Double-diffusive convection in groundwater wells

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[1] Double-diffusive convection caused by variations in solute concentration and temperature within a fluid body has previously been studied in connection with oceanic mixing processes, astrophysics, metallurgy, geology, and vadose zone hydrology but has not previously been studied in connection with thermohaline transport in a groundwater well. This paper considers whether double-diffusive convection induced by salinity and/or temperature variations is a plausible mechanism for heat and solute transport in a groundwater well. This is examined theoretically using Rayleigh number stability "onset" criteria for fluid in a cylinder that considers the cylindrical well geometry and geothermal/solute boundary conditions. Theoretical results suggest that both monotonic and oscillatory double-diffusive convection are plausible transport phenomena in groundwater wells. These analyses have important implications for hydrogeology because they provide another theoretically plausible mechanism by which heat and solute may mix in a well. This previously unaccounted for thermohaline mixing phenomenon may therefore be critical in the interpretation of well hydrogeologic and hydrochemical data.

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1. Introduction

[2] Groundwater wells are the most basic instrument for measuring hydrogeologic and hydrochemical parameters in a groundwater system. It is well known, however, that measurements made in these wells may not always be representative of the adjacent aquifer especially where intrawell mixing induced by vertical hydraulic gradients occur [see, e.g., *Elci et al.*, 2001]. The driving forces for intrawell mixing are typically assumed to be advective, dispersive and diffusive transport phenomena. However, to the best of our knowledge, the potential effects of thermohaline double-diffusive convection (DDC) have not been studied in connection with a groundwater well in previous literature.

[3] Some simple observations suggest that the thermohaline mechanism clearly warrants attention as a potential thermohaline transport mechanism in a well. First, all groundwater wells exist in the presence of a geothermal gradient in which groundwater temperature increases with depth. In terms of the groundwater density, this is unstable since the temperature transitions from colder fluid at shallow depths (greater density) to warmer fluid at depth (lesser density). It is clear that the potential exists for gravitational unstable density gradients to drive convective heat transport in a groundwater system and this phenomenon has been studied in aquifers and porous media in previous literature [*Rubin*, 1981; *Wood and Hewitt*, 1992; *Pestov*, 2000]. Given that it is widely accepted that geothermal gradients may drive fluid circulations in geologic settings, a logical question then follows. To what extent can the geothermal gradient drive convective flow in a groundwater well? One may expect that since the groundwater well represents a zone of very low resistance to fluid flow it may be possible that even moderate density contrasts may lead to fluid circulations. One of the earliest studies in relation to convective motion in geysers was a theoretical analysis by *Hales* [1937]. One may begin to draw an analogy between the theoretical treatment by *Hales* [1937] and the problem we consider here. Hales' analysis predicted that the onset of instability in a tube filled with water would occur when the temperature gradient exceeded a critical value related to the tube radius and the viscosity of the fluid. His theory predicted that thermal convection was more likely in larger diameter tubes. His theoretical development was tested by field observations in oil wells in the 1960s [*Diment and Robertson*, 1963; *Diment*, 1967; *Gretner*, 1967]. Observation of temperature profiles in large diameter wells were shown to be unstable as theoretically predicted. It appears that the potential for thermal mixing to occur in a groundwater well has received little attention in groundwater literature since these pioneering studies but may be more important than we currently recognize.

[4] These previous studies only considered single component convection driven by heat. However, the interaction of salt and heat (with the diffusivity of heat being approx-

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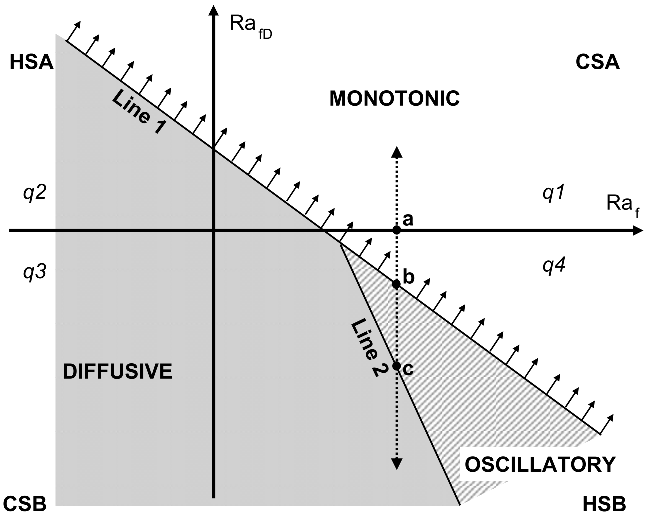

Figure 1. Schematic diagram in $Ra_f - Ra_{fD}$ number space showing the stability regimes for DDC in a vertical cylinder with fluid. The different quadrants represent different thermohaline regimes in a groundwater well: q1, CSA (cold and salty above); q2, HSA (hot and salty above); q3, CSB (cold and salty below); and q4, HSB (hot and salty below). For line 1, $Ra_f + Ra_{fD} = Ra_{f0}$ represents the boundary between stable and monotonic convection. For line 2, $(P_s^2 Ra_f + P_r^2 Ra_{fD})/(P_r P_s + P_r + P_s) = Ra_{f0}$ represents the boundary between the stable and oscillatory modes. The example presented is for a well with $r = 0.01$ m, $H_f = 30$ m, and geothermal gradient 0.02°C/m ($\Delta T = 0.6$°C). Point a is the geothermal gradient only ($\Delta C = 0$). Note: The upward arrow indicates that any increase in ΔC will result in further unstable monotonic conditions. At point b, the boundary between monotonic and oscillatory convection will occur by increasing the salinity difference to $\Delta C = 1.7686$ mg/L in a stable configuration. At point c, the boundary between oscillatory and diffusive flow will occur by increasing the salinity difference to $\Delta C = 14{,}188.2$ mg/L in a stable configuration. Note: The downward arrow indicates that any increase in ΔC (beyond point c) will result in stable conditions.

imately two orders of magnitude greater than salt) means that one must also consider the potential for double-diffusive convection in a well, a previously unaccounted for phenomenon. Interestingly, DDC has been studied previously in oceanography [*Stern*, 1960; *Stern and Turner*, 1969; *Turner*, 1979, 1985], astrophysics [*Spiegel*, 1972] metallurgy [*Azouni*, 1981], geophysics [*McKenzie and Richter*, 1981] and the formation of magma chambers [*Turner*, 1985; *Brandt and Fernando*, 1995]. Critically, DDC has also been studied theoretically and experimentally in porous media [*Nield*, 1968; *Rubin and Roth*, 1979; *Griffiths*, 1981; *Imhoff and Green*, 1988; *Murray and Chen*, 1989; *Ronen et al.*, 1988; *Ronen et al.*, 1995; *Cooper et al.*, 1997, 2001; *Nield and Bejan*, 2006]. A very important point follows. In terms of "flow freedom" as determined by resistance to flow, oceanic systems are expected to be the least resistive; porous media flow most resistive; and flow in a groundwater well might intuitively represent an intermediate point between these two systems.

