DISPERSION IN VARIABLE-DENSITY FLOW

DISSERTATION

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By

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To Janet and Alison

for their never-ending love and support
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CHAPTER I

INTRODUCTION

The goal of this study is to develop an improved understanding of the origin and propagation of instabilities in unstable, variable-density flow systems. Unstable fluid density stratification may develop in a variety of hydrogeologic situations, such as: the migration of a dense plume of contaminants in a porous medium (Schincariol and Schwartz, 1990; Oostrom et al., 1992; Koch and Zhang, 1992), the intrusion of "freshwater" noses along permeable units in sedimentary basins (Domenico and Robins, 1985), the circulation of fluids around salt domes (Bennett and Hanor, 1987; Herbert et al., 1987), salt-leaching of soils due to irrigation (Mulqueen and Kirkham, 1972), or in shallow groundwater due to evaporation (Stein and Schwartz, 1990). Unstable flows are often influenced by buoyancy forces, which under some conditions superimpose perturbations on the evolving concentration distributions. The process of instability development causes the fluids to mix to achieve a stable density gradient.

This study looks specifically at interfacial unstable conditions, that often form in relation to contamination problems, where a more dense plume is found to be enclosed by and moving along
in a body of less dense fluid. The particular geometry of the "plume" problem, characterized by mean flow geometry perpendicular to the gravity vector and a long horizontal interface (along which the instabilities develop), differentiates this from previous work on interfacial instabilities.

The potential impact that instability development might have on contaminant transport is not well understood. Experimental studies (Schincariol and Schwartz, 1990, Oostrom et al., 1992) have shown that instabilities can play an important role in the mixing or dispersion process, at the laboratory scale. Those works, however, addressed only to a limited extent what conditions are necessary for instabilities to form, and how they are manifest in a plume geometry. Only once the mechanism of instability formation and propagation is better understood in the "laboratory" domain can one address the question of how instabilities form in natural systems, and their role in promoting contaminant mixing.

To understand the conditions under which instabilities form, and how they are manifest in a plume geometry, requires a theoretical or model based study. The experimental studies of variable-density groundwater flow by Schincariol and Schwartz (1990) provided a convenient starting point, and a set of calibration data for the model study. Unfortunately, limitations in the original image analysis techniques used by Schincariol and Schwartz (1990) only made it possible to differentiate two concentration zones from the photographic data. Although these data were useful for the purposes
of the initial study of instabilities in variable-density flow, it was apparent from visual inspection that the photographs contained much more useful information on concentration than the initial image processing was able to extract. Therefore, as part of my present study, more sophisticated image analysis techniques were developed to reinterpret the imagery from the original flow-tank experiments.

Chapter II of this thesis describes the new image analysis approach that permitted much more detailed resolution of concentration distributions within the flow tank. These refined data created a better understanding of mixed convective flow and instability development, and enabled transport parameters for the present work (dispersivity, tortuosity, bulk diffusion coefficient) to be calculated from the original experiments.

Early in the studies, it became obvious that actually creating instabilities within a model framework provided a formidable challenge. Chapter III presents the results of studies concerned with generating instabilities. It describes the conditions that lead to instabilities and how instabilities are manifest in a plume geometry, and establishes whether the classical Rayleigh stability criterion for convective flow is generally applicable to problems of interface instability.

With the fundamentals in place, it was possible in Chapter IV to address the question of whether instabilities can be expected to form in natural geologic systems. The basic approach involved a sensitivity analysis with both deterministic and probabilistic
conceptualizations of the medium to establish what hydrogeologic conditions, represented in terms of conventional transport parameters, promote the growth of instabilities in variable-density flow. The use of a probabilistic approach, for representing local scale variability in permeability, provides a realistic representation of actual media.
CHAPTER II

DEVELOPMENT OF VALIDATION DATA SETS

Many recent advances in the study of mass transport processes rely on extremely detailed sampling to map temporal and spatial variations in concentration distributions. In field-scale experiments the state-of-the-art remains with multi-level samplers. However, in the laboratory photographic/image processing provides a useful way to accurately estimate concentration distributions at a very fine scale. This method provides an essentially continuous distribution of sampling points, over a transparent wall of a flow tank, with two to three orders of magnitude more sampling points than would be available with conventional sampling/analysis methods. Furthermore, the procedure is non-intrusive and does not disturb the flow field.

The goal of this portion of the study was to develop new image processing procedures and software that would allow the generation of detailed concentration distributions from photographic data. The photographic data were originally collected as part of a study on variable-density groundwater flow (Schincariol and Schwartz, 1990). Black and white photographs recorded the spreading of dense plumes within a Flexiglas flow tank. The first attempt to interpret the
concentration distributions (Schincariol and Schwartz, 1990) only differentiated two gray levels or groups of levels within the tracer mass. These zones represented a high concentration zone, 50-100% of the source concentration and second, a low-concentration zone, 10-25% of the source concentration. Although useful for preliminary analysis, it was apparent from visual inspection that the photographs contained much more useful information on concentration than the initial processing was able to extract.

This chapter describes a more sophisticated approach that was developed to reinterpret the imagery from the concentration distributions of the original flow-tank experiments (Schincariol and Schwartz, 1990). Most of the work involved development of image processing software to convert output from an Elkornix 78/99 digital scanning system into concentration maps. These procedures and programs allowed the correction of much of the lighting nonuniformity that plagued the preliminary effort, and permitted more detailed resolution of concentration distributions within the flow tank. For experiments with heterogeneous media, the computer processing is complicated by the need to account for different sizes of glass beads, and thus differing dye thicknesses along the tank walls. Experience shows that on-screen interactive processing facilitates the interpretation of the large data base of information that comes from the analysis.
Experimental Method

The original flow visualization experiments were conducted in a Plexiglas flow tank filled with porous media consisting of various sizes of industrial glass beads. Details of the experimental method are given in Schincariol and Schwartz (1990). In the experiments, a dense NaCl solution was introduced into the middle of a less dense fluid, and the subsequent pattern of mixing was monitored photographically.

The dense fluid is marked with a colored dye to differentiate the plume visually from the ambient porewater. The tracer is Rhodamine WT liquid (Crompton and Knowles Corporation, Charlotte, North Carolina), which is nonabsorbing, nondegrading, relatively inert, and mostly nonreactive with NaCl. Schincariol (1989) discusses pertinent literature and testing to demonstrate the suitability of the tracer. A solution of 500 mg/L Rhodamine WT liquid in water served as the carrier for various concentrations of solute.

Control of room lighting is important when a photograph is used for image analysis. Although the image processing techniques discussed in the following sections can correct for spatial and temporal lighting nonuniformity, errors in estimating concentration are minimized and the ability to differentiate concentrations are maximized if lighting is controlled. Lighting uniformity can be determined by placing strips of a constant optical density or gray level across the area to be photographed. Eighteen percent gray
cards commonly are available for this purpose. During image processing these reference points on the photographic negative provide the basis for correcting for variability in the lighting. Other problems can be reduced through appropriate care when the photographs are taken. For example, to eliminate reflections of the camera or other peripheral equipment on the flow tank walls a black curtain or sheet of black felt can be placed in front of the tank. Photographs are taken through a slit or hole in the curtain.

To correct for small differences in lighting, exposure or film development, and to compute necessary standard curves, a gray scale must be present in every photograph. The computation of the optical density standard curves, which allow all images to be brought to constant lighting conditions, and the conversion of a given optical density value to a concentration of solute or dye, are discussed in the following sections.

Image Analysis Procedure

Photographs of the spreading tracer from the original experiments provided the black and white negatives used for the analyses. The negatives were scanned on a Eikonix 78/99 digital scanning system at a resolution of 1024 by 1024 by 12 bits. The image analysis system is comprised of a Digital Equipment Corporation Microvax II computer and a Gould IP9527 image processor. It transforms the scanned images, whose pixels represent dye intensity,
into images whose pixels represent solute concentration. The image analysis process involves eight steps: (1) scanning the negative on digital scanning system, (2) computing an optical density standard curve, (3) rotating and transforming the image to standard sized matrix (800x555), (4) median smoothing on a 3x3 window, (5) subtraction of a background image, (6) median smoothing on a 3x3 window, (7) computing an optical density versus concentration standard curve, and (8) using a standard curve to convert optical density values on scanned images to concentration. These eight steps are discussed in detail in the following sections.

Scanning negatives

The first step in the image analysis procedure is to scan the black and white negatives. When the negatives are scanned, the incident light on the negative is first adjusted to maximize the variation in intensity over the zone of interest. For example, putting too much light through a negative may wash out the lighter gray tones and the loss of detail may render these areas useless for image processing. If detail is required in the darker areas of the negative, the loss of detail in the lighter areas may be acceptable.

When negatives are scanned at 12 bits, the light intensities across the negative are divided into 4096 different gray levels from darkest to lightest. The scanner is actually measuring transmittance. Transmittance (T) is the quantity that defines how well light is transmitted through a photographic negative, and is
defined mathematically as (Stimson, 1974):

\[ T = \frac{I_i}{I_f} \]  

(1)

where \( I_i \) is the transmitted light or luminous intensity, and \( I_f \) is the incident luminous intensity. Optical density (D) is related to transmittance by (Stimson, 1974):

\[ D = \log_{10} \left( \frac{1}{T} \right) \]  

(2)

Scanning at this resolution is necessary because only a small number of the 4096 gray levels may represent the plume. In general, the number of concentration zones that can be differentiated in the plume depends directly on the number of gray levels.

A monochrome negative can only record a certain range of luminance in a particular scene. It is the luminance of a surface that determines its brightness. This range is much less than the range that the human eye can register (Williamson and Cummins, 1983). The light absorptive property of a particular region of a photographic negative can be described by its optical density. The greater the density the less light is transmitted through the negative. The characteristic curve of the film (Figure 1) describes how the optical density increases with exposure. With exposure \( (E_p) \) defined mathematically as (Williamson and Cummins, 1983):

\[ E_p = c \cdot E_v \]  

(3)
Figure 1. Example of a characteristic curve for monochrome film. Over the central region (B to C) the optical density increases in proportion to the logarithm of exposure.
where \( t \) is the exposure time and illuminance \( (E_v) \) is defined as:

\[
E_v = \frac{\text{incident luminous flux}}{\text{surface area receiving it}}
\]

(4)

The unit for expressing illuminance is the lumen per meter squared \((\text{lm/m}^2)\), which is sometimes called the "lux". Over the linear portion of the characteristic curve (B to C) density increases in proportion to the logarithm of exposure (Williamson and Cummins, 1983). It is over this linear portion of the curve that one can develop equations that equate optical densities to dye concentrations. Because the exposure time is constant for a given image of a plume, it is variations in illuminance that control the exposure and, thus, the optical density of that particular region of the negative. Detail is lost in regions such as the toe and knee portions of the curve (Figure 1) as optical density varies only slightly for large differences in exposure (Williamson and Cummins, 1983). In the image analysis of a plume, this behavior results in a loss of the ability to predict accurately concentrations in the very dilute (high illuminance or exposure) portions of the plume. In regions of low illuminance (toe of curve), the maximum dye concentration, typically the source concentration, can be chosen to fall on the linear portion of the curve. Thus, concentrations can be accurately predicted up to the maximum concentration of the tracer in the experiment.
Computation of optical density standard curve

Values of transmittance are recorded, from the negative, during the scanning process. Because small differences in lighting, exposure or film development always occur and cause the optical density to vary from photograph to photograph, a gray scale must be present in each negative or image. Based on this gray scale, one can create a transmittance versus optical density standard curve (Figure 2) for every image. In this way, transmittance values for each pixel are standardized among the collection of photographs. The values of transmittance in Figure 2 are not actual transmittance values as defined by equation 1. The Eikonix digital scanner actually records a binary number in the range of 0 to 4095, which is proportional to the actual transmittance, and is referred to as "binary transmittance" in Figure 2.

The work presented here utilized a Kodak gray scale, which has 20 bars each 0.10 density increments apart from a nominal white of 0.0 optical density to a practical printing black of 1.90 density. The optical density standard curve is formed by computing the average transmittance value for each bar and plotting this value against the known optical density value (Figure 2). This procedure is repeated for each image so that the transmittance values for pixels within the image can be converted to optical density units. In this way, each image has its own calibration curve from which values of optical density can be calculated from the transmittance values.
Considerable variability can exist in the standard curves of transmittance versus optical density in a series of photographs. For example, the three curves shown in Figures 2 and 3 illustrate typical variation in standard curves from three photographs at 0, 54, and 72 hours for experiments with 500 mg/L Rhodamine WT (Figure 2) and with 5000 mg/L NaCl (in a solution of 500 mg/L Rhodamine WT, Figure 3). In these cases, the differences among the curves result from changes in lighting or film development. Although such differences are difficult to see on the negative with the naked eye, they must be accounted for in the image analysis process if a comparison study is to be made among several different images.

