimensionality is an extremely important control on the onset of free convection in heterogeneous geologic media. The findings from the SEPSH analyses represent a significant advance in our understanding of how spatial dimensionality controls the onset of free convection in highly heterogeneous geologic systems. In particular, the potential for unbounded behavior in 3D is quite striking and is an extremely important new finding. This new finding also allows us to draw a very important and new conclusion regarding the use of Rayleigh numbers based on mean quantities for predicting the onset of convection in heterogeneous geologic media. An important consequence of this unbounded behavior in 3D systems is that if all we know is the average value of $\widetilde{K}$ calculated over the big cube, then no matter how small the Rayleigh number for the entire cube is, we are unable to conclude that convection is not occurring. It could be occurring within one or more small sub-regions of the big cube. We would, however, be confident that there was no significant motion outside those particular

Table 2. Values of the Mean of Ra_{NO} for Various SGSIM Input Values of σ and τ[a]

	$\tau = 0.05$		$\tau = 0.2$		$\tau = 0.3$		$\tau = 0.5$	
	2D	3D	2D	3D	2D	3D	2D	3D
$\sigma = 0.1$	1.000 (0.0002)	0.981 (0.008)	1.000 (0.001)	0.981 (0.008)	1.000 (0.001)	0.981 (0.008)	1.000 (0.001)	0.981 (0.008)
$\sigma = 0.3$	1.000 (0.001)	0.978 (0.007)	1.002 (0.004)	0.979 (0.007)	1.003 (0.005)	0.979 (0.007)	1.004 (0.007)	0.979 (0.007)
$\sigma = 1.0$	1.051 (0.007)	0.984 (0.008)	1.046 (0.079)	0.994 (0.051)	1.066 (0.099)	0.989 (0.021)	1.081 (0.103)	0.984 (0.016)
$\sigma = 1.5$	1.101 (0.167)	1.158 (0.364)	1.398 (0.485)	1.771 (0.841)	1.436 (0.436)	1.597 (0.711)	1.383 (0.336)	1.306 (0.529)
$\sigma = 2.0$	2.213 (0.874)	3.279 (1.834)	2.302 (1.012)	5.000 (3.183)	2.169 (0.934)	4.098 (2.456)	1.900 (0.724)	3.019 (1.834)
$\sigma = 2.5$	4.472 (2.085)	8.838 (6.22)	3.522 (1.562)	11.324 (6.82)	3.181 (1.500)	8.828 (5.07)	2.656 (1.171)	6.110 (3.87)
$\sigma = 3.0$	7.675 (3.845)	18.79 (14.38)	4.999 (2.134)	21.982 (16.35)	4.402 (2.104)	16.20 (11.56)	3.562 (1.662)	10.80 (7.83)

[a]Comparison of 2D and 3D results. The 2D results are "exact" results obtained with a grid number $N = 101$. The 3D results are obtained using the Monte Carlo method with a grid number $N = 49$ and a sample size $N_s = 10^7$. Standard deviation is given in parentheses.

sub-regions, and that may be enough information for some practical purposes. We can also make some general comments on the usefulness of Ra_{av} as a prediction criterion, where Ra_{av} is the Rayleigh number based on mean quantities. This depends on what one wants to use the Rayleigh number for and what supplementary information one has available. If convection in small sub-regions is deemed to be important and one knows that strong 3D localization is possible then Ra_{av} is useless. At the other end of the spectrum, if one has weak heterogeneity then Ra_{av} is very useful. In an intermediate situation, if one is fairly sure that Ra_{NO} may be as large as some number $Ra_{NO\max}$ but no larger, then one can make the following predictions. If Ra_{av} is greater than the critical $Ra = 40$ one probably has convection. If Ra_{av} is less than $40/Ra_{NO\max}$ then one probably has no convection. If Ra_{av} is between $40/Ra_{NO\max}$ and 40 then one cannot draw any conclusion one way or the other. Here spatial dimensionality is critical. Our results to date demonstrate that it may be possible to put reasonable bounds on Ra_{NO} in a 2D analysis, and hence make some predictions about the likelihood of convection in 2D heterogeneous systems. However, the onset of convection in a 3D heterogeneous system may in fact not be amenable to any form of reasonable prediction using Rayleigh number criteria. This is because we expect that it will be very difficult, and perhaps impossible, to put reasonable bounds on Ra_{NO} in the 3D case. This will be especially true where a heterogeneous geologic structure contains strong 3D localization which leads to unbounded results for Ra_{NO}. Given the matters discussed above, in the best case scenario the use of a Rayleigh number based on mean quantities should be applied with extreme care and caution in strongly heterogeneous geologic field settings. In the worst case scenario where strong localization leads to unbounded behavior the Rayleigh number will not be a valid predictor for the onset of convection and should not be applied to strongly heterogeneous geologic field settings. The major difficulty therefore lies in an ability to adequately quantify whether Ra_{NO} is bounded or unbounded and in the bounded case, making a reasonable determination of this upper bound. A-priori knowledge of the heterogeneous geologic structure is required in order to reasonably apply predictive Rayleigh stability analyses such as those employed by SEPSH in practical field settings. As is the case with many areas of hydrogeology, this represents a major challenge.