[5] The aim of this paper is to theoretically examine whether thermohaline double-diffusive transport induced by salinity and/or temperature variations is a plausible mechanism for heat and solute transport in a groundwater well. We adapt previous theoretical fluid mechanics studies based on convection in a cylinder [*Gershuni and Zhukhovitskii*, 1970, 1976] to develop the steady state onset conditions (required temperature, salinity, and well geometry) for DDC in a groundwater well. The Rayleigh number stability criteria that consider the cylindrical well geometry and appropriate geothermal and solute boundary conditions are formulated. We apply the theoretical treatment to groundwater wells using realistic data to determine whether, from a theoretical viewpoint at least, thermohaline double-diffusive convection is a plausible phenomenon; that is, do typical hydrogeologic data theoretically satisfy the various onset criteria. Here we determine whether onset of convection will or will not occur. We do not consider the temporal behavior of these phenomena once they are established in this first analysis.

2. Double-Diffusive Convection

[6] DDC can occur where the density of the fluid is affected by at least two components with different diffusivities. Combined heat and salt transport (thermohaline convection) is one specific subset of the more general DDC problems. In thermohaline phenomena, the thermal diffusivity is approximately two orders of magnitude higher than the solute diffusivity. Under certain conditions, this may result in gravitational instabilities due to the phase lag between the faster diffusing heat and the slower diffusing solute. For exhaustive treatments on DDC phenomena, the reader is referred to *Turner* [1979], *Nield and Bejan* [2006], and *Diersch and Kolditz* [2002]. A conceptual diagram of the different convection regimes are shown in Figure 1 in $Ra_f - Ra_{fD}$ space, where Ra_f is the thermal Rayleigh number of the fluid, and Ra_{fD} is the solute Rayleigh number of the fluid. These are defined in the formal mathematical treatment that follows (equations (81) and (82)). Briefly, there are broadly two regimes that are of interest. They are referred to as: (1) monotonic convection (sometimes referred to as the fingering regime) and (2) oscillatory convection.

2.1. Monotonic Convection

[7] Monotonic convection can occur when the sum of the solute and thermal Rayleigh number exceeds a critical Rayleigh number. This can potentially occur in thermohaline regimes where temperature and salinity are destabilizing with respect to the net density gradient or when the faster diffusing component is stabilizing. For the configuration of hot and salty water stratified above cold and fresh water, the density contribution from the temperature component is stable and from the solute component is unstable. A small perturbation of fluid moving vertically down will result in long narrow lobes of descending saltier water that cools alternating with thin lobes of fresher warmer water that rise. Monotonic instabilities are sometimes referred to as fingering instabilities that provides a physical description of the convective motion.

2.2. Oscillatory Convection

[8] Oscillatory motions can only occur for the configuration of cold fresh water overlying hot and salty water, where the density contribution from the temperature component is destabilizing and from the solute component is stabilizing. If one considers a parcel of hot salty water that is displaced upward, the parcel will diffuse heat more rapidly than it diffuses salt, which will result in instability across the interface. As the perturbed parcel of water continues to rise (losing heat more rapidly than it loses salt) it eventually becomes heavier than the surrounding fluid at which point it begins to descend. The parcel of water will descend beyond its original position, warming as it sinks. The parcel eventually becomes less dense than the surrounding fluid at which point it begins to rise. An oscillatory motion will result. This results in a "staircase" like profile with sharp interfaces of density separated by well mixed layers that have been studied extensively in previous literature [*Tait and Howe*, 1971; *Turner*, 1979; *Schmitt*, 1995]. (Oceanic salt fingers may also result in a staircase profile, but in this case another mechanism is involved.)

3. Theory of a Thermohaline Well in a Geothermal Field

[9] We first present some basic theory for thermal convection published by *Gershuni and Zhukhovitskii* [1970, 1976]. Since the original publications are in Russian, and the translated book is not readily available, we present more detail than we would have done normally in order to provide a complete theoretical analysis.

[10] For the benefit of readers who are unfamiliar with linear instability theory, we outline the basic methodology that is involved. The Oberbeck-Boussinesq approximation is invoked. A basic solution is obtained. This solution is perturbed by a small amount, and the system is linearized. When account of the basic solution is made, a set of homogeneous linear equations results. This permits the application of the method of separation of variables. (In this context, this means the introduction of normal modes.) In particular, the time dependence in such a mode appears as a factor involving an exponential term. The sign of the real part of the coefficient in the exponent determines whether the perturbation grows (instability) or decays (stability) with time. A good book on this subject is the one by *Chandrasekhar* [1961].

3.1. General Vertical Cylindrical Channel Infinite Height, Thermal Problem

[11] Suppose that the well can be modeled as a vertical cylindrical channel, with solid walls in which heat conduction is modeled by Laplace's equation. If the fluid and the walls are heated from below and the temperature gradient A is constant and vertical then the basic velocity and temperature distributions are given as functions of the upward vertical coordinate by

$$\mathbf{v} = 0,\ T_0 = -Az + \text{constant}. \tag{1}$$

[12] In the absence of normal heat flux at the walls, it follows from the continuity of temperature that the temperature in the walls is also a linear function of z, and moreover the equilibrium temperature gradients in the walls and the fluid coincide.