Optical density provides a useful characterization of the light absorptive property of a filter or a portion of a photographic negative (Williamson and Cummins, 1983). It has been noted that the greater the optical density the less light is transmitted. In addition, optical densities have an important additive property. Once the pixel values are in terms of optical density any background subtraction can be done directly as optical densities are additive.

Ultimately, it is the corrected optical density values for the plume that are correlatable with concentration. In other words, the optical density of a filter composed of dye is proportional to the concentration of the dye (Williamson and Cummins, 1983). This relationship requires the development of an optical density - concentration standard curve, which is the aim of the processing exercise.
Figure 2. Binary transmittance vs. optical density standard curves for three images (500 mg/L Rhodamine WT at 0, 54, and 72 hours).

Figure 3. Binary transmittance vs. optical density standard curves for three images (5000 mg/L Rhodamine WT at 0, 54, and 72 hours.)
Rotation and transformation of the image

The scanned negative may contain considerable unwanted information, such as the flow tank or peripheral equipment. A useful step in the processing involves "trimming" the computed optical density data to provide only that portion of the image over which the concentration distribution is determined. The resulting matrix of pixel values is available for other operations such as background subtraction or contouring.

In this application, four fiducial points were marked on the image with a tracing program. These represent the four corners of the flow tank. These fiducial points should be clearly marked on the tank or photographic subject so that the corresponding points can be identified on each of the negatives. A software program (Cornhill et al., 1990) then rotates and translates the image to its correct orientation (in this case horizontal) and maintains a consistent size. This step corrects for any errors introduced while scanning the negative or camera movement from one photograph to another. For the marked area defined here the basic data set is a 800 by 555 pixel matrix. Therefore, for the experimental tank, individual concentration estimates are available for square areas approximately 1.3 by 1.3 mm in size over the entire area of the tank.

Median smoothing

Median smoothing is performed on two occasions in the image processing. Median smoothing takes the neighboring pixels around a
given pixel, sorts all nine values in this 3 by 3 window, and then places the median value in this pixel. In this way no value is placed in the window that was not an actual value. The smoothing calculation is performed for every pixel in the matrix. The effect of median smoothing is to reduce much of the noise from grain size in the photographic emulsion and bead size without moving any concentration boundaries.

Background subtraction

As mentioned previously, the images originally suffered from uneven lighting. The top of the tank/plume was closer to the ceiling lights and this resulted in a lighting drop-off. One of the best ways to adjust for this falloff was to subtract an appropriate background image. The background image was the flow tank containing only the porous medium and water. As this image suffered from the same falloff, subtracting an image of a tank with a plume in it from a “blank” tank results in an image that contains only a plume.

To test the effectiveness of the background subtraction an image with a known concentration was examined. The particular example involved a tank filled totally with 500 mg/L Rhodamine WT dye, the concentration used as the source fluid in all runs. Figure 4, a nine pixel wide vertical transect, illustrates the problem with lighting “falloff”. Optical density values decrease from approximately 250 to 175 from the top to the bottom of the tank. Figure 5 illustrates the same transect after correction using the background subtraction.
Figure 4. Optical density values along a vertical transect taken from the uncorrected image.

Figure 5. Optical density values along the same vertical transect in Fig. 4 after background subtraction.
Although nonuniformity is not totally eliminated, the nonuniform lighting is reduced by approximately a factor of three (optical density range approximately 145 to 170).

Computations of optical density-concentration standard curve

In order to equate a given value of optical density with a concentration of solute or dye, calibration runs were made in which predetermined concentrations of the dye (Rhodamine WT) were photographed and image processed. The known concentrations of dye were injected as a slug source. Minimal dispersion of the slug occurred due to the very low dispersivity of the medium. The longitudinal and transverse dispersivities were determined to be $3.0 \times 10^{-4}$ m and 0.0 m, respectively, from numerical simulations of tracer experiments, which are discussed in chapter III and Appendix A. Diffusion was minimal as only a few hours elapsed between slug injection and the photographing of the slug. Furthermore, only a small zone in the center of the slug was equated with the source concentration.

Theoretically, if the dye is acting as a true filter, the optical density of the dye is proportional to concentration. As the concentration of the colorant molecules in the solution is increased, there are more molecules to provide selective absorption. If $T$ is the transmittance at a given wavelength for a given concentration, increasing the concentration $N$-fold yields a transmittance of $T^N$ (Williamson and Cummins, 1983). This relationship is known as Beer's
law. Expressing Beer's law in terms of optical density provides a linear relationship between optical density and concentration. This linear relationship is evident for the experimental data when the average optical density of a region of dye of known concentration is plotted against concentration (Figure 6). The best-fit line through the points has an $R^2$ value of 0.976. In practice, a quadratic function with a slightly higher $R^2$ value of 0.982 (Figure 6) was used. This function resulted in less error at the low end of the spectrum. At the low end of the concentration range the gray level of the dye is approaching the gray level of the light green glass beads and this effect causes some scatter in the data. Figure 6 shows that certain concentrations have multiple points. For these concentrations separate images were used as the zone of known concentration travelled through the tank. The differences may represent the slight lighting variations that were not completely corrected by background subtraction.

Using the function calculated in Figure 6, the optical density value for each pixel can be converted to a concentration value for the dye in each image. The concentration of NaCl then can be scaled from the dye concentrations.

To estimate the error in computed concentrations that would encompass most of the errors present in the image analysis process, the optical density-concentration function was used to predict values of known concentration. As Table 1 shows, the greatest error is at low concentrations where there is low level noise. Due to the
Figure 6. Linear and quadratic fit through optical density values of various known concentrations of Rhodamine WT dye.
large amount of noise at the low end, all concentrations below 50 mg/L Rhodamine WT (10% source concentration) were set to background for the "color shade" images that will be shown in the next section. Overall a maximum error of approximately 7% resulted from the image processing the data.

Image Processing of Heterogeneous Media

The image processing is much more complicated when more than one size of glass beads are present in the image. In the experiments with a lenticular medium, four different sizes of glass beads were used to obtain the variable hydraulic conductivity field (Table 2). Size #13 was not used in the lenticular medium experiments, although it was used in the calibration runs to be discussed later.

The optical density of a filter (dye) is proportional to its thickness (Williamson and Cummins, 1983). Thus, if a thicker layer of dye is present along the wall of the tank due to a larger pore size, the optical density of the dye will be different than for a small pore, concentration being the same. Effectively, the larger the bead or pore size the darker the dye or the greater the optical density.

The luminance of a colored light source (or colored object illuminated by a standard source of white light) is calculated from its spectral power distribution. When light passes through a filter the spectral power distribution of the incident light is altered as
Table 1. Errors in Predicted Concentration Values

<table>
<thead>
<tr>
<th>Concentration Rhodamine WT (mg/L)</th>
<th>Optical Density</th>
<th>Predicted Concentration (mg/L)</th>
<th>Percent Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>242.115</td>
<td>27.95</td>
<td>11.8</td>
</tr>
<tr>
<td>50</td>
<td>236.657</td>
<td>48.54</td>
<td>2.9</td>
</tr>
<tr>
<td>100</td>
<td>226.181</td>
<td>93.15</td>
<td>6.9</td>
</tr>
<tr>
<td>150</td>
<td>216.292</td>
<td>141.39</td>
<td>5.7</td>
</tr>
<tr>
<td>200</td>
<td>206.992</td>
<td>192.20</td>
<td>3.9</td>
</tr>
<tr>
<td>250</td>
<td>198.279</td>
<td>244.58</td>
<td>2.2</td>
</tr>
<tr>
<td>300</td>
<td>190.154</td>
<td>297.59</td>
<td>0.8</td>
</tr>
<tr>
<td>350</td>
<td>182.617</td>
<td>350.36</td>
<td>0.1</td>
</tr>
<tr>
<td>400</td>
<td>175.667</td>
<td>402.08</td>
<td>0.5</td>
</tr>
<tr>
<td>450</td>
<td>169.305</td>
<td>452.01</td>
<td>0.5</td>
</tr>
<tr>
<td>500</td>
<td>163.532</td>
<td>499.46</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 2. Porous Medium Data

<table>
<thead>
<tr>
<th>Manufacturer's Bead Size</th>
<th>Median Grain Size $d_{50}$ (mm)</th>
<th>Hydraulic Conductivity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.650</td>
<td>$3.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>5</td>
<td>0.310</td>
<td>$5.6 \times 10^{-2}$</td>
</tr>
<tr>
<td>7</td>
<td>0.210</td>
<td>$2.2 \times 10^{-2}$</td>
</tr>
<tr>
<td>10</td>
<td>0.150</td>
<td>$1.2 \times 10^{-3}$</td>
</tr>
<tr>
<td>13</td>
<td>0.085</td>
<td>$1.9 \times 10^{-3}$</td>
</tr>
</tbody>
</table>
the filter (dye) absorbs differing amounts of power across the spectrum. The spectral transmittance curve of the filter specifies the fraction of incident light that is transmitted for each wavelength across the spectrum. In the particular experimental setup examined here, light could not penetrate the tank due to the thickness of the porous medium. The incident light shining on the surface of the tank is reflected by the layer of dye and porous medium that is present along the wall, and a few grain diameters inward. The altering of the spectral power distribution and thus the luminance of the incident light is characterized by the "objects" spectral reflectance curve in an analogous manner to the spectral transmittance curve for a filter. Therefore, the thickness of the layer of dye and its reflectance characteristics can be considered analogous to thickness characteristics of a filter. In effect, increasing the thickness of the dye layer allows more colorant molecules to provide selective absorption and reflection.

To take these effects into account an additional group of experiments using various sizes of glass beads placed in layers were conducted with the original flow tank. Different concentrations of Rhodamine WT were injected into the tank and the photographs taken and processed as described in the previous section. In these experiments a line source was applied to the entire inflow end of the tank. Figure 7 shows a plot, for the various bead sizes listed in Table 2, of optical density versus concentration. This plot shows clearly the effect of bead size on optical density. Thus, in
Figure 7. Optical density vs. concentration curves using known Rhodamine WT concentrations in various bead sizes.
heterogeneous experiments, a correction is necessary to avoid large errors in the estimated concentration distribution. It should be noted that in Figure 7, and the other standard curves, one is plotting concentration of the dye versus optical density of the film. Because the film is a negative image the greater the optical density of the dye the lower the optical density on the negative.

These experiments also showed the effect of the color of the glass beads on the optical density of the dye. Several bead sizes (0.650 mm, 0.310 mm and 0.150 mm) were represented by multiple layers in the tank. The two lowermost curves in Figure 7 are for the 0.650 mm (#3-Table 2) bead size. The curves are different because a different bag of beads was used for each layer. The greenish color of the glass beads sometimes varies slightly from bag to bag and this affects the optical density. The two curves for the 0.310 mm (#5) bead size also represent beads from different bags but these had a much smaller color difference than the #3 beads. The two curves for the 0.150 mm (#10) glass beads are nearly identical as they represent two layers (in different regions of the flow tank) that came from the same bag. These color variations can be eliminated as long as optical density versus concentration standard curves are constructed for each porous medium setup. This is discussed in detail in the following sections.

The complicating effect of color variation is not corrected by subtracting the optical density of a "blank tank" as was the case with uneven lighting. The problem is more complicated because the
laws of subtractive color mixing come into play. However, one can utilize the main principles to interpret the particular optical phenomena associated with this work. As discussed previously, the luminance of the glass beads in the "blank tank" image is determined from the spectral power distribution of the light leaving the surfaces of the glass beads. The light green color that is seen, and the resulting luminance recorded on the film, was produced from the interaction of the "white light" in the laboratory with the glass beads. When the Rhodamine WT dye is present within the pore spaces of the beads, the dye colorant molecules selectively absorb certain wavelengths of the incident "white" light and reflects other wavelengths. Therefore, the spectral power distribution of the light hitting the glass beads is altered by the spectral transmittance curve of the dye, and is no longer the "white" light that determined the luminance of the beads in the "background image". The color mixing and changes to the spectral power distribution of the incident light, due to the spectral reflectance/transmittance of the dye and glass beads, is very complicated. The effects of grain size and color on the optical density of the plume should be mostly eliminated by calculating a separate optical density versus concentration standard curve for each region of the porous medium that has a different grain size or "color". In addition, as the spectral power distribution of the incident light affects the luminance, one should try to always maintain a spectrally consistent light source. For example, one should prevent sunlight from entering the room.
Sunlight would alter the incident spectral power distribution by providing a blend of, for example, fluorescent light and sunlight during the day, and fluorescent light at night.