[24] We then applied the Monte Carlo procedure to investigate the effect of variation of the correlation length parameter τ in the 3D situation, with the results presented in Table 2. Table 2 also provides a comparison with corresponding results for the 2D case for which the Monte Carlo procedure was not necessary. We see that the 3D results are qualitatively similar to the 2D results. As we have just observed for the special case reported in Table 1, for σ less than unity the value of Ra_{NO} differs little from unity, but for larger values of σ the values of the mean and standard deviation of Ra_{NO} increase substantially. For the 3D case, the rate of increase is quite dramatic. These results are likely to be indicative of the unbounded behavior described earlier that is associated with the permeability distribution becoming increasingly localized. We now also observe that the dependence of τ is not strong when compared to the effect of changing the standard deviation of the lognormal permeability field. Using the SEPSH analysis has allowed the relative sensitivity of the different controlling parameters of the heterogeneous geologic distribution (standard deviation, correlation length) on the onset of free convection to be quantified and this is important new information. Results show that larger values of correlation length appear to be subtly more destabilizing at lower values of standard deviation ($\sigma < 1$) of the lognormal permeability field. Smaller values of correlation length appear to be noticeably more destabilizing at higher values of standard deviation ($\sigma \geq 2.5$) of the lognormal permeability field. In the intermediate range of standard deviation ($1.5 \leq \sigma \leq 2$) of the lognormal permeability field, intermediate values of the correlation length scale appear somewhat more destabilizing. Without more rigorous statistical testing of these results we are aware that these apparent differences, for any given standard deviation of the lognormal permeability field, may not be statistically significant. The subtle effects at smaller values of standard deviation of the lognormal permeability distribution should be interpreted with caution and we do not wish to draw any conclusions from these results, especially at lower values of standard deviation. However, at higher values of standard deviation ($\sigma \geq 2.5$) where the effect of changing correlation length is most significant, we note that our results are consistent with *Prasad and Simmons* [2003] who observed that smaller correlation length scales were generally destabilizing and larger values of correlation length scales were generally stabilizing. This is because the larger correlation length of the permeability structure leads to laterally more extensive low permeability regions. These low permeability regions are more effective at dampening the downward and upward motion required for instability growth. *Prasad and Simmons* [2003] also observed some cases where intermediate values of correlation length very slightly enhanced destabilization. More generally, *Prasad*

and Simmons [2003] noted that in comparison to the effect of the standard deviation of the lognormal permeability field that their results appeared to be relatively insensitive to the correlation length of the permeability distribution which is in agreement with our current assessment.

[25] It is useful to remark a little further on the relative insensitivity of the correlation length parameter when compared with that of the standard deviation of the lognormal permeability field. Since large scale free convection is determined by the overall layer properties such as the permeability in the vertical direction, it is important to note that changing the correlation length in both the horizontal and vertical direction while holding all other properties constant and maintaining the condition of correlation length isotropy does not change the overall layer permeability in either the horizontal or vertical direction. Importantly, the overall permeability of the system remains isotropic when the correlation length structure is isotropic. No significant changes to the onset conditions on the layer scale are therefore expected by simply changing the correlation length in both directions when overall correlation length isotropy and hence permeability isotropy is maintained. However, as noted earlier, as σ increases there is a transition from layer scale convection to increasingly localized convection. This is the critical phenomenon which controls the convection behavior and hence the results for the onset conditions and stability criteria. Changing the correlation length at low values of σ does not result in localized behavior and therefore has little effect on overall convection onset conditions. Larger layer scale averaging for properties still holds and since simultaneous changes to the correlation length in both directions does not change the layer scale properties, little effect is observed. However, for much larger values of σ increasingly localized convection behavior occurs. Larger layer scale averaging no longer applies. At these higher values of σ, correlation length is seen to have more effect, but it is still far less pronounced than that of σ which is the principal cause for the transition from layer scale to local scale convective behavior.