[13] Small disturbances from the basic solution satisfy the set of equations

$$-\lambda\mathbf{v} = -\nabla p + \nabla^2\mathbf{v} + RT\mathbf{k} \tag{2}$$

$$-\lambda P_r\mathbf{v} = \nabla^2 T + \mathbf{v}\cdot\mathbf{k} \tag{3}$$

$$\text{div }\mathbf{v} = 0 \tag{4}$$

$$-\lambda P_r\bar{\kappa}T_w = \nabla^2 T_w, \tag{5}$$

where the velocity $\mathbf{v}$, fluid temperature T and the wall temperature T_w are assumed to vary with time as $\exp(-\lambda t)$. Here $\overline{\kappa} = \kappa/\kappa_w$ is the fluid-to-wall thermal diffusivity ratio and $P_r = \nu/\kappa$ is the fluid Prandtl number, and R is a Rayleigh number defined by

$$R = \frac{g\beta AL^4}{\nu\kappa}. \tag{6}$$

[14] Here ν is the fluid kinematic viscosity, β is the volumetric coefficient of expansion, g is the gravitational acceleration. The equations have been scaled in terms of the characteristic length L, time L^2/ν, velocity κ/L and pressure $\rho_0\nu\kappa/L^2$, where ρ_0 is the reference density.

[15] In the thermal problem with heating from below, λ is real. Gershuni and Zhukhovitskii refer to this as the "monotonicity principle for disturbances". In the Western literature the term used is "the principle of exchange of stabilities." At the onset of convection (that is, for a "neutral mode"), $\lambda = 0$, and the equations simplify to

$$\nabla^2\mathbf{v} + RT\mathbf{k} = \nabla p \tag{7}$$

$$\nabla^2 T = -v_z \tag{8}$$

$$\text{div }\mathbf{v} = 0 \tag{9}$$

$$\nabla^2 T_w = 0. \tag{10}$$

[16] Let us now consider motions parallel to the channel axis, assuming that the temperature disturbance is independent of the z coordinate:

$$\begin{aligned} &v_x = v_y = 0,\ v_z = v(x,y)\\ &T = T(x,y),\ T_w = T_w(x,y). \end{aligned} \tag{11}$$

[17] Taking the x and y components of the equation of motion, we find that $p = p(z)$, and the z component then gives

$$\nabla_H^2 v + RT = \frac{dp}{dz} = C, \tag{12}$$

where $\nabla_H^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is the two-dimensional Laplacian and C is a separation constant that defines the longitudinal pressure gradient. Hence we obtain the system of critical motions

$$\nabla_H^2 v + RT = C \tag{13}$$

$$\nabla_H^2 T + v = 0 \tag{14}$$

$$\nabla_H^2 T_w = 0. \tag{15}$$

[18] The velocity vanishes at the boundary Γ of the horizontal cross section of the channel, and there the temperature and normal heat flux satisfy the continuity conditions

$$v = 0,\ T = T_w,\ \bar{k}\frac{\partial T}{\partial n} = \frac{\partial T_w}{\partial n}, \tag{16}$$

where $\bar{k} = k/k_w$, the thermal conductivity ratio.

[19] In the walls at large distances from the channel, the temperature disturbances are damped out, so

$$T_{w\infty} = 0. \tag{17}$$

[20] We assume that the channel is closed, so that the volume flux through any cross section is zero:

$$\int_S v\, dS = 0. \tag{18}$$

[21] Since the vertical pressure gradient is constant, we can eliminate the constant C in equation (13) by a suitable change of reference temperature, introducing a new temperature. Then, at the walls the new temperature is $T - C/R$. Hence without loss of generality we can assume that the right-hand side of equation (13) is zero, with equation (17) replaced by $T_{w\infty}$ = constant. This constant is found by solving the boundary value problem. Thanks to symmetry properties of the flow, the condition (18) is automatically fulfilled for a wide range of critical motions, in such a way that the longitudinal pressure gradient is zero.

3.2. Circular Cylinder, Infinite Height, Thermal Problem

[22] For a cylinder of circular cross section, we can choose cylindrical coordinates with the *z axis* drawn upward along the channel axis. This problem allows solutions of the form

$$v(r,\phi) = u(r)\cos n\phi \tag{19}$$

$$T(r,\phi) = \theta(r)\cos n\phi \tag{20}$$

$$T_w(r,\phi) = \theta_w(r)\cos n\phi, \tag{21}$$

where $n = 0, 1, 2, \ldots$.

[23] Substituting (19)–(21) into (13)–(15), and with an appropriate choice of reference temperature so that the constant C is eliminated from equation (13), we obtain equations for the radial functions u, θ and θ_w:

$$Du + R\theta = 0 \tag{22}$$

$$D\theta + u = 0 \tag{23}$$

$$D\theta_w = 0, \tag{24}$$

where D denotes the operator $d^2/dr^2 + (1/r)d/dr - n^2/r^2$ and now R is defined in terms of the radius r_0 of the cylinder:

$$R = \frac{g\beta A r_0^4}{\nu\kappa}. \tag{25}$$

[24] At the interface between the channel and the rigid walls the velocity vanishes and the temperature and the heat flux are continuous:

$$\text{at } r = 1:\ u = 0,\ \theta = \theta_w,\ \bar{k}\partial\theta/\partial r = \partial\theta_w/\partial r. \tag{26}$$

[25] In addition, we need a condition stating that u and θ are finite at the axis, and the temperature disturbances in the walls far from the channel are also finite:

$$\text{at } r = 0:\ u \text{ and } \theta \text{ are finite} \tag{27}$$

$$\text{at } r \to \infty: \theta_w \to \text{constant}. \tag{28}$$

[26] If we eliminate θ from equations (22) and (23) we get

$$\left(D^2 - R\right)u = 0. \tag{29}$$

[27] The general solution of equation (29) that remains finite as $r \to 0$ is

$$u = C_1 J_n(\gamma r) + C_2 I_n(\gamma r), \tag{30}$$

where J_n and I_n are Bessel functions of the first kind, C_1 and C_2 are arbitrary constants, and

$$\gamma = R^{1/4}. \tag{31}$$

[28] Then equation (22) implies that

$$\theta = \frac{1}{\gamma^2}\left[C_1 J_n(\gamma r) - C_2 I_n(\gamma r)\right]. \tag{32}$$

Table 1. Critical Values for $\gamma_n^{(1)}$ and $R_n^{(1)}$

	$\bar{k} = 0$		$\bar{k} = \infty$	
n	$\gamma_n^{(1)}$	$R_n^{(1)}$	$\gamma_n^{(1)}$	$R_n^{(1)}$
0	4.611	452.0	4.611	452.0
1	3.382	215.6	2.871	67.95
2	5.136	695.6	4.259	329.1
3	6.380	1657	5.541	942.5

[29] In view of the condition (27), equation (24) yields

$$\theta_w = \frac{C_3}{r^n}. \tag{33}$$

[30] The boundary conditions (26) lead to a homogeneous system for the three integration constants:

$$C_1 J_n(\gamma) + C_2 I_n(\gamma) = 0 \tag{34}$$

$$C_1 J_n(\gamma) - C_2 I_n(\gamma) - \gamma^2 C_3 = 0 \tag{35}$$

$$C_1 J_n'(\gamma) - C_2 I_n'(\gamma) + \frac{n\gamma}{\bar{k}} C_3 = 0. \tag{36}$$

[31] There will be a nontrivial solution only if the determinant of this system vanishes. This condition leads to the eigenvalue equation

$$\frac{J_n'(\gamma)}{J_n(\gamma)} + \frac{I_n'(\gamma)}{I_n(\gamma)} = -\frac{2n}{\gamma\bar{k}}. \tag{37}$$

[32] For a given value of n, this equation has roots (in increasing magnitude) $\gamma_n^{(1)}, \gamma_n^{(2)}, \gamma_n^{(3)}, \ldots$.