To take into account the differences in grain size a mathematical relationship to correct for varying bead size was developed. From Figure 7 the functional relationship can be expected to take the form of equation (5) where the dye concentration \(c\) and the bead size \(\beta\) are the independent variables and the optical density \(D\) is the dependent variable.

\[
D = b_0 + b_1 \cdot c + b_2 \cdot \beta + b_3 \cdot c \cdot \beta + b_4 \cdot c^2 + b_5 \cdot \beta^2
\] (5)

Using a statistical analysis software package (Statistical Analysis System, SAS Institute Inc., Cary, N.C. 27512) the coefficients \(b_k\) were determined to have the following values:

\[
D = 245.9 - 0.1678 \cdot c - 121.1 \cdot \beta - 0.1105 \cdot c \cdot \beta + 0.00017 \cdot c^2 + 112.2 \cdot \beta^2
\] (6)

When equation (6) is used to predict the optical density values from the concentration and grain size data, the root mean square error \(R^2\) is 0.985. When the lenticular medium images are processed, each lens or layer must be identified on the image and the applicable correction applied. This step greatly increases the computational difficulty and execution times. Once a template is created delineating the various zones, the inverse of equation 6 can be applied where the concentration is predicted from the optical density value and the grain size. This inverse equation (7) has a slightly
smaller $R^2$ value of 0.956. In equation 7 the optical density ($D$) and the grain size ($\beta$) are the independent variables, whereas the concentration ($c$) is the dependent variable.

$$c=5531-38.31\cdot D-4525\cdot \beta+14.23\cdot D\cdot \beta+0.3648\cdot D^2+1645\cdot \beta^2$$  (7)

In the previous example a single equation was developed that takes into effect the bead size and was fairly successful with an $R^2$ of 0.936. This equation, though, averaged in the effect of the slight color variation in the glass beads. Alternatively, as discussed previously, a separate optical density versus concentration standard curve could be developed for each bead size/color.

Examples of Processed Experimental Data

The image processing of an negative produces a matrix of concentration values, in this case an 800x555 matrix. Contour plots or color shade plots can then be made on the matrix.

Color shade maps provide a good way to view the concentration distribution within a plume and to recognize various plume structures. Figure 8 shows a broad overview of the entire range of concentrations observed in a 1000 mg/L NaCl plume where density effects become noticeable. At this density, though, the instabilities (lobe-shaped protuberances) only slightly perturb the concentration distribution. Notice as well at the snout of the plume, and around the edges, the small effect of mixing due to dispersion (Figure 8). With an initial concentration of 2000 mg/L
(Figure 9) the density effects are much more noticeable. The plume sank noticeably, is more dispersed, and the instabilities are narrower than those in the 1000 mg/L source plume. The small zones of variable concentration visible at the source inlet in Figures 8 and 9, which should be at source concentration, are due to the progressive staining of the glass beads over several runs. This staining or residue is limited to the first few centimeters of the porous medium adjacent to the injection chamber, and affects the image processing when a stained "blank tank" image is used for background subtraction.

The image processing approach also lets one examine specific ranges in concentration in more detail. For example, consider the 5000 mg/L NaCl case where the low concentration end (from 500 to 2500 mg/L) is examined in detail in Figure 10, and the high concentration end (from 2500 to 5000 mg/L) is examined in Figure 11. Effectively one is just adjusting the concentration ranges of the legend color maps. This allows one to highlight certain concentration ranges. For example, the internal instabilities within the low concentration zone (Figure 10), are wider and more dispersed compared to those within the high concentration zone (Figure 11), which are very narrow and nearly vertical. Figure 11 also shows clearly how the highest concentrations of solute occur in the lower portions of the plume.

With the concentrations now stored in digital form, it is a simple matter to construct a variety of derivative plots from the data. For example, concentration versus distance plots can be made
Figure 8. Color shade map for a 1000 mg/L NaCl source plume, at 72 hours, in a homogeneous medium.

Figure 9. Color shade map for a 2000 mg/L NaCl source plume, at 72 hours, in a homogeneous medium.
Figure 10. Color shade map (detail- low concentration end) for a 5000 mg/L NaCl source plume, at 54 hours, in a homogeneous medium.

Figure 11. Color shade map (detail- high concentration end) for a 5000 mg/L NaCl source plume, at 54 hours, in a homogeneous medium.
at various locations across the plume in the transverse direction and along the longitudinal axis of the plume. Figures 12 and 13 are transverse and longitudinal plots, at selected transects, from a 500 mg/L Rhodamine WT plume, in a homogeneous medium, at 54 hours (Schincariol and Schwartz, 1990). The horizontal axis shows the position along a 3 pixel wide transect where x=0, y=0 is defined as the lower left corner of the tank, and the horizontal and vertical orientations are defined as the x and y directions, respectively. Figure 13 shows the degree of scatter or error that exists at the high concentration end. The first portion of the plot, along the centerline of the plume from approximately 200 to 380 mm, should be equal to the source concentration of 500 mg/L. This scatter is due to the nonlinearity of the optical density versus concentration curve (Figure 6) near the 400 to 500 mg/L area. In this area small differences in light intensity result in large differences in concentration. Thus the degree of error that was seen for the low concentration end (Table 1) is also present, although due to different reasons, in the high concentration end. It is also thought that some of the scatter or errors seen here are due to the portion of lighting nonuniformities that were not eliminated with background subtraction (Figure 5).
Figure 12. Plot of concentration vs. distance for a vertical (x=249 mm) transect (transverse) through a 500 mg/L Rhodamine WT plume at 54 hours.

Figure 13. Plot of concentration vs. distance for a horizontal (centerline) transect through a 500 mg/L Rhodamine WT plume at 54 hours.
CHAPTER III

THE GENERATION OF INSTABILITIES IN VARIABLE-DENSITY FLOW

Mixed convective flows, where both free and forced convection operate to control solute concentrations (Gebhart et al., 1988), may become unstable under certain conditions. Instabilities which form due to variability in density or viscosity superimpose perturbations on the evolving concentration distributions. The stability of a groundwater flow system is reflected by how flow responds to small perturbations in variables such as pressure, concentration, or temperature. Flow is considered stable if, when the system is disturbed slightly from initial condition, the variation in the movement of the system remains similar to the initial perturbation or decays in time. Flow is considered unstable if the perturbation grows or continues to displace the position of the system from its initial state (Harle, 1981). An unstable system will attempt to return to stability through fluid mixing that eventually produces stable density or viscosity gradients.

Researchers historically have classified unstable flows into broad categories. For example, instabilities or convective motions within a whole bounded region or layer have been called Benard, Rayleigh, or thermal instabilities (Gebhart et al., 1988).
Variations on this theoretical problem have been studied for nearly a century (e.g., Raleigh, 1916; Horton and Rogers, 1945; Lapwood, 1948; Pratts, 1966; Combaronous and Bories, 1975). Another classical instability problem relates to the stability of fluid-fluid interfaces along which fingers may develop to produce a corrugated interface. The most important early work on this problem was done by Saffman and Taylor (1958), who considered the stability of the interface between immiscible fluids moving vertically through a porous medium. These concepts of interfacial instabilities were generalized to miscible systems by Wooding (1962) who examined the effects of longitudinal dispersion across the interface of two miscible fluids.

Interfacial instabilities have been studied recently in relation to contamination problems where a more dense plume is found to be enclosed by and moving along in a body of less dense fluid (Schincariol and Schwartz, 1990; Oostrom et al., 1992; Koch and Zhang, 1992; Schincarioi et al., 1993). They are manifest by a complex concentration distribution that develops as lobes of dense fluid move downward from the plume, while less dense fluid moves upward into the plume to balance the denser fluid movement (Figures 8 to 11). Although initially developed as an interface instability, these convolutions lead to similar motions within the plume. To date only List (1965) has analyzed theoretically interfacial instabilities for miscible fluids; however, by virtue of his analytical approach and need for simplifying assumptions, his analysis is limited in its
practical applicability.

The geometry of the "plume" problem, with mean flow generally perpendicular to the gravity vector and a long horizontal interface, differentiates this from previous work on interfacial instabilities. For example, Wooding (1962, 1969), Bachmat and Elrick (1970), and Bues and Aachib (1991) studied the effects of density and viscosity contrasts on miscible vertical displacements (flow parallel to the gravity vector). The problem of fingering in secondary petroleum recovery, which has been studied extensively, involves instabilities that develop along a moving vertical interface. It is this relatively limited understanding, concerning the formation of instabilities in a plume geometry, that is the motivation for this theoretical study. The specific objectives of this chapter are first to present an approach for generating instabilities within a numerical modeling framework, second to describe the conditions that lead to instabilities and how these instabilities are manifest in a plume geometry, and third to establish whether the classical Rayleigh stability criterion for convective flow is generally applicable to problems of interface instability.

Perturbing Functions and the Concept of Critical Wavelength

Both experimental (e.g., Bues and Aachib, 1991; Schincariol and Schwartz, 1991; Oostrom et al., 1992; Schincariol et al., 1993) and numerical modeling studies (Koch and Zhang, 1992) have illustrated
how unstable flows may result in complex patterns of mass spreading in variable-density systems. However, questions remain concerning the relationship between how the system is perturbed, and whether instabilities form and grow. This result is not surprising in the experiments given that the system is self-perturbing. That is, if conditions are appropriate, instabilities will simply develop in the experiment as the dense plume is transported in the less dense ambient flow. Essentially, in flow through a natural porous medium, interfacial disturbances are continuously generated due to the heterogeneities of the medium (Hoissia and Wheeler, 1990). These random perturbations to flow occur over many scales, from slight differences in pore geometry to larger heterogeneities on the scale of the problem under consideration, and are sufficient to generate instabilities.

List’s (1965) theoretical analysis, unlike the experiments, provides useful information about the relationship between the instabilities that form and the nature of the perturbation. The reason is that the spectrum of mathematical functions representing the perturbations in the shape of the interface and velocity are formally defined as part of the analysis. Mathematically these perturbations are created through the superposition of spatially oscillatory terms, which in List’s case have a sinusoidal form. In this representation of the disturbance, if any one of these Fourier modes is unstable, the disturbance will grow (Phillips, 1991). List’s (1965) work provides important physical insight about critical
features of the perturbing function. Of particular importance is the wavelength of the disturbance along the fluid-fluid or plume interface. In addition, List's theoretical analysis shows that not all wavelengths in a perturbing function are unstable for a given system. Thus, perturbations with a wavelength greater than some "critical wavelength" grow, whereas those below decay. An analogous concept, based on the periodicity of instabilities along the interface, also applies to fingering in immiscible displacement.

Marle (1981) looked at a simple case of immiscible flow that illustrated the importance of a critical wavelength. Along the vertical interface between two immiscible fluids, capillary forces tend to equalize the saturations in a displacement front, and may suppress the formation of fingers before they have time to grow. If it is assumed that instability creates fingers with a regular spatial periodicity, the stabilizing effect of the capillarity will depend on the wavelength of the fingers. The smaller the wavelength, the greater the stabilizing effect of capillarity. At a certain wavelength, deemed the critical wavelength, the fingers or perturbations will grow and the displacement will be unstable. In geologically relevant situations, it will be the heterogeneity of the porous media, from the pore scale to the reservoir scale, that will control the perturbations. Here the maximum wavelength should be somewhat similar to the dimensions of the reservoir (Marle, 1981).

The concept of a critical wavelength requires modification for application to miscible fluid systems. With miscible fluids,
dispersion tends to enhance the stability of a displacement and is comparable to the effects of capillarity for immiscible fluids. The shorter the wavelength, the more effective dispersion is at smoothing out or eliminating the fingers before they have a chance to grow. The existence of a mixing zone, where the viscosity and density of the fluid varies progressively from that of the displacing fluid to that of the displaced fluid, diminishes the principal cause of the instability, namely differences in fluid properties (Marle, 1981).

In approaching this problem analytically, List (1965) had to make many assumptions including (1) flow is steady, (2) the rate of growth of the mixing layer or dispersion zone is very small over some length, so the problem will be investigated for a zone where the sides of the mixing zone are parallel, and (3) diffusion is negligible, so that the solution is valid only at large velocities. With these assumptions List (1965) presents a local theory, assessing the stability of an interface over a length where the dispersion zone is assumed not to widen. His analysis cannot address, for example, the two-dimensional character of any instabilities that are generated, the problem of evaluating how an arbitrary disturbance at x=0 decays or grows as it is swept downstream, or how instabilities behave as a function of transport, where the zone of dispersion significantly increases.