[26] It is useful to consider the application of these results to a field based system. As noted earlier, only very recently has primary evidence of free convection in a natural field setting been reported in the literature [*Van Dam et al.*, 2009]. These authors presented electrical resistivity measurements from a sabkha aquifer near Abu Dhabi, United Arab Emirates, where large density inversions exist. The geophysical images from this site provided, for the first time, compelling field evidence of fingering associated with natural free convection in groundwater. The field results are quite illustrative of the nature of natural convection behavior. However, the field site studied in Abu Dhabi is extremely homogeneous. The sabkha sediments below the water table consist of uniform, fine sand (0.16–0.22 mm) from reworked dunes. The material has a nearly homogeneous porosity of 0.38 and hydraulic conductivity of 1.0 ± 0.2 m/day [*Van Dam et al.*, 2009]. The nearly perfect homogeneous conditions in the site did not necessitate any mapping of the heterogeneity within the sabkha sediments and one may assume that the system is essentially perfectly homogeneous. In this case, the Rayleigh number may be calculated in the traditional way. *Van Dam et al.* [2009] showed that the Rayleigh number is orders of magnitude greater than the common stability criterion $Ra = 4\pi^2 = 39.48$. These Rayleigh number calculations showed that free convection was therefore expected to occur in this system [see *Van Dam et al.*, 2009, Text S1]. In a sense, the Abu Dhabi system permits the simplest application of our latest theoretical work in a homogeneous setting. While the results suggest that free convection should be observed in the sabkha on the basis of the Rayleigh stability criterion this application is not a test of the newly proposed strongly heterogeneous stability criterion. Unfortunately, due to the severe lack of primary field based measurements of free convection in the literature at this time, a meaningful application of the strongly heterogeneous stability criterion to a heterogeneous field based application is currently not possible.

3.2. Two-Dimensional Anisotropic Correlation Length

[27] We then turned our attention to the effect of anisotropy of correlation length. We confined our investigation to the 2D case. This was because we were very limited by the number of nodes we could use in the 3D situation. Strongly anisotropic cases require either the horizontal domain to be increased in order to fit a sufficient number of horizontal correlation lengths within the overall domain and/or a reduction in the vertical correlation length accompanied by reduced vertical discretization in order to adequately resolve the reduced vertical correlation length. These requirements were computationally prohibitive in the 3D situation. We were, however, able to obtain a much better spatial resolution in the 2D case which was therefore much better suited to the anisotropic analysis.

[28] We investigated the particular case where the aspect ratio (the ratio of horizontal domain length to vertical domain length) was increased to $A = 10$. That meant that instead of the physical domain being a square ($A = 1$) it was now a shallow rectangle which could be divided into 10 squares. We made this adjustment to the domain in order to allow anisotropic correlation structures to be meaningfully tested. Here we refer to correlation length anisotropy (τ_x/τ_y) as the ratio of the correlation length in the horizontal direction (τ_x) to the correlation length in the vertical direction (τ_y). For realistic geologic media, we expect layers and lenses to be horizontally elongated, thus giving correlation length anisotropy values greater than unity. The core SEPSH code operates on a square, and so a square selection procedure (a cube selection procedure in 3D) must now be involved. SEPSH was modified accordingly so that we could run it for each of the 10 square subdomains in turn using the same SGSIM output. We obtained the results that are reported in Table 3. The Monte Carlo procedure was not used. The values $\tau_x = 0.30$ and $\tau_y = 0.03$ were chosen so that their ratio was 10. The headings Case 1, …, Case 10 refer to the square subdomains, taken in order of increasing value of x, while Case 0 refers to the case where the original domain is a square (a rectangle whose aspect ratio $A = 1$). To be explicit, the whole domain is given by (x in [0,10], y in [0,1]). Case 1 applies to the left-hand square (x in [0,1]), Case 2 applies to the next square (x in [1,2]), and so on. Case 10 applies to the right-hand square (x in [9,10]). By symmetry, one would expect that the results for Cases 1 and 10 would be essentially the same, and inspection reveals that this is indeed the case. When one looks at the differences between calculated means in comparison with the calculated standard deviations, a rough statistical analysis immediately