[33] From these the critical Rayleigh number $R = \gamma^4$ is determined.

[34] The corresponding eigenvector is constituted by

$$u = \frac{J_n(\gamma r)}{J_n(\gamma)} - \frac{I_n(\gamma r)}{I_n(\gamma)} \tag{38}$$

$$\theta = \frac{1}{\gamma^2}\left[\frac{J_n(\gamma r)}{J_n(\gamma)} + \frac{I_n(\gamma r)}{I_n(\gamma)}\right] \tag{39}$$

$$\theta_w = \frac{2}{\gamma^2 r^n}. \tag{40}$$

[35] Equations (38)–(40) define the velocity and temperature only to within a constant factor. The flux closure condition (18) is trivially fulfilled if $n \neq 0$, while if $n = 0$ it follows from equation (37).

[36] In fact, if $n = 0$ one deduces from equation (37)) that the criterion for instability is independent of $\bar{k}$. This is consistent with the fact that then $\theta'(1) = 0$ so that the radial heat flux at the boundary is zero.

[37] Returning to the case of $n \neq 0$, one has the following limiting cases.

[38] Case A: conductivity of the walls much higher than the conductivity of the fluid: $\bar{k} = k/k_w \to 0$.

[39] The characteristic equation is

$$J_n(\gamma) = 0, \; n = 1, 2, 3, \ldots. \tag{41}$$

[40] Case B: conductivity of the walls much lower than the conductivity of the fluid: $\bar{k} = k/k_w \to \infty$

[41] The characteristic equation is

$$\frac{J_n'(\gamma)}{J_n(\gamma)} + \frac{I_n'(\gamma)}{I_n(\gamma)} = 0. \tag{42}$$

[42] Numerical values of the roots are presented in Table 1. It is apparent that the smallest value for R is obtained with $n = 1$ in each case. For highly conducting boundaries this value is 215.6, while for poorly conducting boundaries it is 67.95.

3.3. Vertical Circular Cylinder of Finite Height, Thermal Problem

[43] Let the cylinder have height h and define the parameter

$$h = H/2r_0. \tag{43}$$

[44] Then $h \to \infty$ gives the problem just treated while $h \to 0$ gives the Rayleigh-Bénard problem.

[45] Now three-dimensional modes are important. Thus the velocity approximation must allow for all of the components of the velocity vector **v** to be nonzero. Considering motions periodic in ϕ and satisfying the no-slip condition at the rigid boundaries $z = \pm h$, we write approximate expressions for the velocity components thus:

$$v_z = \frac{1}{4}\left(h^2 - z^2\right) u(r) \cos n\phi \tag{44}$$

$$v_r = z\left(h^2 - z^2\right) v(r) \cos n\phi \tag{45}$$

$$v_\phi = z\left(h^2 - z^2\right) w(r) \sin n\phi \tag{46}$$

for $n = 0, 1, 2, \ldots$.

[46] The radial functions u, v, w must vanish at the rigid lateral surface of the cylinder ($r = 1$). The continuity equation yields

$$\frac{1}{r}\frac{d}{dr}(rv) + \frac{n}{r} w - u = 0. \tag{47}$$

[47] A solution of this equation is given by the following functions:

$$u = \frac{J_n(kr)}{J_n(k)} - r^n \tag{48}$$

$$v = -\frac{1}{kJ_n(k)}\left[J_n'(kr) - J_n(k) r^{n+1}\right] \tag{49}$$

$$w = \frac{n}{k^2 J_n(k)}\left[\frac{1}{r} J_n(kr) - J_n(k) r^{n+1}\right], \tag{50}$$

where the parameter k satisfies the equation

$$kJ_n''(k) = (n+1)J_n'(k). \tag{51}$$

[48] An increase in k implies an increase in the number of nodes of the radial velocity.

[49] To determine the temperature, we must solve the thermal energy equation

$$\nabla^2 T = -v_z. \tag{52}$$

$$R = \frac{124\alpha^4(k^2+\alpha^2)^2}{121h^4k^2} \times \frac{2h^4(k^8+k^6-20k^4)+3h^2(4k^6-k^4-112k^2+64)+21(4k^4+k^2-104)}{72k^6+9\alpha^2k^6+2\alpha^4(k^4-2k^2-44)+\alpha^6(2k^4-k^2-64)-36k^6\alpha\frac{I_0(\alpha)}{I_1(\alpha)}}. \tag{60}$$

[50] Setting $T = f(r, z)\cos\phi$, we obtain an equation for f:

$$\frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} - \frac{n^2}{r^2}f + \frac{\partial^2 f}{\partial z^2} = -\frac{1}{4}\left[\frac{J_n(kr}{J_n(r)} - r^n\right](h^2-z^2)^2. \tag{53}$$

[51] We shall assume that the end surfaces are perfect conductors, so that the temperature disturbances vanish there. We also assume that $\partial^2 f/\partial z^2$ vanishes at the ends, so we have

$$\text{at } z = \pm h: \; f = 0, \; \frac{\partial^2 f}{\partial z^2} = 0. \tag{54}$$

[52] Hence we may choose the following approximation:

$$f(r,z) = (h^2 - z^2)(5h^2 - z^2)\theta(r). \tag{55}$$

[53] The function $\theta(r)$ is determined by inserting (55) into (53), multiplying by the part of $f(r, z)$ that depends on z, and integrating with respect to z from $-h$ to h. We then obtain

$$\theta'' + \frac{1}{r}\theta' - \left(\frac{n^2}{r^2} + \alpha^2\right)\theta = -\frac{11}{248}\left[\frac{J_n(kr)}{J_n(k)} - r^n\right], \tag{56}$$

where $\alpha^2 = \frac{153}{62h^2}$.