In spite of the geometric simplifications and approximations that are typically required for analytical analyses of stability, the results, at least qualitatively, seem more or less correct (Marle,
1981). However, the general applicability of several conclusions drawn by List (1965) need to be evaluated. Thanks to powerful numerical-computational tools, this study is able to further evaluate the following aspects: (1) horizontal two-dimensional flow in a saturated porous medium with denser fluid on top are always unstable, although instability may not be manifest because the perturbing waves are below the critical wavelength, (2) longer perturbing wavelengths are more unstable, and (3) an increase in density contrast increases the spectrum of unstable wavelengths and increases the growth rate of the instabilities.

Modeling Methodology

Several numerical codes exist that solve the problem of flow and transport in variable-density systems. Here, a finite-element code (Vapour?), originally developed by Mendoza and Frind (1990a) to simulate the transport of dense vapors in the unsaturated zone, is utilized. Because the processes of density-dependent mass transport in the unsaturated and saturated zones are similar, only minor modifications to the code were required for the variable-density groundwater flow problem. The code uses triangular elements with linear basis and weighting functions, and efficient iterative, preconditioned conjugate gradient and orthogonal minimization techniques for solving the matrix equations (Mendoza et al., 1992). The solver efficiency was an important consideration in choosing this
code due to the large size of the grids, typically involving 170,000 elements. Simulations were performed on a CRAY Y-MP8/864, a HP 9000/750, and a DEC 5400, with run times averaging 25 to 50 CPU hours @ 9.2 Mflops (CRAY operating in scalar mode). Simulation time very strongly depends on the density contrast of the scenario under consideration.

Mathematical formulation

Using the equivalent head formulation (Frind, 1982), and assuming that the principal directions of permeability are aligned with the coordinate axes, the continuity equation for fluid flow may be written as:

\[
\frac{\partial}{\partial x} \left[ k_x \frac{\partial \theta^*}{\partial x} \right] + \frac{\partial}{\partial z} \left[ k_z \frac{\partial \theta^*}{\partial z} \right] = \frac{\partial}{\partial t} \left( \frac{\partial \theta^*}{\partial t} + \frac{\partial \rho_e}{\partial \rho_e} \right)
\]

where \( x \) and \( z \) are the horizontal and vertical coordinate directions, respectively, \( t \) is time, \( k_{ij} \) is the permeability, \( \rho_e \) is the density of a reference fluid, \( g \) is the gravitational constant, \( \rho = \rho(c) \) is the fluid density, \( \mu = \mu(c) \) is the viscosity of the fluid mixture, with \( c \) being the solute concentration, \( \theta^* \) is the equivalent freshwater head, and \( S_n \) is the specific storage.

The continuity equation governing advective-dispersive mass transport in porous media is:
\[
\frac{\partial}{\partial x} \left[ nD_{xx} \frac{\partial c}{\partial x} \right] + \frac{\partial}{\partial x} \left[ nD_{xy} \frac{\partial c}{\partial y} \right] + \frac{\partial}{\partial x} \left[ nD_{xz} \frac{\partial c}{\partial z} \right] + \frac{\partial}{\partial x} \left[ nD_{zz} \frac{\partial c}{\partial z} \right] = R \frac{\partial}{\partial x} (nc)
\]

where \( n \) is the porosity, and \( R \) is the retardation factor. The average interstitial velocity is determined from Darcy’s equation and the dispersion tensor is defined following Bear (1969). Because density is defined to be an average elemental property, the code uses a consistent formulation that is physically correct according to the discussion of Voss and Souza (1987). The time derivative in both the flow and transport equations is approximated by finite differences. The model uses fully implicit time weighting for flow, although a Crank-Nicolson time weighting is applied to the density terms. Crank-Nicolson time stepping also is used in the transport solution to obtain second-order accuracy in time (Huyakorn and Pinder, 1983) and lumped mass matrices improve stability (Fridn, 1982) and enhance convergence rates (Mendoza et al., 1992).

Coupling between the flow and transport equations is implemented via a sequential iterative procedure where the flow and transport equations are solved repeatedly, using updated information, until convergence is achieved. Advection and dispersive mass balance calculations are performed for each time step to quantify mass fluxes, determine mass fate, and to verify mass conservation in the model. Details of the numerical solution and mass balance calculations are provided in Mendoza and Fridn (1990a) and Mendoza.

**Code verification**

The code has undergone verification tests in earlier work (see Mendoza, 1992) and has been validated in laboratory and field applications. Several laboratory, field, and theoretical studies have involved the successful application of the code [see Mendoza and Frind (1990a,b), Mendoza et al. (1990a,b), Mendoza and McAalay (1990), MacPherson (1991), and Hughes (1991)]. In a qualitative manner, the code has been cross-verified through comparison to the numerical results of Falta et al. (1989).

Because of the application to saturated flow and transport, further verification testing of this code was undertaken as part of this study. The code was successfully verified against analytical solutions for a simple Thies flow problem, and for a one-dimensional transport problem for an ideal tracer with no density difference or sorption (Wexler, 1989). Details of these tests are presented in Appendix A. Another verification test involved comparison to Henry's (1964) approximate analytic solution for steady-state saltwater intrusion. However, as discussed by Voss (1984), and Voss and Souza (1987), no code has successfully matched the analytic solution; possibly due to inaccuracies caused by dropping higher order terms. Therefore, the common practice of cross-verifying the code for Henry's problem with another numerical model - in this case SUTRA (Voss, 1984), is followed here. Voss and Souza (1987) show that the
SUTRA solution to Henry's problem, where the molecular diffusion coefficient is set equal to 6.6x10^{-6} m^2/s, closely matches that of other variable-density flow models such as Pinder and Cooper (1970), Segal et al. (1975), Dersi and Contractor (1977), and Frind (1982). The reader is referred to Voss and Souza (1987) for details of the problem in terms of boundary conditions, parameters, and simulation results.

The simulation of Henry's problem utilizes a 200x100 grid (each of size 0.01 m by 0.01 m) consisting of 20,301 nodes defining 40,000 triangular elements. The time step was a constant 0.0025 hrs with Crank-Nicolson time stepping. The model was run to a simulation time of 100 minutes so that direct comparison could be made with Voss (1984). Voss (1984) determined 5-100 minutes to be approximately steady state. As can be seen from Figure 14 the two codes compare very well.

Model system and parameter values

To facilitate comparisons with the previous experimental work, all simulations are based on the experimental system of Schincariol and Schwartz (1990). The region (Figure 15) is 106.25 cm long and 50 cm high with impermeable boundaries along the top and bottom. The left and right boundaries are modeled as specified equivalent freshwater heads, while the left transport boundary condition is specified concentration and the right is a zero-dispersive flux boundary (Figure 15). To avoid the buildup of dispersive mass within
Figure 14. Match of isochlors along the bottom of aquifer for "Henry's" saltwater intrusion problem from SUTRA and VapourT at t=100 minutes.
Figure 15. Model domain and boundary conditions for numerical simulation of tank experiments. $C_0$ and $h_0$ are specified values of concentration or equivalent freshwater head, and $n$ designates the direction normal to the domain boundary. The dashed line indicates the subdomain used for some simulations. Boundary conditions on this subdomain were as for the full domain.
the flow domain, the plume is not allowed to reach the far exit boundary during the simulation period. All simulations in this chapter involve a homogeneous, isotropic medium, and use the set of experimental parameters in Table 3. The dispersion parameters (Table 4) were determined as part of this study by a trial and error fitting procedure, documented in Appendix B, using concentration data from Schincariol's (1989) experiments.

Numerical Errors and the Creation of Instabilities

In experiments the perturbations necessary for instabilities growth along an interface are generated due to heterogeneities in porous media. However, in contrast, List (1965) perturbed the interface mathematically in order to create instabilities. Interestingly, this work has shown that the problem of numerical spatial oscillations, commonly associated with codes, also can serve as a perturbation capable of creating instabilities. Because these errors essentially form by themselves, one is not sure whether the instabilities they create are physically realistic, nor is one able to control their formation. More importantly, however, because the numerical errors may go undetected, a surprising array of physically unrealistic instabilities may result. These issues provide the motivation for the analyses presented in this section.
Table 3. Known Tank Parameter Values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydraulic conductivity(^1)</td>
<td>(5.6 \times 10^{-4}) m s(^{-1})</td>
</tr>
<tr>
<td>permeability(^1)</td>
<td>(3.7 \times 10^{-11}) m(^2)</td>
</tr>
<tr>
<td>porosity(^1)</td>
<td>0.38</td>
</tr>
<tr>
<td>aqueous diffusion coefficient for dilute NaCl solution ((D_a))(^2)</td>
<td>(1.61 \times 10^{-8}) m(^2) s(^{-1})</td>
</tr>
<tr>
<td>average linear groundwater velocity(^1)</td>
<td>(2.75 \times 10^{-6}) m s(^{-1})</td>
</tr>
<tr>
<td>viscosity of H(_2)O @ 20(^°) (^3)</td>
<td>(1.002 \times 10^{-2}) g cm(^{-1}) s(^{-1}) ((1.002 \times 10^{-2}) Pa s)</td>
</tr>
<tr>
<td>viscosity: 500 mg/L Rh(WT) sol’n (^3)</td>
<td>(1.002 \times 10^{-3}) Pa s ((1.004 \times 10^{-3}) Pa s)</td>
</tr>
<tr>
<td>viscosity: 1000 mg/L NaCl sol’n (^3)</td>
<td>(1.006 \times 10^{-3}) Pa s ((1.008 \times 10^{-3}) Pa s)</td>
</tr>
<tr>
<td>viscosity: 3000 mg/L NaCl sol’n (^3)</td>
<td>(1.011 \times 10^{-3}) Pa s ((4.8 \times 10^{-12}) m(^2) N(^{-1}))</td>
</tr>
<tr>
<td>compressibility of H(_2)O @25(^°) (^4)</td>
<td>(0.9982) g cm(^{-3})</td>
</tr>
<tr>
<td>relative density of H(_2)O @ 20(^°) (^3)</td>
<td>(0.9983) g cm(^{-3})</td>
</tr>
<tr>
<td>relative density: 500 mg/L Rh(WT) @ 20(^°) (^1)</td>
<td>(0.9989) g cm(^{-3})</td>
</tr>
<tr>
<td>relative density: 1000 mg/L NaCl sol’n @ 20(^°) (^3)</td>
<td>(0.9997) g cm(^{-3})</td>
</tr>
<tr>
<td>relative density: 3000 mg/L NaCl sol’n @ 20(^°) (^3)</td>
<td>(1.0004) g cm(^{-3})</td>
</tr>
<tr>
<td>relative density: 5000 mg/L NaCl sol’n @ 20(^°) (^3)</td>
<td>(1.0018) g cm(^{-3})</td>
</tr>
</tbody>
</table>

1. Schincariol and Schwartz (1990)
2. Robinson and Stokes (1970)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>longitudinal dispersivity $a_L$</td>
<td>$3.00 \times 10^{-4}$ m</td>
</tr>
<tr>
<td>transverse dispersivity $a_T$</td>
<td>0.0 m</td>
</tr>
<tr>
<td>tortuosity $\tau$</td>
<td>0.35</td>
</tr>
<tr>
<td>bulk diffusion coefficient ($rD_{$B$}$)</td>
<td>$5.635 \times 10^{-10}$ m$^2$ s$^{-1}$</td>
</tr>
</tbody>
</table>
Accuracy criteria

In advection-dominated transport problems, based on finite-element and finite-difference codes, numerical-spatial oscillations often may develop near a concentration front (Huyakorn and Pinder, 1983). For weakly coupled flow and transport (i.e. linear) problems, adherence to accuracy criteria for time/space discretization can control these problems. For example, Huyakorn and Pinder (1983) suggest that numerical oscillations in a finite-element solution, using linear basis functions, can be virtually eliminated if the element size is selected so that the local grid Peclet number ($P_e$) does not exceed 2, where $P_e$ is given as:

$$ P_e = \frac{v A_f}{D} \quad (10) $$

with $A_f$ in two-dimensional problems given as $\max(AX,AY)$. Further, for some linear problems, a grid Peclet number as large as 10 may result in only mild oscillations (Huyakorn and Pinder, 1983). A second criterion is related to the size of the time step, which should be selected so that the local Courant number ($Cr$) defined as:

$$ Cr = \frac{v A_f}{A_t} \quad (11) $$

is less than or equal to one (Huyakorn and Pinder, 1983).

Numerical solutions are typically oscillation free and numerical errors small with $P_e < 2$ and $Cr < 1$. These criteria for linear problems are typically not rigid requirements for solution accuracy; however, progressively greater violation leads to a gradual deterioration in
solution accuracy (Daua et al., 1985). Both Courant number and Peclet number violations lead to oscillations in calculated concentrations and numerical errors, although to different degrees. The oscillations and errors, however, dampen out with time as the concentration gradient at the front decreases due to dispersion. Although minor oscillations will not overly affect the plume shape in linear problems, in non-linear density-dependent flow problems, oscillations create interfacial instabilities.