leads to the conclusion that the results are consistent with the hypothesis that the results for Cases 2, 3, … come from the same population as for Cases 1 and 10, and further that the results for Case 0 are also a sample from that population. We therefore conclude that the aspect ratio is not a significant factor in this context. This could be expected, since in the Horton-Rogers-Lapwood problem [*Nield and Bejan*, 2006] the extension of the layer laterally adds more convection cells but does not change the critical Rayleigh number significantly. Importantly, when comparing the Ra_{NO} results for $\tau_x = 0.30$ and $\tau_y = 0.03$ (Table 3) with the isotropic case $\tau_x = \tau_y = 0.30$ for the 2D system (Table 2) little difference can be seen. This suggests that the onset of convection is relatively insensitive to the anisotropy of correlation length.

[29] To further confirm our conclusion that the anisotropy of correlation length is not a significant factor we repeated the calculation but with τ_y given the value 0.003 rather than 0.03, so that the ratio τ_x/τ_y was now 100 rather than 10. The aspect ratio of the domain was kept at $A = 10$. The new results are reported in Table 4. The results in Table 4 are not significantly different from those shown in Table 3. We can reasonably conclude that our results are not sensitive to the anisotropy of correlation length.

[30] *Simmons et al.* [2001] made the qualitative observation that instabilities tended to be dampened in cases with hydraulic conductivity fields with low vertical correlation length scales (for a fixed value of the horizontal correlation length). All of the current and previous observations, irrespective of whether the anisotropy of correlation length is manipulated by variation of correlation lengths in the horizontal and/or vertical direction, are consistent in showing that long, laterally extensive low permeability layers dampen instability and that there is some effect of the anisotropy of correlation length [*Schincariol et al.*, 1997; *Simmons et al.*, 2001; *Prasad and Simmons*, 2003]. However, they have not adequately quantified its effect relative to other ones. We now clearly see that the value of σ is the most significant parameter controlling the onset of free convection. It is this parameter which controls the transition from larger layer scale convection to local convection and hence when averaging across larger regions breaks down. When local scale convection is dominant, it is clear that the geometrical structure and hence parameters such as τ will be important in determining the dominant mode(s) of convection which occur in the system.

4. Conclusion

[31] We have used the Stability Exploration Package for Strong Heterogeneity (SEPSH) to study the applicability of an average Rayleigh number as a criterion for the onset of convection in realistic and strongly heterogeneous geologic porous media. We have quantitatively assessed the importance of spatial dimensionality and geologic controls.

[32] Our results quantitatively demonstrate for the first time that spatial dimensionality is a dominant control on the onset of convection in a strongly heterogeneous geologic medium. A comparison of 2D and 3D results suggest that, for identical geostatistical properties, 3D systems are inherently more unstable than 2D systems. In contrast to their 2D counterparts, the 3D systems have larger mean Ra_{NO} values and hence more widespread instability overall on average as well as larger standard deviation in Ra_{NO} values suggesting that there is also a greater range in observed behavior. For larger values of standard deviation of the lognormal permeability field, the values of the mean and standard deviation of Ra_{NO} increase substantially and for the case of 3D the rate of increase is quite dramatic. Unbounded Rayleigh number behavior is observed in 3D. This leads to the important new conclusion that a Rayleigh number based on mean quantities is unlikely to be a valid predictor for the onset of convection in 3D strongly heterogeneous porous media. In the best case scenario the use of a Rayleigh number should be applied with extreme care and caution in strongly heterogeneous geologic field settings. In the worst case scenario where strong localization leads to unbounded behavior the Rayleigh number will not be a valid predictor for the onset of convection and should not be applied to strongly heterogeneous geologic field settings. The major difficulty therefore lies in an ability to adequately quantify whether Ra_{NO} is bounded or unbounded and in the bounded case, making a reasonable determination of this upper bound. A-priori knowledge of the heterogeneous geologic structure is required in order to reasonably apply predictive Rayleigh stability analyses such as those employed by SEPSH in practical field settings.