[54] We confine our attention to a cylinder with an ideally conducting lateral surface. We must find a solution of equation (56) that is finite at $r = 0$ and such that $\theta(1) = 0$. The solution is

$$\theta = \frac{11}{248\alpha^2(k^2+\alpha^2)}\left[\alpha^2\frac{J_n(kr)}{J_n(k)} + k^2\frac{I_n(\alpha r)}{I_n(\alpha)} - (k^2+\alpha^2)r^n\right]. \tag{57}$$

[55] The approximate formulas for v and T enable us to calculate the critical Rayleigh number using the integral relation

$$R = -\frac{\int \mathbf{v}\cdot\nabla^2\mathbf{v}\; dV}{\int v_z T \; dV}. \tag{58}$$

[56] For the mode $n = 0$ one finds that

$$R = \frac{31\alpha^2(k^2+\alpha^2)^2}{121h^4k^2} \cdot \frac{4k^4h^4 + 24k^2h^2 + 189}{4k^4 + \alpha^2k^2 + \alpha^4 - \frac{8k^2}{\alpha}\frac{I_1(\alpha)}{I_0(\alpha)}}. \tag{59}$$

[57] It should be noted that here, in contrast to the case of a layer of infinite extent, there is no horizontal wave number that can be varied to minimize the value of R.

[58] For the mode $n = 1$ one finds that (60)

[59] Equation (51) may be solved numerically. One finds that the smallest root for the case $n = 0$ is $k = 5.1366$, while for the case $n = 1$ it is $k = 2.8064$.

[60] Similar results for the mode $n = 2$ are presented by *Gershuni and Zhukhovitskii* [1976], while the expressions (59) and (60) and the similar result for $n = 2$ are plotted in their Figure 46. The plots show that as $h \to \infty$ (and in practice for $h > 5$) the critical Rayleigh number becomes independent of h and approaches the limiting value for the case of an infinite cylinder. As h decreases, the critical Rayleigh number for each mode increases monotonically. This represents the stabilizing effects of the ends. For $h \gg 1$ one has the approximation

$$R \approx R_\infty\left(1 + \frac{c}{h^2}\right), \tag{61}$$

where R_∞ is the number for an infinite cylinder and the coefficient c is positive. For example $c = 0.96$ for the case $n = 1$.

[61] The plots show that at $h_* = 0.74$ the $R(h)$ curves for $n = 0$ and $n = 1$ intersect. When $h > h_*$ instability appears in the form of the antisymmetric mode ($n = 1$), but for $h < h_*$ it is the axisymmetric mode ($n = 0$) that is the more dangerous. It is probable that for $h < 0.2$ further exchanges of the instability mode occur.

[62] *Gershuni and Zhukhovitskii* [1976] present a similar figure for the case of a thermally insulated lateral surface.

3.4. Vertical Circular Cylinder, Infinite Height, Double-Diffusive Problem

[63] We now adapt the above theory to the case of double-diffusive convection. It is assumed that the equation of state takes the form

$$\rho = \rho_0\left(1 - \beta T^* - \beta_C C^*\right), \tag{62}$$

where T^* and C^* represent the dimensional temperature and concentration. We consider the case where the temperature and concentration gradients are vertical:

$$\nabla^* T_0^* = -A\mathbf{k}, \nabla * C_0^* = -B\mathbf{k}. \tag{63}$$

[64] The dimensionless equations (2) and (3) are now replaced by the three equations

$$-\lambda \mathbf{v} = -\nabla p + \nabla^2 \mathbf{v} + (RT + SC)\mathbf{k} \tag{64}$$

$$-\lambda P_r \mathbf{v} = \nabla^2 T + \mathbf{v} \cdot \mathbf{k} \tag{65}$$

$$-\lambda P_s \mathbf{v} = \nabla^2 C + \mathbf{v} \cdot \mathbf{k}, \tag{66}$$

where the solutal Rayleigh number S (compare equation (25)) and the Schmidt number P_s are defined by

$$S = \frac{g\beta_C B r_0^4}{\nu D} \tag{67}$$

$$P_s = \frac{\nu}{D}, \tag{68}$$

where D is the diffusivity of the solute. Appending to equations (19), (20) the equation

$$C(r, \phi) = \gamma(r) \cos n\phi, \tag{69}$$

and setting λ equal to the pure imaginary number $i\omega$ (rather than zero) for the case of neutral stability, we have in place of equations (22) and (23) the three equations

$$(D + i\omega)u + R\theta + S\gamma = 0 \tag{70}$$

$$(D + i\omega P_r)\theta + u = 0 \tag{71}$$

$$(D + i\omega P_s)\gamma + u = 0. \tag{72}$$

[65] Then, eliminating θ and γ from these three equations one has

$$[(D + i\omega)(D + i\omega P_r)(D + i\omega P_s) - R(D + i\omega P_s) - S(D + i\omega P_r)]u = 0. \tag{73}$$

[66] Taking the real and imaginary parts of this equation one has

$$\left[D^2 - \omega^2(P_r + P_s + P_r P_s) - (R + S)\right]Du = 0 \tag{74}$$

$$i\omega\left\{(1 + P_r + P_s)D^2 - \omega^2 P_r P_s - P_s R - P_r S\right\}u = 0. \tag{75}$$

[67] Equations (74) and (75) must be satisfied simultaneously.

[68] Either $\omega = 0$, and so equation (75) is satisfied identically and on integration equation (74) gives

$$\left[D^2 - (R + S)\right]u = 0, \tag{76}$$

or $\omega \neq 0$ and then

$$\left[(1 + P_r + P_s)D^2 - \omega^2 P_r P_s - P_s R - P_r S\right]u = 0, \tag{77}$$

and then, eliminating ω from equations (77) and (74) one obtains, after some algebra,

$$\left[D^2 - \frac{P_s^2 R + P_r^2 S}{P_r P_s + P_r + P_s}\right]u = 0. \tag{78}$$

[69] We now consider the case where the θ satisfies the perfectly conducting boundary conditions, namely the isothermal condition $\theta = 0$ on all of the boundaries, and γ satisfies the isosolutal condition $\gamma = 0$ on the boundaries. Then any linear combination of θ and γ (including the combination $R\theta + S\gamma$) also vanishes on the boundaries. Further, one notes that equation (76) is obtained from equation (29) if R is replaced by $R + S$. One concludes that one has the same boundary value problem as before but with R replaced by $R + S$. Hence if $R = R_c$ is the criterion for the onset of convection in the thermal problem then

$$R + S = R_c \tag{79}$$

is the criterion for the case of double diffusion for the case of nonoscillatory (monotonic) convection.