Simulation experiments

Presented here are two sets of simulation trials. The first encompasses four different model runs in which all parameters remain the same except the grid spacings, which give rise to approximate maximum Pe values of 14, 9.4, 4.7 and 2.3. The time steps are adjusted so that the maximum Courant number is close to one. The parameters of the simulation are those in Tables 3 and 4, except for values of $a_x$ and $a_y$ which are increased slightly to $1.0 \times 10^{-3}$ m and $2.0 \times 10^{-4}$ m respectively. The magnitude of the dispersivities had to be increased slightly, so that error free simulations could be performed within computer memory/time constraints.

The results for these simulations (Figures 16 to 19) illustrate how the formation of instabilities is directly linked to the numerical errors, which are predicted by the grid Peclet stability criterion. With Pe values of approximately 14 and 9 (Figures 16 and 17) oscillations develop at the source, produce relative
Figure 16. Concentration shade map for a 2000 mg/L NaCl source at 90 hours (15mm x 15mm grid, maximum $\text{Pe}(x)=14.0$, $\text{Pe}(z)=14.2$, $\text{Cr}(x)=1.0$, $\text{Cr}(z)=0.5$).

Figure 17. Concentration shade map for a 2000 mg/L NaCl source at 90 hours (10mm x 10mm grid, maximum $\text{Pe}(x)=9.4$, $\text{Pe}(z)=9.5$, $\text{Cr}(x)=1.0$, $\text{Cr}(z)=0.5$).
Figure 18. Concentration shade map for a 2000 mg/L NaCl source at 90 hours (5.0mm x 5.0mm grid, maximum Pe(x)=4.7, Pe(z)=4.7, Cr(x)=1.0, Cr(z)=0.5).

Figure 19. Concentration shade map for a 2000 mg/L NaCl source at 90 hours (2.5mm x 2.5mm grid, maximum Pe(x)=2.3, Pe(z)=2.4, Cr(x)=1.1, Cr(z)=0.5).
concentrations above 1.0, and move with the plume creating large instabilities, particularly at the nose of the plume. With time (t), the magnitude of the errors at the source decreases as the solution becomes smoother. For example at t=12 hours (Figure 17), there are large errors, which produce maximum (c/c₀) values of approximately 1.15. The magnitude of errors at the source gradually decreases with time. For example, after 90 hours, c/c₀ is 1.05.

The reduction of the numerical errors in time leads to instabilities only being propagated early in the simulation. As a result, instabilities form only in the frontal portions of the plume. Toward the source no other instabilities develop even after long times. This pattern of instability development is different than patterns obtained in laboratory experiments (Figures 8 to 11), and in cases where instabilities are generated by mathematical perturbation; here instabilities form along the entire bottom edge of the plume.

As the grid Peclet number is reduced, the numerical errors decline (Figure 18) and essentially disappear (Figure 19). In these latter two cases the small solution errors that remain cannot perturb the solution sufficiently to create instabilities. Thus, for unstable flow problems, the stability criteria may have more bearing on the solution than for stable problems. Further, in unstable simulation problems, one cannot rely on numerical errors to create instabilities because the process is inherently unpredictable.

Note that in Figure 19 the lobe at the end of the plume remains even though the numerical errors have disappeared. This instability,
which was also observed in the experimental investigations of Schincariol and Schwartz (1990), is caused by the very large boundary perturbation that is produced as the flow system responds to the entry of more dense water. Thus, it is technically different than the instabilities that follow.

The next simulation illustrates another facet of this issue of unpredictability. In this model run (Figure 20) the Pedlet number (s=13) is comparable to the model run illustrated in Figure 16 (Pe=14), except that values of longitudinal and transverse dispersivity are reduced to 3x10^-4 m and 0.0, respectively. The results (Figure 16 vs. Figure 20) show that as the dispersivity is reduced the number of instabilities increase, and they become narrower in shape. This result is not totally unexpected because List's (1965) theoretical work shows that increasing dispersion reduces concentration gradients and the potential for instabilities to form.

These results show that there is no doubt that instabilities can be generated in variable-density flow problems through the propagation of numerical errors. As an operational approach, however, one has to be concerned that the instabilities are not physically realistic, are relatively uncontrollable, and are difficult to reproduce from one numerical method, or simulation, to another.
Figure 20. Concentration shade map for a 2000 mg/L NaCl source at 90 hours (5.0mm x 5.0mm grid, maximum Pe(x)=12.7, Pe(z)=13.0, Cr(x)=1.1, Cr(z)=0.5).
Creation of Instabilities by Interface Perturbations

Various theoretical analyses have shown how stability can be addressed by examining the response of a system to perturbations of fundamental variables, such as concentration, velocity, and pressure. This theory extends naturally to numerical studies and forms the basis of the analysis on the creation of instabilities through perturbations of the interface. More specifically, the series of computer experiments that follow examine how features of the interface perturbations determine whether instabilities form, and what influence they have on the velocity field and concentration distribution.

Given the power of the numerical procedure, it would be possible to add perturbations to the interface, velocities, and concentrations. However, a problem in this approach is that arbitrary perturbing functions may not preserve the inherent coupling among the variables. The approach, then, is to perturb the interface and let the coupling create the appropriate perturbations of the other variables. A simple sinusoidal perturbation was applied to the lower edge of the plume by increasing and decreasing the height of the inflow zone, for the dense fluid, through an adjustment of the specified concentrations of the lowest two nodes forming the 21 node inflow zone. The resulting sinusoidal perturbation was 2.5 mm or 5% of source width. The wavelength of the perturbation was altered by defining the concentration of the lower two nodes as a function of
times as either \( c_0 = 100.0 \) or \( c_0 = 0.0 \).

Manifestations of the interface perturbations

The first model simulation illustrates how sinusoidal perturbations of the interface are manifest in the concentration distribution. For this simulation, the dense fluid at the source is assumed to have a concentration of 2000 mg/L NaCl. Again, the region size and boundary conditions are shown in Figure 15, and the parameters are those in Tables 3 and 4, except for values of \( \alpha_L \) and \( \alpha_T \) which are increased slightly to \( 1.0 \times 10^{-7} \) m and \( 2.0 \times 10^{-4} \) m, respectively. The interface perturbation is a sine function with a wavelength of 71.5 mm. The region is discretized by 200 rows and 425 columns at a grid spacing of 2.5 mm. The resulting maximum grid Peclet and Courant numbers for this simulation are \( Pe(x) = 2.3 \), \( Pe(z) = 2.4 \) and \( Cr(x) = 1.1 \), \( Cr(z) = 0.5 \), respectively.

The perturbations at the interface grew rapidly and formed lobe shaped instabilities (Figure 21). A particular feature of these instabilities, as compared to those created by numerical errors, is that they are present all along the bottom of the plume not just at the nose. The system, thus, is unstable because the perturbation or slight disruption to the system grew, or continued to displace the position of the system from its initial state. The growth of the disturbance also can be illustrated by examining the vertical linear groundwater velocity field (Figure 22). The velocity field illustrates alternating zones, which correspond to upward (positive)
Figure 21. Concentration shade map for a 2000 mg/L NaCl source at 90 hours (perturbation wavelength=71.5mm; perturbation amplitude=2.5mm).

Figure 22. Vertical velocity shade map of plume illustrated in Fig. 21.
and downward (negative) vertical velocities. These zones of velocity variability coincide with places where the lobes of denser fluid, initially created by the small perturbation to the system, are moving downwards and the lighter ambient fluid is moving upwards to balance the denser fluid movement.

Sensitivities in the concentration distribution

The next trials examine how the style of instabilities that form depends on characteristics of the perturbing function, and the density of the dense fluid. For all simulations the base set of parameters apply and the domain is discretized (Δx, Δz) at 2.5 mm, which results in grid Peclet numbers below 2.4. The first parameter, the amplitude of the perturbation, was investigated with two simulations utilizing the subset grid (shown by the dashed lines in Figure 19). The subset grid represents exactly the same problem over a piece of the larger domain (Figure 15). The only difference between the two simulations is the amplitude of the perturbing function, 2.5 mm in the first case and 5.0 mm in the second. The two concentration distributions at 48 hours (Figures 23 and 24) show only minor differences. Effectively, a 100% increase in the perturbation amplitude caused the rate of growth of the instability to increase by only 15 to 20%. Thus, the concentration distribution is not particularly sensitive to the amplitude of the interface perturbation.
Figure 23. Contoured concentration distribution for a 2000 mg/L NaCl source plume at 48 hours (perturbation wavelength=71.5mm; perturbation amplitude=2.5mm).

Figure 24. Contoured concentration distribution for a 2000 mg/L NaCl source plume at 48 hours (perturbation wavelength=71.5mm; perturbation amplitude=5.0mm).
The next trials examine how instabilities depend on the wavelength of the perturbing function. The first trial consisted of eight model simulations using wavelengths of 119.2, 95.4, 71.5, 59.6, 53.7, 47.7, 41.7, 35.8 mm and a source with a concentration of 2000 mg/L. Figures 25, 26, and 27 illustrate concentration distributions at 48 hours for wavelengths of 119.2, 59.6, and 41.7 mm. The largest perturbation wavelength, 119.2 mm (Figure 25), is associated with the greatest growth rate of the instabilities. The growth rate is much smaller when the wavelength is reduced to 59.6 mm (Figure 26), and at a perturbation wavelength of 41.7 mm (Figure 27) the perturbations rapidly decay. Thus, the transition between stability and instability occurred at a wavelength of 59.6 mm. At the next smaller wavelength of 53.7 mm (as allowed by the time step; results not shown), initial perturbations to the interface slowly degrade from the input amplitude of 2.5 mm and no upward fluid motions are present except at nose of the plume, which, as discussed previously, is a boundary effect. The two criteria used for stability are (1) the amplitude of the initial perturbation as represented in the concentration fields grows in time, and (2) obvious zones of upward and downward fluid motions are evident in the velocity plot. Thus, the concept of a critical wavelength holds even for this more complicated transport problem. In the case of disturbances with a shorter wavelength, dispersion is increasingly more efficient at smoothing out or eliminating the "finger" or perturbation lobes before they have a chance to grow.
Figure 25. Contoured concentration distribution for a 2000 mg/L NaCl source plume at 48 hours (perturbation wavelength=119.2mm; perturbation amplitude=2.5mm).

Figure 26. Contoured concentration distribution for a 2000 mg/L NaCl source plume at 48 hours (perturbation wavelength=59.6mm; perturbation amplitude=2.5mm).
Figure 27. Contoured concentration distribution for a 2000 mg/L NaCl source plume at 48 hours (perturbation wavelength=41.7mm; perturbation amplitude=2.5mm).
The rate at which perturbations grow or decay is dependent on the perturbation wavelength. Plotted in Figure 28 are growth rate curves for the 2000 mg/L NaCl case. The growth rate factor (normalized amplitude) is defined, for a particular wave or instability, as the amplitude at a given time divided by the original input amplitude (2.5 mm). Below the critical wavelength the perturbations rapidly decay (Figure 28). Just below the critical wavelength a pseudo-stable state is reached where the perturbations maintain the input amplitude with time and slow degradation occurs due to dispersion. The growth rate is very rapid for wavelengths significantly above the critical wavelength.

The next trial considers how the critical wavelength changes as a function of plume density. Density contrasts are created with plume concentrations varying from 1000 mg/L to 3000 mg/L NaCl. A stability diagram, summarising the results of 22 simulations (Figure 29), illustrates that irrespective of concentration the flow is unstable above the critical wavelength, which is shown by the stability/instability line on Figure 29. However, as the concentration decreases an increasingly longer perturbing wavelength is required to produce an instability. The plot is in agreement, conceptually, with List's (1965) general stability theory presented earlier; the greater the density difference the larger the spectrum of unstable wavelengths. The smaller the density difference, the longer the perturbing wavelength required to generate instabilities.
Figure 28. Growth rate curves for a 2000 mg/L NaCl source plume perturbed with a 2.5 mm amplitude function at various wavelengths.
Figure 29. Stability diagram depicting the dependence of stability/instability, for various concentrations, on perturbation wavelength.
The curve outlining the first instance of instabilities in Figure 29 appears to be becoming asymptotic to both axes. Therefore, one could conclude that, when the density differences are very small, only a very small spectrum of long wavelengths will be unstable, and when the density difference is large, most disturbing wavelengths will be unstable. The experimental work (Figures 8 and 9) also illustrate this concept. The instabilities generated by the 1000 mg/L NaCl plume (Figure 8) have a longer wavelength than instabilities generated by the 2000 mg/L plume (Figure 9), in the identical homogeneous medium, under the same flow conditions.