[33] We have demonstrated that the onset of convection in a heterogeneous geologic medium is highly sensitive to changes in the standard deviation of the lognormal permeability field, moderately sensitive to changes in the level of correlation length, and relatively insensitive to the anisotropy of correlation length. These relative sensitivities have not been elucidated in quantitative terms in previous studies and are important new findings. On the basis of the systematic and quantitative analyses presented in this paper, we conclude that the onset of convection in a strongly heterogeneous porous medium is largely controlled by spatial dimensionality and the standard deviation of the lognormal permeability field, and to a much lesser degree by the correlation length and anisotropy of correlation lengths of the permeability field. These are important new findings which have not been presented in previous literature.

[34] This paper has presented the first 3D theoretical treatment of the Rayleigh stability criteria for the onset of convection in realistic, strongly heterogeneous porous media. It represents a significant advance over the earlier highly mathematized treatments and therefore leads to a much more realistic set of stability criteria than that which has been presented in earlier work. Our results quantitatively demonstrate for the first time that spatial dimensionality is a dominant control on the onset of convection in a strongly heterogeneous geologic medium. Given that real geologic systems are 3D in nature, and that previous theoretical analyses have been exclusively 1D or 2D treatments only, this 3D study was clearly warranted and its findings are significant. In particular, the potential for unbounded Rayleigh number behavior in 3D is quite striking and is an extremely important new result. The fact that this behavior then severely limits and quite possibly prohibits the use of the classical Rayleigh number based on mean quantities for determining the onset of convection in strongly heterogeneous geologic field settings is a fundamental new result. These are very important new findings for the field of free convection in porous media.

Table 3. Values of the Mean of Ra_{NO} for Various SGSIM Input Values of σ, for $\tau_x = 0.30$, $\tau_y = 0.03$ With Grid Number $N = 101$ and With Aspect Ratio $A = 10$ for the 2D Case[a]

σ	Case 0	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case10
0.1	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.001 (0.001)	1.000 (0.001)
0.3	1.002 (0.003)	1.002 (0.005)	1.004 (0.006)	1.003 (0.006)	1.002 (0.006)	1.004 (0.004)	1.004 (0.004)	1.004 (0.007)	1.004 (0.006)	1.005 (0.007)	1.003 (0.005)
1.0	1.015 (0.013)	1.100 (0.158)	1.108 (0.170)	1.055 (0.081)	1.062 (0.089)	1.095 (0.117)	1.056 (0.084)	1.083 (0.134)	1.087 (0.117)	1.066 (0.072)	1.044 (0.052)
1.5	1.085 (0.133)	1.597 (0.757)	1.590 (0.717)	1.416 (0.443)	1.440 (0.443)	1.521 (0.531)	1.440 (0.424)	1.475 (0.530)	1.495 (0.416)	1.436 (0.446)	1.315 (0.350)
2.0	1.864 (0.882)	2.419 (1.387)	2.371 (1.341)	2.076 (0.942)	2.142 (0.913)	2.260 (1.076)	2.124 (0.840)	2.122 (1.014)	2.174 (0.828)	2.178 (0.944)	1.909 (0.810)
2.5	3.583 (2.180)	3.297 (1.826)	3.248 (1.814)	2.866 (1.391)	2.919 (1.368)	3.071 (1.536)	2.920 (1.225)	2.902 (1.454)	2.923 (1.236)	3.098 (1.378)	2.653 (1.251)
3.0	5.950 (4.028)	4.137 (2.077)	4.113 (2.082)	3.613 (1.715)	3.642 (1.686)	3.826 (1.841)	3.694 (1.532)	3.669 (1.817)	3.647 (1.539)	4.059 (1.710)	3.407 (1.619)

[a]Standard deviation is given in parentheses.