[70] Similarly a comparison of equations (78) and (29) leads to the conclusion that in the case of oscillatory double-diffusive convection the criterion for the onset of convection is

$$\frac{P_s^2 R + P_r^2 S}{P_r P_s + P_r + P_s} = R_c, \tag{80}$$

subject to the constraint that the vanishing of the expression within the square brackets in equation (77) yields a real value of ω.

[71] It appears that the same argument is valid for the case of a cylinder of finite height.

[72] If one now defines Rayleigh numbers in terms of the height of water in the cylinder above the base of the well (H_f) and the temperature and concentration differences from top to bottom,

$$\mathrm{Ra}_f = \frac{g\beta H_f^3 \Delta T}{\nu\kappa} \tag{81}$$

$$\mathrm{Ra}_{fD} = \frac{g\beta_C H_f^3 \Delta C}{\nu D}, \tag{82}$$

then one concludes that the criterion for the onset of nonoscillatory convection is

$$\mathrm{Ra}_f + \mathrm{Ra}_{fD} = \frac{215.6}{r_a^4}\left(1 + 3.84 r_a^2\right), \tag{83}$$

the approximation being a good one for $r_a < 0.2$, where r_a is the radius-to-height aspect ratio. Similarly the criterion for the onset of oscillatory convection is

$$\frac{P_s^2 \mathrm{Ra}_f + P_r^2 \mathrm{Ra}_{fD}}{P_r P_s + P_r + P_s} = \frac{215.6}{r_a^4}\left(1 + 3.84 r_a^2\right). \tag{84}$$

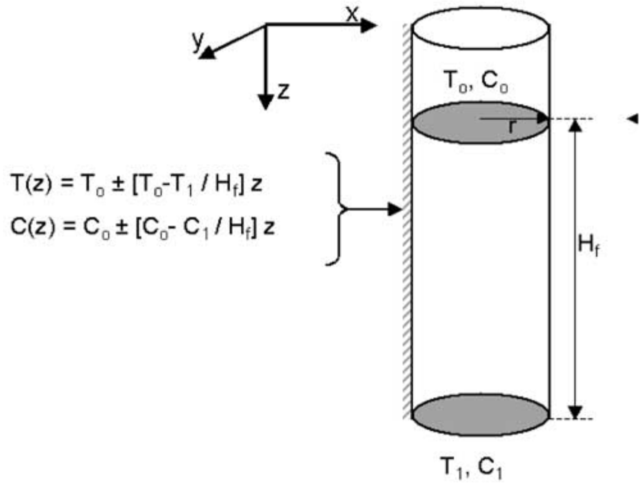

Figure 2. Conceptual model of the groundwater well and associated boundary conditions. The well is modeled as a vertical circular cylinder whose top and bottom are rigid and at constant temperature (zero perturbation temperature, the "conducting" condition) and constant concentration and whose lateral wall is impermeable and rigid and at constant temperature and constant concentration. Constant gradients are applied in both $T(z)$ and $C(z)$ boundary conditions on the lateral wall.

3.5. Applicability of the Theory to a Geothermal Well

[73] One thing can be said at the outset. The criteria expressed in equations (83) and (84) give upper bounds on the true critical Rayleigh number. The reason for this is that among the class of physically plausible thermal boundary conditions the perfect conducting condition is the most restrictive. Similarly, among the class of physically plausible hydrodynamic boundary conditions the no slip condition is the most restrictive. The more restrictive the boundary conditions in a boundary value problem such as we have been treating, the higher the eigenvalue. Hence a move to less restrictive boundary conditions lowers the eigenvalue, i.e., reduces the value of the critical Rayleigh number.

[74] More precisely, a more adequate model of a geothermal well would be a circular cylinder occupied by fluid surrounded by a sheath of porous medium of finite conductivity, say a concentric cylinder of outer radius r_m. We could model this as a conjugate conduction-convection problem. The expected net effect of this is that the Dirichlet boundary condition (boundary condition of the first kind) $\theta = 0$ on the boundary Γ would be replaced by a Robin (third kind) condition of the form $\partial\theta/\partial n + \lambda_T\theta = 0$ on Γ, where λ_T is a Biot number dependent on the conductivity ratio k_m/k and the radius ratio r_m/r_0, where k_m is the effective conductivity of the porous medium. The case $\lambda_T = \infty$ is that we have just examined. The case $\lambda_T = 0$ corresponds to an insulating wall. In the case of an infinitely tall cylinder, this change produces a reduction of the critical Rayleigh number for the thermal problem in the ratio 67.95/215.6, other things being equal. In a geothermal situation λ_T is likely to be large compared with unity, and hence the finite (rather than infinite) conductivity of the wall is not expected to substantially reduce the value of the critical Rayleigh number.

[75] Likewise, the replacement of a rigid wall by a Darcy porous medium is expected to change the hydrodynamic tangential boundary condition from first kind to third kind, of the form

$$\partial u/\partial n + \lambda_H u = 0, \tag{85}$$

containing a parameter λ_H defined by

$$\lambda_H = \frac{\alpha_{BJ} r_0}{K^{1/2}}, \tag{86}$$

where α_{BJ} is the Beavers-Joseph coefficient and K is the permeability of the porous medium. In the geothermal situation λ_H is expected to be large compared with unity, and thus the reduction in the value of the critical Rayleigh number, as a consequence of the replacement of a solid wall by a porous medium, is expected to be small.

4. Application to Groundwater Wells

[76] In this section, we apply the theoretical treatment developed above to groundwater wells using realistic data to determine whether, from a theoretical viewpoint at least, thermohaline double-diffusive convection is a plausible phenomenon. The critical elements of the analysis presented in section 3 can now be drawn out in order to apply it to groundwater wells. For the final cases considered in this section, the conceptual model of our groundwater well and associated boundary conditions are illustrated in Figure 2. The well is modeled as a vertical circular cylinder whose top and bottom are rigid and at constant temperature (zero perturbation temperature, the "conducting" condition) and constant concentration and whose lateral wall is impermeable and rigid and at constant temperature and constant concentration. Constant gradients are applied in both T(z) and C(z) boundary conditions on the lateral wall. The aspect ratio of the well is defined as the ratio of the radius of the well to the height of the fluid filled column above the well base. It is critical to note that it is the height of the water column in the well that governs the fluid circulation and not the total height of the well (i.e., the "dry" space above the water table does not contribute and should not be included in Rayleigh number analyses).