By looking at the results in a different way, one can examine how the density difference between the plume and the ambient water influences stability. Let us consider the growth rate curves of three of the plumes simulated in the previous trials. The wavelength of the perturbing function is kept constant and only the density difference is varied. The growth rate curves for three simulations (Figure 30) show that the greater the density difference, the greater the growth rate of the instabilities. This increased growth rate, and increased intensity of the upward and downward fluid motions, is clearly illustrated when plots of concentration distribution and vertical fluid velocities for a 3000 mg/L source plume (Figures 31 and 32) are compared to those compared to similar plots for the 2000 mg/L source plume (Figures 21 and 22). The growth rate falls off relatively rapidly for the 3000 mg/L plume after reaching a maximum, as intense plume mixing caused by the
Figure 30. Growth rate curves for a 71.5 mm wavelength perturbation function applied to 1000, 2000, and 3000 mg/L NaCl source plumes.
Figure 31. Concentration shade map for a 3000 mg/L NaCl source at 90 hours (perturbation wavelength=71.5 mm; perturbation amplitude=2.5 mm).

Figure 32. Vertical velocity shade map of plume illustrated in Fig. 31.
instabilities diminishes the density difference. When the concentration is reduced to 1000 mg/L, again with the same 71.5 mm wavelength perturbation, the disturbances to the plume decay rapidly (Figure 30), and the plume is nearly identical to an unperturbed plume.

Interestingly, instabilities created using a spectrum of perturbing functions (here the sum of three sine waves - each with a different wavelength), depend upon those component wavelengths above the critical wavelength. The instabilities evident in Figure 33 were created with a perturbation function that was the sum of three sinusoidal functions with amplitudes of 2.5 mm and wavelengths of 29.8, 71.5, and 99.4 mm (Figure 34). Given a source concentration of 2000 mg/L, Figure 29 shows that the 29.8 mm wavelength function would be below the critical wavelength, while the 71.5, and 99.4 mm wavelengths would be above. The complex function resulting from the addition of these three waves contains a wide range of wavelengths from much smaller than the critical wavelength to much larger. Small wavelength perturbations are dampened out by dispersion and coalesce with larger perturbations to form the complex instabilities shown in Figure 33. Apparently, if the correct perturbation function could be found for a given porous medium, for example the experimental study shown in Figure 9, one could more closely reproduce the actual concentration distribution.
Figure 33. Concentration shade map for a 2000 mg/L NaCl source plume at 72 hours, when subjected to a variable perturbing function.

Figure 34. Perturbing function for the plume illustrated in Fig. 33.
Dimensionless Parameters as Indicators of Stability

It is tempting in both experimental and theoretical analysis to utilize dimensionless parameters, such as the Rayleigh number, to try and predict the stability. For discussion purposes, the Rayleigh number developed by Wooding (1959) describing the stability of a more dense viscous liquid overlying a less dense liquid, in a vertical tube containing porous material, will be considered here. It has the form:

\[ \lambda = \frac{d\rho}{dz} \frac{skb^3}{\mu D'} \]  \hspace{1cm} (12)

where \( \frac{d\rho}{dz} \) is the vertical density gradient, \( g \) is the gravity constant, \( k \) is permeability, \( b \) is the radius of the column, \( \mu \) is the mean viscosity of the two fluids initially present in the column, and \( D' \) is the apparent diffusivity of the solute through the medium (Backnæst and Elrick, 1970). The Rayleigh number, thus, is proportional to permeability and density gradient and inversely proportional to the apparent diffusivity. For a system, comparison of the calculated Rayleigh number to some critical Rayleigh number may establish whether or not the system is stable.

Because Wooding's (1959) study dealt only with "free" convection his Rayleigh number was very similar to those obtained in classical studies of convective heat flow (Rayleigh, 1916; Horton and Roger, 1945; Lapwood, 1948). The Rayleigh number, in heat flow, expresses
the ratio of the transport of energy by free convection to the transport by conduction, and theory provides the conditions for the onset of free convection. In most one-dimensional cases, the characteristic length is taken as equal to the thickness over which the temperature difference ΔT is measured. In two-dimensional problems, it will be some length associated with fluid movement (Domonico and Schwartz, 1990).

Both List's (1965) results and those shown here suggest that dimensionless Rayleigh numbers, by themselves, cannot be used as predictors of stability of interface problems. In essence, this result is evident in Figure 29, which shows that irrespective of the density contrast, a critical wavelength exists that separates stable and unstable plume behaviors. Granted, as dρ/dz becomes smaller there is a much smaller spectrum of only long wavelengths capable of making the plume unstable, but it is still possible for instabilities to develop. Even for very small density differences (500 mg/L NaCl) instabilities can be generated given a perturbation with a long enough wavelength. However, the instabilities are very weak and difficult to assess, which is why a critical wavelength was not determined for the 500 mg/L NaCl trials.

In experiments that rely only on the porous medium to create near-source perturbations of the interface, there probably is a natural upper limit to the size of perturbations that are created. Thus, as the density of the plume decreases, the porous medium eventually becomes incapable of creating a long enough wavelength to
make the interface unstable. In other words, the maximum wavelength of the perturbation created by the porous medium becomes less than the critical wavelength. This feature provides the illusion of density control on the origin of stability, as Rayleigh stability theory would predict. However, if the source boundary were controllable, an experimenter could simply perturb the interface (as was done mathematically in this study) to make the plume unstable.

The Rayleigh number comes about through a dimensional analysis of the steady-state transport-conduction equation in combination with a buoyancy driven velocity term. This equation has been solved for certain boundary and initial conditions, and various simplifying assumptions. Therefore, the validity of the Rayleigh number as a predictor of stability is tied to these assumptions and boundary conditions. The present problem of interfacial stability is a very different problem with different boundary conditions. For example, one of the boundary conditions, for the problem investigated here, obviously relates to the wavelength of perturbations along the interface. Thus, a dimensionless stability criterion, pertaining to this problem, would depend critically on the wavelength of the perturbing function.

There is other evidence that suggests that the complexity of the stability criterion increases with the complexity of the problem. Recall for example Wooding's (1959) experiment of free convective mixing and the resulting stability criterion (Eqn. 12). Once a vertical flow is imposed on this system, the nondimensional
parameters governing instability become much more complex. For example, Bues and Aachib (1991) investigated miscible displacement processes in a vertical column with a uniform velocity distribution, and established a criterion of stability that is defined as a function of two dimensionless numbers \((G^*, Rm^*)\). The nondimensional parameter \(G^*\):

\[
G^* = \frac{k g \Delta \rho}{n \mu U}
\]  

(13)

where \(n\) is porosity, \(U\) is the mean pore or linear velocity, \(\mu_m\) is the mean dynamic viscosity, reflects the ratio of gravitational forces to viscosity forces. The dimensionless number \(Rm^*\) is referred to as a modified Rayleigh number:

\[
Rm^* = \frac{(\rho_1 - \rho_2) g k h}{\mu_m D_1} + \frac{Pe^*(\mu_1 - \mu_2)}{\mu_m}
\]  

(14)

where the first term is a solute Rayleigh number and the subscript 1 refers to the fluid above the mixing zone and the subscript 2 to the fluid below, \(h\) is the length of the mixing zone, \(D_1\) is the apparent longitudinal dispersion coefficient, and \(Pe^*\) is a modified Peclet number \(Pe^* = (nU h) / D_1\). In the functional relationship of these parameters, a change in slope, defined by the couple \((G^*, Rm^*)\) denotes the critical threshold of stability (Bues and Aachib, 1991).

The problem investigated here is yet more complicated than Bues and Aachib (1991), in that (1) the problem is two-dimensional, (2) the gravity vector is located perpendicular to the flow field, (3) the dispersion zone widens downstream, and (4) the experimental
studies (Schincariol and Schwartz, 1990, and Costrom et al., 1992) show the flows are unsteady. Carrying the analytical analysis of stability beyond List (1965) is a challenging and perhaps intractable problem; however, it is clear that Rayleigh theory cannot stand as a substitute.
CHAPTER IV

FACTORS INFLUENCING THE PROPAGATION OF INSTABILITIES IN POROUS MEDIA

Chapter III illustrated how small perturbations, imposed mathematically on the interface between fluids of differing densities, may result in instabilities that grow with time. The analysis established how features of the initial perturbation, particularly the wavelength and the magnitude of the density difference between the two fluids, determined the growth rate of the perturbation. Further, it demonstrated how important elements of the local theory of instability formation in a porous medium, proposed by List (1965), appear to hold for much more complicated systems.

Several unanswered questions, however, remained in relation to instability formation which are addressed in this chapter. By far the most important is whether instabilities can be expected to form in natural geologic systems. One approach for addressing this issue is to establish what hydrogeologic conditions, represented in terms of conventional transport parameters, promote the growth of instabilities in variable-density flow. The extent to which these environments occur in nature provides a preliminary basis for the analysis.
There are at least two different choices available as how to go about parameterizing the system. The first is the classical deterministic approach in which geologic units are represented in terms of a set of average properties. Effectively, this approach avoids dealing with the particular pattern of local variation in parameters like hydraulic conductivity. The second choice is a probabilistic approach that attempts to represent features of the local variability in parameters using geostatistical concepts. Because both of these parameterizations are legitimate conceptualizations of real systems, the analysis of the potential for instability development presented in this chapter will involve both of these conceptual models.

Besides addressing the question of the legitimacy of instability growth as a process promoting contaminant mixing, this chapter also examines how instabilities form in natural systems. As Chapter III emphasizes, in theoretical systems that are truly isotropic and homogeneous, a slight perturbation of the interface must be supplied for instabilities to form. The fact that instabilities form in experiments with "isotropic and homogeneous" media (Schincariol and Schwartz, 1990) was attributed to local scale variability in hydraulic conductivity. Fortunately, development of the probabilistic approach for representing local scale variability in parameters provides the opportunity to test this hypothesis in this chapter.
Modeling Approach

There are two accepted ways of defining local properties of a porous medium. With the deterministic conceptualization, properties are defined with reference to a representative elementary volume (REV). With the probabilistic approach, properties are defined as random functions (RF).

*Deterministic conceptualization*

This section describes the deterministic conceptualization where some mean property applies to the domain of interest. The governing equations for fluid flow (equation 1, chapter III) and physical mass transport (equation 2, chapter III) define the main parameters of interest in the sensitivity analysis, namely, permeability, velocity of ambient flow field (gradient in head), and dispersivity. The analysis involves varying these parameters one at a time over some predetermined range and assessing the sensitivity of instability growth to realistic changes in these flow and transport parameters. The modeling uses the modified VapourT code discussed in Chapter III with the model domain and boundary conditions shown in Figure 15. The parameters of the simulation are also the same (see Tables 3 and 4) except for those parameters that are varied as part of the sensitivity analysis.

The sensitivity analysis with the deterministic conceptualization involves three sets of model trials, which examine
system behavior in terms of changes in dispersivity, average linear flow velocity, and permeability. In all cases parameter values are varied around a base case, which is represented by the parameters in Tables 3 and 4.

**Probabilistic conceptualization**

The probabilistic conceptualization assumes that porous medium is a realization of a random process (de Marsily, 1986). The concept of a "mean", used in a deterministic sense, is replaced by the "ensemble average" of multiple realizations of that porous medium. Essentially, a parameter such as permeability, or porosity, is defined in value and space as a random function. To exploit these geostatistical concepts, a random field generator is required to generate the realization from statistical parameters such as mean, variance, and correlation lengths. In this work, the cross-correlated random field generator, FGEN version 9.2, by M.J.L. Robin (Robin, 1991; and Robin et al., 1992), was utilized. This code is computationally efficient, and avoids the difficulties with lineation problems that can be encountered with the turning bands method (Mantoglou and Wilson, 1982). The algorithm is based on the direct power spectral estimation method, which estimates the spectral density function (the frequency domain equivalent of autocovariance functions) directly from the input statistical parameters. The spectral density of a parameter is the Fourier transform of its autocovariance function. The spatial covariance, or autocovariance,
specifies the spatial persistence of a given parameter in space. Although FGEN can produce three-dimensional cross-correlated random fields, only a two-dimensional single-field generation (permeability) is used here. Readers can refer to Robin et al. (1992) for details concerning the theory and implementation of the code.

Realizations of the permeability field are generated from a set of user-supplied geostatistical parameters, including mean, variance, and correlation length scales for the population. All the simulations presented here were produced using a power spectral density function based on a exponential-decay covariance function. As is normally held, permeability is assumed to have a log-normal probability distribution function (Freeze, 1975). In addition, the porous medium is assumed to be weakly stationary. A random function is said to be weakly stationary (or second-order stationary) if the mean is constant and does not vary in space, and the function of covariance only depends on the separation distance, or lag distance, and not the points of reference (de Marsily, 1986).