Table 4. As for Table 3 but With $\tau_y = 0.003$

σ	Case 0	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case10
0.1	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.000 (0.001)	1.001 (0.001)	1.000 (0.001)
0.3	1.001 (0.002)	1.002 (0.003)	1.003 (0.004)	1.003 (0.005)	1.003 (0.005)	1.003 (0.005)	1.001 (0.003)	1.003 (0.005)	1.004 (0.006)	1.005 (0.006)	1.002 (0.004)
1.0	1.008 (0.008)	1.084 (0.186)	1.055 (0.085)	1.083 (0.138)	1.049 (0.098)	1.063 (0.107)	1.105 (0.206)	1.031 (0.026)	1.086 (0.205)	1.086 (0.149)	1.046 (0.072)
1.5	1.075 (0.182)	1.587 (0.789)	1.459 (0.548)	1.528 (0.756)	1.382 (0.557)	1.521 (0.570)	1.584 (0.844)	1.224 (0.260)	1.577 (0.763)	1.534 (0.606)	1.400 (0.466)
2.0	1.766 (1.023)	2.465 (1.375)	2.242 (1.071)	2.304 (1.435)	1.990 (1.120)	2.318 (1.062)	2.419 (1.427)	1.731 (0.620)	2.363 (1.258)	2.326 (1.090)	2.104 (0.937)
2.5	3.338 (2.217)	3.412 (1.767)	3.162 (1.486)	3.101 (1.955)	2.716 (1.574)	3.237 (1.392)	3.247 (1.835)	2.414 (0.971)	3.184 (1.581)	3.192 (1.495)	2.878 (1.370)
3.0	5.406 (3.458)	4.283 (2.020)	4.106 (1.746)	3.794 (2.266)	3.431 (1.888)	4.188 (1.721)	3.963 (2.080)	3.116 (1.320)	3.956 (1.801)	4.055 (1.804)	3.612 (1.676)

[35] Unfortunately, due to the severe lack of primary field based measurements of free convection in the literature at this time, a meaningful application of the strongly heterogeneous stability criterion to a strongly heterogeneous field based application is currently not possible. However, it is clear that the theory does provide a useful end-member for application in the near-homogeneous setting studied recently by *Van Dam et al.* [2009]. In this case, the traditional use of the Rayleigh number showed that free convection was expected to occur in the Abu-Dhabi sabkha system. Further field studies to measure free convection in strongly heterogeneous geologic systems are warranted. This is a necessary precursor to application of the current theoretical findings in field based settings. However, the results of this study may also usefully serve to guide field scale exploration of free convection in strongly heterogeneous geologic settings.

Notation

A aspect ratio of the domain.
A_x aspect ratio in x-direction, H/L_x.
A_y aspect ratio in y-direction, H/L_y.
A_{sx} aspect ratio of a sub-box in x-direction, $(z_B - z_A)/(x_B - x_A)$.
A_{sy} aspect ratio of a sub-box in y-direction, $(z_B - z_A)/(y_B - y_A)$.
b parameter defined by equation (3).
D effective solute diffusion coefficient.
g acceleration due to gravity.
H height of the box or layer.
k thermal conductivity.
k_r value of k normalized in terms of its mean value.
k_s mean of k_r taken over the sub-box.
K permeability.
K_r value of K normalized in terms of its mean value.
K_s mean of K_r taken over the sub-box.
$\widetilde{K}$ potential convectivity.
$\widetilde{K}_{\mathrm{SEPSH}}$ transformed SGSIM value for input as potential convectivity to SEPSH.
$\widetilde{K}_{\mathrm{SGSIM}}$ SGSIM data generated from a standard normal distribution.
L length of the box.
L_x dimension of the box in the x-direction.
L_y dimension of the box in the y-direction.
N grid number for SEPSH grid.
N_s sample size for Monte Carlo sampling procedure.
p nonnegative integer.
q nonnegative integer.
Ra critical Rayleigh number.
$\mathrm{Ra}_{\mathrm{av}}$ Rayleigh number based on mean quantities.
Ra_g geometrically adjusted Rayleigh number defined by equation (6).
Ra_l local sub-box Rayleigh number.
Ra_{NO} overall normalized Rayleigh number defined by equation (11).
$\mathrm{Ra}_{NO\max}$ upper bound to overall normalized Rayleigh number.
Ra_{Ns} normalized Rayleigh number defined by equation (9).
Ra_{Nsg} geometrically adjusted Rayleigh number for a particular sub-box, defined by equation (10).
Ra_O overall Rayleigh number defined by equation (7).
Ra_S solute Rayleigh number.
Ra_T thermal Rayleigh number.
S solute concentration.
T temperature.

Greek symbols

α_T thermal expansion coefficient.
α_S density-concentration coupling coefficient.
β applied vertical temperature gradient.
β_r value of β normalized in terms of its mean value.
β_s mean of β_r taken over the sub-box.
ε the order of a fractional change in some quantity.
κ thermal diffusivity of the porous medium.
δ length of the side of a small cube.
Δ change in some quantity.
μ dynamic viscosity.
ρ_o reference density.
σ standard deviation.
τ relative correlation length.

Subscripts

x parameter based on length or dimension x.

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