[77] From equation (83) it can be seen that the critical Rayleigh number for a well (Ra_{f0}) is a function of the well aspect ratio and is given by

$$Ra_{f0} = \frac{215.6}{r_a^4}\left(1 + 3.84 r_a^2\right). \tag{87}$$

[78] A conceptual diagram showing the critical Rayleigh numbers for a vertical well, versus the well aspect ratio ($r_a = r/H_f$) is shown in Figure 3. The restricted boundary conditions imposed by the well results in the critical Rayleigh numbers being much larger than would be the case for an infinite horizontal layer. At a glance, one can see that the critical Rayleigh numbers appear enormous. As the well aspect ratio increases, the critical Rayleigh number reduces; that is, the propensity for DDC is greatest in wells with a higher aspect ratio, namely, larger radii and shorter height.

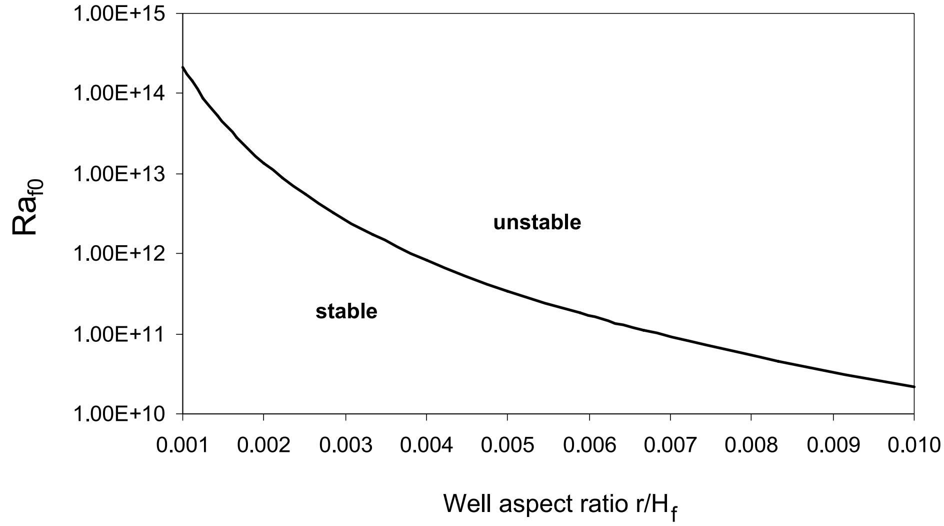

Figure 3. Critical Rayleigh number (Ra_{f0}) versus the well aspect ratio (r/H_f) for fluid in a vertical cylinder. Well aspect ratios above the line are unstable, and those below the line are stable. Increasing the well aspect ratio results in a reduction in the value of Ra_{f0} required for the onset of convection.

[79] In particular, monotonic convection will occur when the inequality given by equation (88) is satisfied, namely,

$$Ra_f + Ra_{fD} \geq Ra_{f0}, \quad (88)$$

while oscillatory convection will occur when both inequalities given by equations (89) and (90) are simultaneously satisfied,

$$\frac{P_s^2 Ra_f + P_r^2 Ra_{fD}}{P_r P_s + P_r + P_s} \geq Ra_{f0} \quad (89)$$

$$Ra_f + Ra_{fD} \leq Ra_{f0}. \quad (90)$$

[80] It is important to note that the critical Rayleigh number criterion is a function of the well aspect ratio only (i.e., radius and height of well). However, the thermal and solute Rayleigh numbers that are summed to provide the overall well Rayleigh number are a function of the height of the water column only. In this way, for each configuration of well aspect ratio and temperature/salinity gradients, a separate computation of both critical Rayleigh numbers and thermal/solute Rayleigh numbers are required (i.e., the thermal and solute Rayleigh number of the well change each time the height of the water column is changed, even if the overall aspect ratio of the well remains constant).

[81] We now consider various scenarios that may be most relevant to groundwater wells. These applications of the theory are not intended to be exhaustive. Rather, they are provided to demonstrate the plausibility of DDC phenomena in groundwater wells. In the following we consider the most common thermal regime that would occur in a groundwater well. This being where cold water transitions into warmer water at depth, we assume a geothermal gradient of 0.02°C/m (typical of groundwater wells [see *Domenico and Schwartz*, 1998]). In our demonstrations we also assume that a typical monitoring well has the dimensions of r = 0.01 m and H_f = 30 m. Keeping all variables constant we then vary ΔC (resulting in all cases being parallel to Ra_{fD}) and assess the impact of concentration gradients on the predicted convective modes. We utilize various parameters in our analyses that are shown in Table 2. Results for different thermohaline regimes (temperature and salinity gradients), well geometries and critical Rayleigh numbers, as well as actual thermal and solute Rayleigh numbers are presented in Table 3 and also plotted schematically in $Ra_f - Ra_{fD}$ parameter space (Figure 1). Examples are presented for three important cases: (1) the geothermal gradient only, (2) the boundary between monotonic and oscillatory convection, and (3) the boundary between oscillatory convection and diffusive flow.

[82] Here we attempt to answer some very fundamental questions. These include: Can the geothermal gradient alone drive thermal convection in a well in the absence of any solute gradient? In the presence of the geothermal gradient, what are the salinity distributions (both configuration and magnitude) required for two types of DDC (monotonic and oscillatory)?

[83] In the following analysis, we ignore the seasonal variations in the geothermal gradient that usually exist at the surface. Our analysis applies at depths below which the geothermal gradient may be assumed time invariant. We assume a constant geothermal gradient of 0.02°C/m and set ΔC = 0 in the following demonstration (Case a in Table 3).