The analysis with this conceptual model involves four different realizations. The calculated statistical properties of the generated field for each realization are shown in Table 5. As is often the case in generating heterogeneous fields, the calculated statistics can differ slightly from those specified. Thus, random field generators generally only reproduce the input statistical parameters in an ensemble-average sense (Robin et al., 1992).
Table 5. Realization Field Data

<table>
<thead>
<tr>
<th></th>
<th>#1</th>
<th>#2</th>
<th>#3</th>
<th>#4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>-23.58</td>
<td>-23.58</td>
<td>-23.58</td>
<td>-23.68</td>
</tr>
<tr>
<td>$\mu$ (m²)</td>
<td>5.7x10⁻¹¹</td>
<td>5.7x10⁻¹¹</td>
<td>5.7x10⁻¹¹</td>
<td>5.2x10⁻¹¹</td>
</tr>
<tr>
<td>$\sigma_y^2$</td>
<td>0.05</td>
<td>0.05</td>
<td>0.11</td>
<td>0.18</td>
</tr>
<tr>
<td>$\lambda_x$ (m)</td>
<td>0.05</td>
<td>0.15</td>
<td>0.05</td>
<td>0.25</td>
</tr>
<tr>
<td>$\lambda_y$ (m)</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.05</td>
</tr>
<tr>
<td>$e$</td>
<td>0.20</td>
<td>0.067</td>
<td>0.20</td>
<td>0.20</td>
</tr>
</tbody>
</table>

$\mu_y$ = mean of the log-transformed permeability field ($Y-\ln(k)$)
$\mu$ = mean permeability
$\sigma_y^2$ = variance of the log-transformed permeability field ($Y-\ln(k)$)
$\lambda_x$ = longitudinal correlation length
$\lambda_y$ = transverse (vertical) correlation length
$e = \lambda_z/\lambda_x$
Most commonly, one employs a probabilistic conceptualization of a random field in some type of stochastic analysis, that attempts to capture the ensemble behavior of the transport process. However, the long run times associated with the variable-density flow and transport simulations make a stochastic analysis of the system infeasible. For example, the variability in the velocity field due to the heterogeneities result in longer CPU times because the Courant and Peclet criteria, for stability, must apply locally over the domain. The 5000 mg/L simulations, in heterogeneous permeability fields, typically required CPU time equivalent to the total simulation time (i.e., a 72 hour simulation on the Cray Y-MPA/864, operating in linear mode at 9.2 Mflops, took approximately 53 CPU hours). Thus, the analyses that follow are based on a single realization for each set of statistical parameters.

Sensitivity of Dispersivity

The first trial examines how the growth/decay of instabilities depends upon the dispersive characteristics of the medium. Dispersivity was varied in a series of five simulations. As indicated, the base set of parameters were those in Tables 3 and 4, and only dispersivity was varied. The source concentration in these simulations was 2000 mg/L NaCl with perturbations applied as a sine wave (wavelength=71.5 mm, amplitude=2.5 mm), as described in Chapter III.
Because changing the dispersivity changed the grid Peclet numbers, the modal grid had to be adjusted to accommodate the smaller dispersivity values. The first three simulations employ the previous domain (Figure 15) discretized \((\Delta x, \Delta z)\) at 2.5 mm, which results in grid Peclet numbers below 2.4. The last two simulations, with dispersivities smaller than the base-case values, were run with grid spacings \((\Delta x, \Delta z)\) of 1.25 mm. This discretization kept grid Peclet numbers below 2.1. However, due to memory and CPU time constraints, reducing the grid size cut the size of the model domain by one half. Therefore, the growth characteristics could only be sampled for approximately 30 hours.

Shown in Figure 35 are the growth rate curves for the five simulations, which are plotted in terms of normalized amplitude versus time. Normalized amplitude is the ratio between the amplitude of a designated instability and the amplitude of the initial perturbing function. By following the particular instability in time, one interprets instability growth by normalized amplitudes that increase with time, and instability decay by normalized amplitudes that decline in time. The growth curves for these simulations (Figure 35) show that instability growth and decay are highly sensitive to changes in dispersivity. Reducing the dispersivities by a factor of 0.75 (curve d) from the base case (curve c) increased the growth rate by a factor of 2.1, as sampled at t = 24 hrs. Reducing the dispersivity even more (0.5 of the base case) increased the growth rate by a factor of 3.3 (curve e, sampled at t = 24 hrs). Although the
fining of the grid prevented calculation of growth rates past approximately 30 hours, the trend of the curves (d) and (e) in Figure 35 indicate that growth rates will continue increasing until intense plume mixing, caused by instabilities, diminishes the density difference. At that point the growth rate would be expected to fall off rapidly, as illustrated in chapter III (Figure 30) with the 3000 mg/L plume.

Increasing dispersivity above the base-case value significantly reduced the growth rate of instabilities (Figure 35). An increase by a factor of 1.5 (curve b), over the base case (curve c), resulted in perturbations only growing to a maximum normalized amplitude of 1.4. After just 45 hours the perturbation decays to below the amplitude of the source perturbation. When the dispersivities are increased by a factor of 2 (curve a), the perturbation rapidly decays and the plume is never unstable.

Clearly, there are other adjustable parameters such as fluid density, which, like dispersivity, have the potential of promoting greater or less stability in the plume. An obvious question is the extent to which factors promoting instability are able to compete with each other. For example, how does a plume respond to increasing the density contrast (a destabilizing factor), and increasing the dispersivity (a stabilizing factor). This issue was examined with a separate simulation where the initial concentration was increased to 3000 mg/L NaCl, and dispersivities ($\alpha_p=0.002m$, $\alpha_r=0.0004m$) were double the base case values. Although perturbations did grow and the plume
became unstable, the growth rate of the instability was greatly reduced (results not shown). At t=24 hours the normalized amplitude was approximately 2, 5 times less than the normalized amplitude (≈10) of the same simulation with \( \alpha_x=0.001 \) m, \( \alpha_y=0.0002 \) m.

Sensitivity of Velocity

The influence of the velocity of the groundwater flow field was investigated with three simulations with a 2000 mg/L NaCl plume in three different velocity fields. The average linear groundwater velocity was reduced by a factor of 0.75 (\( v=2.07\times10^{-6} \) m/s) and increased by a factor of 1.5 (\( v=4.16\times10^{-5} \) m/s) with respect to the base velocity of \( 2.76\times10^{-6} \) m/s. The growth rate curves for the three 2000 mg/L NaCl simulations are shown in Figure 36. Here, the normalized amplitude is plotted versus distance, as compared to versus time in the previous plots, so that growth rates can be compared to a common point of reference. Clearly instabilities are also very sensitive to the velocity field. Increases in velocity dampen instability growth, whereas decreases in velocity enhance instability growth.

Hydrodynamic dispersion (\( D \)) occurs as a consequence of two processes, mechanical dispersion and diffusion (Domenico and Schwartz, 1990):

\[
D = D' + D''
\]  

(15)

The coefficient of mechanical dispersion (\( D' \)) can be defined parallel
Figure 35. Growth rate curves for perturbations to a 2000 mg/L NaCl source plume, simulated with homogeneous media and five different dispersivities: a) $\alpha_l=2.0 \times 10^{-3} \text{ m}$, $\alpha_d=4.0 \times 10^{-4} \text{ m}$; b) $\alpha_l=1.5 \times 10^{-3} \text{ m}$, $\alpha_d=3.0 \times 10^{-4} \text{ m}$; c) $\alpha_l=1.0 \times 10^{-3} \text{ m}$, $\alpha_d=2.8 \times 10^{-4} \text{ m}$; d) $\alpha_l=7.5 \times 10^{-4} \text{ m}$, $\alpha_d=1.5 \times 10^{-4} \text{ m}$; e) $\alpha_l=5.0 \times 10^{-4} \text{ m}$, $\alpha_d=1.0 \times 10^{-4} \text{ m}$

Figure 36. Growth rate curves for perturbations to a 2000 mg/L NaCl source plume, simulated with a homogeneous medium and three different velocity fields.
and perpendicular to the direction of mean flow in a homogeneous and isotropic medium as:

\[ D'_x = \alpha_x v \quad D'_y = \alpha_y v \]  \hspace{1cm} (16)

where \( v \) is the linear groundwater velocity. The contribution of diffusion to the process is represented by the bulk diffusion coefficient \( (D'_x)' \). Therefore, because the coefficient of mechanical dispersion is the product of dispersivity and velocity, changing the velocity in this series of runs also changes the dispersion coefficient. If \( D'_x \) or \( D'_y \) was studied to establish its influence on instability behavior, the effects of changing dispersivity by a constant is the same as changing velocity by the same constant. When the growth rate curves for increasing/decreasing dispersivity by a factor of 1.5 and 0.75, respectively, are plotted along with the same curves for increasing/decreasing velocities by the same factor (Figure 37), it can be seen that although the growth rates are fairly similar, they are not identical. Clearly, instability growth/decay is slightly more sensitive to changes in dispersivity than they are to changes in velocity. In addition, the effect of the two parameters is different and not represented by their product in the form of the coefficient of hydrodynamic dispersion. This could be, in part, due to the appearance of both \( D' \) and \( v' \) separately in the continuity equation governing advective-dispersive mass transport (equation 9).
Sensitivity of Permeability

The sensitivity of instability development to changes in permeability was investigated with four simulations. The first three involved a homogeneous/isotropic simulation (i.e., $k_x = k_z = \text{constant}$) and a 2000 mg/L NaCl source, which is perturbed with a 71.5 mm wavelength sinusoidal perturbation. These three simulations employ the subset grid (shown by the dashed lines in Figure 13) discretized ($\Delta x$, $\Delta y$) at 2.5 mm. Permeability values, $k_x$ and $k_z$, are increased/decreased by a factor of 1.5 and 0.75, respectively, over the base-case permeability of $5.7 \times 10^{-11}$ m$^2$. A plot of the growth rate curves for the three simulations (Figure 38) shows that increasing permeability enhances instability growth, whereas decreasing permeability dampens instability growth. The small reduction in permeability by a factor of 0.75, for this particular combination of perturbation wavelength and plume density, resulted in a plume that is essentially stable. The perturbations grew to a normalized amplitude of 1.6 after approximately 33 hours. This result can be compared to a normalized amplitude of 1.4, after approximately 33 hours, for an increase in permeability by a factor of 1.5. This direct relationship was expected from the form of the Rayleigh number (equation 12) shown in chapter III. Although the Rayleigh number may not be a predictor of stability, the equation correctly expresses the relationships among the variables, that is, proportionality (or inversely proportionality).
Figure 37. Growth rate curves for changing dispersivity by a factor of 0.75 and 1.5 (from Figure 35) plotted together with growth rate curves for changing velocity by a factor of 0.75 and 1.5 (from Figure 36).

Figure 38. Growth rate curves for perturbations to a 2000 mg/L NaCl source plume, simulated with homogeneous media and three different permeabilities: a) \( k_x = k_z = 8.55 \times 10^{-11} \text{ m}^2 \) (1.5x base \( k \)); b) \( k_x = k_z = 5.7 \times 10^{-11} \text{ m}^2 \) (base \( k \)); c) \( k_x = k_z = 4.275 \times 10^{-11} \text{ m}^2 \) (0.75x base \( k \)).
As was the case for dispersivity, it is possible to compare the impact of variables that contribute similarly to stability or instability. In this respect, a comparison can be made between the impact of increasing the permeability to increasing salinity. Both of these changes push the plume towards being more unstable. Figure 39 compares the growth curves for cases where permeability is increased by a factor of 1.5, and the source concentration is increased to 3000 mg/L NaCl (increase in concentration/density by a factor of 1.5; permeability=5.7x10^{-11} m^2, base value). The curves are remarkably similar. They overlap at early times and slowly diverge (Figure 39). Therefore, initially the effect of increasing the permeability by a factor of 1.5 is the same as increasing the plume density by a factor of 1.5. The divergence at later times occurs because dispersion reduces the plume density, reducing the tendency for instabilities to grow. However, the effect of permeability remains the same for all time.

The permeability of natural geologic media often has a directional quality due to the way materials are deposited and lithified. Excluding fractured rocks, the anisotropy typically is such that horizontal permeability is larger than vertical permeability. To examine the effect of anisotropy on instability propagation, the case of a 3000 mg/L source that was reported in Figures 30 to 32, was re-run with the vertical permeability reduced by a factor of 5 (k_x=5.7x10^{-11} m^2, k_z=1.4x10^{-11} m^2). Unlike the earlier results that exhibited instability growth, anisotropy
produces the opposite effect. Perturbations rapidly decay and density effects are negligible (Figure 40). In fact, the plume resembles a neutral density plume with a slight downward trajectory. This result is actually quite understandable in light of the earlier discussion on the origin of instabilities. Recall that in order for instabilities to form, more dense fluid must move downward and less dense fluid must move upward to balance the denser movement. This condition was evident from the plots of vertical groundwater velocities (e.g., Figure 32). When an anisotropic \( (k_x > k_y) \) but homogeneous domain is simulated, downward or upward fluid motions are resisted with preferential fluid flow in a more horizontal direction. Therefore, deterministic anisotropy greatly dampens instability growth.