Table 2. Parameters Used in All Demonstration Calculations

Parameter	Value
Thermal expansion coefficient β, K^{-1}	2×10^{-4}
Solute expansion coefficient β_c, m^3 kg^{-1}	0.755
Thermal diffusivity κ, m^2 s^{-1}	1.4×10^{-7}
Solute diffusivity D, m^2 s^{-1}	1.57×10^{-9}
Fluid kinematic viscosity ν, m^2 s^{-1}	10^{-6}
Acceleration due to gravity g, m s^{-2}	9.81
Prandtl number P_r	7.14
Schmitt number P_s	637

Table 3. Stability Analyses for the Onset of Monotonic and Oscillatory Convection in a Groundwater Well[a]

Case	ΔC, mg/L	Ra_f	Ra_{fD}	Ra^1	Ra^2	Ra_{f0}	Mode
a	0	2.27×10^{14}	–	2.27×10^{14}	–	1.75×10^{12}	M
b	1.7686	2.27×10^{14}	-2.25×10^{14}	2.75×10^{12}	–	1.75×10^{12}	M/O
c	14,188.2	2.27×10^{14}	-1.81×10^{18}	–	1.75×10^{12}	1.75×10^{12}	O/S

[a]We keep the following constant in our demonstration case: $H_f = 30$ m, $r = 0.1$ m, and $\Delta T = 0.6°C$. In the table, ΔC is the change in concentration, Ra_f is the fluid thermal Rayleigh number, Ra_{fD} is the fluid solute Rayleigh number, Ra^1 is the combined thermohaline Rayleigh number for a well ($Ra_f + Ra_{fD}$) for monotonic convection, Ra^2 is the combined thermohaline Rayleigh number for the lower bound of oscillatory convection in a well (defined as $(P_s^2 Ra_f + P_r^2 Ra_{fD})/(P_r P_s + P_r + P_s) = Ra_{f0}$), and Ra_{f0} is the critical Rayleigh number for a well. Convection modes are denoted by M, monotonic convection (unstable); O, oscillatory convection (unstable); and S, stable.

It can be seen that monotonic convection is predicted to occur as the thermal Rayleigh number is much larger than the critical Rayleigh number for this well geometry. Using the above analyses it can be easily be demonstrated that the addition of any salinity gradient in a destabilizing manner will plot in a straight line above the Ra_f axis in q1 and monotonic convection will continue to occur. These observations suggest thermal convection may be much more important in groundwater wells than is currently believed. Other analyses (not shown) suggest a wide range of well geometries are geothermally unstable.

[84] Again using our demonstration well of $H_f = 30$ m, r = 0.01 m and constant geothermal gradient of 0.02°C/m we can now change ΔC in a restoring mode (HSB, q4 of Figure 1). We ask the following question: what change in ΔC is now required to reach the boundary between monotonic-oscillatory convection and oscillatory convection? Case b shows that the boundary between the two convective modes occurs for $\Delta C = 1.7686$ mg/L. Monotonic convection is thus predicted to occur in this quadrant for $0 < \Delta C \leq 1.786$ mg/L (for our typical well configuration). The lower bound between the oscillatory-diffusive (stable) flow regimes can be obtained by imposing a concentration difference of $\Delta C = 14{,}188.2$ mg/L (in the stable salinity configuration). This results in a very large parameter space available for oscillatory convection in the range $1.7686 \leq \Delta C \leq 14{,}188.2$ mg/L. The oscillatory convective regime may be common to many groundwater systems where salinity increases with depth because of the acquisitions of dissolved solutes from water rock interactions and where temperature ubiquitously increases with depth because of the geothermal gradient. Finally, for $\Delta C \geq 14{,}188.2$ mg/L stable flow is predicted.

[85] It should be noted that the term oscillatory convection refers to the small amplitude convection at the onset of convection, and it does not imply that oscillatory flow is predicted to occur in a well. Rather, finite amplitude convection leading to the establishment of a stepwise distribution of temperature and salinity is predicted for this regime.

5. Summary and Conclusions

[86] The possibility that double-diffusive convection driven by thermohaline conditions may occur in a groundwater well has not been studied in previous literature. In this paper we formulated the appropriate stability criteria for DDC and then presented simple demonstration examples using realistic well geometries and temperature and salinity gradients that one could observe in a groundwater well. Critically, our theoretical results suggest that DDC is indeed a plausible mechanism for intrawell mixing. For the realistic well configuration used in this study, it has been shown that:

[87] 1. For a typical well geometry, the geothermal gradient alone is shown to be unstable. This can be further destabilized (monotonic convection) by the addition of salt in the destabilizing configuration, i.e., salty over fresh. This suggests that the geothermal gradient may be a significant driver of intrawell mixing – an observation that we believe has not been recognized fully in previous literature.

[88] 2. In the presence of a geothermal gradient, monotonic convection is predicted to occur for stable salinity contrasts in the range $0 < \Delta C \leq 1.7686$ mg/L (for our demonstration well configuration), i.e., fresh over salty.

[89] 3. In the presence of a geothermal gradient, the lower bound between the oscillatory-diffusive flow regimes can be reached by the addition of $\Delta C = 14{,}188.2$ mg/L in the stable configuration, i.e., fresh over salty. This results in a very large parameter space available for oscillatory convection in the range $1.7686 \leq \Delta C \leq 14{,}188.2$ mg/L.

[90] 4. In the presence of a geothermal gradient, for $\Delta C \geq 14{,}188.2$ mg/L in the stable configuration; that is, fresh over salty, stable diffusive flow is predicted.

[91] What is critical to observe in the above conclusions is that in the presence of the geothermal gradient, only extremely small to negligible salinity differences are required for transitions to occur between stable, oscillatory and monotonic modes of convection. From a theoretical viewpoint, all are practically possible. Clearly, different critical ranges of temperature and salinity gradients should be computed for varying well geometries. The above conclusions simply demonstrate that very realistic temperature and salinity gradients lead to the theoretical possibility that DDC may occur in wells typically encountered in hydrogeologic settings. One does not need to "beg the data".

[92] Some immediate extensions to this current study include: (1) field-based experimentation to support these theoretical analyses, (2) an assessment of the influence of mixed convective phenomena on DDC processes in the presence of advective flows and aquifer heterogeneity, and (3) transient extensions of these steady state concepts in order to explore the spatiotemporal patterns of behavior as well as the persistence of these phenomena once they are established.

[93] This study suggests that DDC processes and their effect on well measurements may be important in understanding and interpreting borehole data in hydrogeologic analyses. We have demonstrated theoretically that the onset of DDC may occur but it is not yet clear to what extent

DDC processes persist and therefore exist (i.e., growth and/or decay processes with time are largely unknown). The findings of this present study are therefore preliminary. In the least, they suggest from a theoretical view point that this DDC phenomenon clearly warrants greater exploration in groundwater hydrology (and in particular connection with groundwater wells) than has been undertaken to date.

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