After looking at this particular simulation, one may hypothesize that because natural geologic media are anisotropic, instabilities may not form very easily or perhaps at all. However, we know from laboratory experiments (Schincariol and Schwartz, 1990) that in layered and lenticular media, which by virtue of their pattern of layering would be expected to have an equivalent \( k_x/k_z > 1 \), instabilities grow and greatly affect plume geometries. The difference between this simulation and the laboratory experiments, or other natural porous media, is that this simulation was perfectly homogeneous, whereas natural porous media are never "perfectly" homogeneous. Therefore, the examination of instability propagation presented thus far, would suggest that it is the heterogeneous nature
Figure 39. Growth rate curve for an increase in permeability by a factor of 1.5 ($k=8.55 \times 10^{-11} \text{ m}^2$, 2000 mg/L - from Figure 35), plotted with the growth rate curve for a increase in density by a factor of 1.5 (3000 mg/L), simulated with the base permeability ($k=5.7 \times 10^{-11} \text{ m}^2$).

Figure 40. Contoured concentration distribution for a 3000 mg/L NaCl source plume, simulated with a homogeneous medium and an anisotropic permeability field, at 72 hours ($k_x=5.7 \times 10^{-11} \text{ m}^2$, $k_y=1.14 \times 10^{-11} \text{ m}^2$).
of porous media that allows vertical fluid exchange and instabilities to propagate in an anisotropic permeability field \((k_x/k_z > 1)\).

**Perturbations and the Heterogeneous Field**

The analysis of the probabilistic conceptualization begins with an examination of how instability formation and propagation depend on the heterogeneous spatial structure in permeability. All of the analyses in this section involve three realizations (#'s 1, 2, and 3), which are represented by the statistics in Table 5. The magnitudes of the variance in the log-transformed permeability field and correlation lengths are small for these realizations, and thus are designed to represent the small scale variability that might exist in natural media at a scale of less than 1 meter (i.e., the domain \(1.1m \times 0.5m\) vertical slice).

This choice of parameters is justified on the basis of data from the Borden aquifer. Sudicky (1986) reported the results of a statistical analysis of a detailed set permeability measurements on a large number of core samples. He found that an exponential covariance model with a variance equal to 0.29, an isotropic horizontal correlation length equal to about 2.8m, and a vertical correlation length of 0.12m, characterized the macro-scale heterogeneous structure of a two-dimensional cross section. The component of the overall variance due to small-scale variability and any measurement error, typically regarded as the "nugget effect", was
0.09. Because the permeability data were on a regular-spaced grid with 0.05m vertical and 1.0m horizontal spatial discretization, this small-scale variability could be considered representative of that seen in a sample of porous media, over relatively small horizontal distances, such as in the simulation domain represented here.

Plots of realizations 1, 2, and 3 are shown in Figures 41, 42, and 43, respectively. All three realizations were generated from the same random number seed. Therefore, the permeability fields are similar, differing only in correlation length and variance, as noted.

Realization #1 (Figure 41) is used as the base case for subsequent analyses. This field has the smallest correlation length of the three (Table 5) Assigning $\lambda_r=0.05m$ provides four nodes per correlation in the "z" or transverse direction. This is about the smallest number of nodes that should be used to keep discretization errors to an acceptable level. In addition, the spatial discretization of the field generator must match that of the transport code. With a variance of 0.05, 95.4 percent of all permeability values would fall from -24.036 to -23.160, or in arithmetic space from 3.6x10^{-11} to 8.9x10^{-11} m^2, which is a contrast in values of approximately 2.5. As Table 5 indicates, realizations 1 and 2 differ only in terms of the correlation length in the x-direction, whereas realizations 1 and 3 differ only in terms of the variance in permeability.

Before beginning the actual analysis, it was necessary to conduct model trials to establish whether instabilities could develop
without perturbing the source. When a 5000 mg/L source plume is developed in realization #1 (Figure 44) the plume sank rapidly and contacted the lower boundary shortly after 36 hours. With a concentration of 2000 mg/L, density effects on plume trajectory were small (Figure 45). In neither case was the heterogeneous structure capable of generating instabilities. However, very slight long-wavelength undulations on the lower plume interface of the 2000 mg/L simulation formed (Figure 45).

These simulation results suggest that in order to create instabilities it is necessary to perturb the lower interface of the source. A 71.5mm wavelength and 2.5mm amplitude perturbation, served the purpose as before with the homogeneous media simulations. When the 2000 mg/L plume is perturbed, instabilities grow very slowly (Figure 46). With a density increase to 3000 mg/L instabilities at first grow slowly, but then growth increases rapidly (Figure 47). When the density is increased to 5000 mg/L, instabilities grow rapidly and contact with the lower flow boundary causes instabilities to coalesce (Figures 48 and 49).

A more detailed analysis of these results shows the influence of local scale heterogeneity on the growth/decay of instabilities. In Figures 50 and 51, c/c_0=0.1 and 0.5 contours for the 2000 mg/L and 3000 mg/L plumes are superimposed on the permeability field, and in Figure 52 the growth rate curves for the two plumes are plotted. In the case of the 2000 mg/L plume instabilities grow slowly and irregularly as they traverse the permeability field. Interspersed
Figure 41. Permeability field realization #1 ($\mu=5.7 \times 10^{-11}$ m$^2$, $\sigma_y^2=0.05$, $\lambda_x=0.05$ m, $\lambda_z=0.01$ m).

Figure 42. Permeability field realization #2 ($\mu=5.7 \times 10^{-11}$ m$^2$, $\sigma_y^2=0.05$, $\lambda_x=0.15$ m, $\lambda_z=0.01$ m).
Figure 43. Permeability field realization #3 (μ=5.7x10^{-11} m², σ_y²=0.11, λ_x=0.05 m, λ_z=0.01 m).

Figure 44. Concentration shade map for a 5000 mg/L NaCl source plume, at 36 hours, simulated with permeability field realization #1.
Figure 45. Concentration shade map for a 2000 mg/L NaCl source plume, at 72 hours, simulated with permeability field realization #1.

Figure 46. Concentration shade map for a perturbed 2000 mg/L NaCl source plume, at 72 hours, simulated with permeability field realization #1.
Figure 47. Concentration shade map for a perturbed 3000 mg/L NaCl source plume, at 72 hours, simulated with permeability field realization #1.

Figure 48. Concentration shade map for a perturbed 5000 mg/L NaCl source plume, at 36 hours, simulated with permeability field realization #1.
Figure 49. Concentration shade map for a perturbed 5000 mg/L NaCl source plume, at 60 hours, simulated with permeability field realization #1.

Figure 50. Overlay of the c/c₀=0.1 and 0.5 contours, for a perturbed 2000 mg/L NaCl source plume, simulated with permeability field realization #1 (the 0.5 contour is not labeled so that instabilities can be defined completely).
Figure 51. Overlay of the $c/c_0=0.1$ and 0.5 contours, for a perturbed 3000 mg/L NaCl source plume, simulated with permeability field realization #1 (the 0.5 contour is not labeled so that instabilities can be defined completely).

Figure 52. Growth rate curves for perturbations to a 2000 mg/L NaCl source plume (curve a), and a 3000 mg/L NaCl source plume (curve b), simulated with permeability field realization #1.
with this modest growth are periods of increased growth that occurs in more permeable zones with fewer low permeability lenses. After approximately 0.35 m, just after a maximum normalized amplitude of approximately 2.0 is reached (Figure 52), instabilities rapidly decay as they enter a zone containing low permeability lenses. With an increase in density to 3000 mg/L the plume follows a different trajectory. Initially, instability growth is slow as instabilities traverse a zone of low permeability. However, approximately 0.2 m into permeability field, the growth rate rapidly increases as instabilities encounter a higher permeability area. Further along the flow path, approximately 0.38 to 0.6 m (or column 150 to 240), this high permeability zone and the overlying low permeability zone result in a more asymmetrical shape to the instabilities (see c/c₀=0.5 contour in Figure 51).

Using the results from simulations with realizations 1 and 2, it is possible to examine how changing the correlation length in the x-direction, λₓ, influences the growth of instabilities. Values of λₓ for these two trials are 0.05 m and 0.15 m respectively. With constant values of λₓ, this parameter choice produces λₓ/λₓ, or "a" values of 0.20 and 0.067, respectively. These ratios are also useful parameters to consider because stochastic process theory indicates that the effective permeability in the x and z-directions, for a heterogeneous medium, changes as a function of e (Dagan, 1989).

The growth-rate curves suggest that with larger values of λₓ or smaller e, perturbations in the 2000 mg/L plume decay much earlier in
time as the low permeability lenses apparently inhibit instability growth (see $c/c_0=0.5$ contour in Figure 53, and growth curve (a) in Figure 54). With a density increase to 3000 mg/L, the larger density-driving forces for instability maintain the slow growth of perturbations through the low permeability zone, until the lower portion of the plume enters a higher permeability area, where growth then increases rapidly (Figures 55 and 54). Overall perturbations continue to grow throughout the simulation, with the growth rates reduced by approximately 10 to 20 percent, as compared to the same simulation in realization #1.

The next simulations with realizations #’s 1 and 3 compare cases that differ only terms of the variance, 0.05 and 0.11, respectively (Table 5). With a variance of 0.11, 95.4 percent of all permeability values would fall from $2.9 \times 10^{-11}$ to $1.1 \times 10^{-10}$ m$^2$, which is a contrast in values of approximately 3.8. When a 3000 mg/L plume is simulated in the field with the greater variance, perturbations initiated at the source initially grow very slowly (Figures 56 to 58), as compared to those propagated in a permeability field with a lower variance (Figure 47 and 52). After nearly dying out, as normalized amplitudes vary slightly above and below the source perturbation amplitude, instability growth rate increases as the plume enters a higher permeability area. Interpreting these results is relatively difficult because differences in behavior appear to be influenced by local variability in the permeability field.
Figure 53. Overlay of the $c/c_0=0.1$ and 0.5 contours, for a perturbed 2000 mg/L NaCl source plume, simulated with permeability field realization #2 (the 0.5 contour is not labeled so that instabilities can be defined completely).

Figure 54. Growth rate curves for perturbations to a 2000 mg/L NaCl source plume (curve a), and a 3000 mg/L NaCl source plume (curve b), simulated with permeability field realization #2.
Figure 55. Overlay of the $c/c_0 = 0.1$ and 0.5 contours, for a perturbed 3000 mg/L NaCl source plume, simulated with permeability field realization #2 (the 0.5 contour is not labeled so that instabilities can be defined completely).

Figure 56. Concentration shade map for a perturbed 3000 mg/L NaCl source plume, at 72 hours, simulated with permeability field realization #3.
Figure 57. Overlay of the $c/(c_0) = 0.1$ and 0.5 contours, for a perturbed 3000 mg/L NaCl source plume, simulated with permeability field realization #3 (the 0.5 contour is not labeled so that instabilities can be defined completely).

Figure 58. Growth rate curve for perturbations to a 3000 mg/L NaCl source plume simulated with permeability field realization #3.
The Formation of Instabilities in Natural Geologic Systems and Their Role in Promoting Contaminant Mixing

The simulation results provide a basis for identifying the hydrogeologic conditions that appear to promote the growth of instabilities in variable-density flow. Instabilities grow most easily in high permeability zones with the effect of increasing permeability being approximately equal to the effect of increasing the density of the plume. From deterministic simulations with varying dispersivity, it was found that reducing dispersivities promotes instability growth, whereas small increases can readily dampen perturbations to the plume interface so instabilities never form. The velocity of the ambient flow field exhibits a similar effect with a slow velocity field promoting instability growth. These results are in line with the approximate analysis presented by List (1965). However, his analysis did not couple the dispersion coefficient and velocity as was done in this study.

The probabilistic simulations allow me to begin to cast the deterministic results in a more realistic geologic framework. In heterogeneous media, it is likely that one will encounter at least two types of instabilities. There will be instabilities that form due to the growth of small fluctuations of the density interface, which predominate in the present analysis. However, other "instability-like" features may form because of the interaction of the variable-density flow with the heterogeneous field. To
illustrate this idea, consider the results of simulations with realization #4 (Figure 59). Unlike the other realizations, the one depicted in Figure 59 has a larger variability that is comparable, for example, to the Borden site, and somewhat larger correlation length scales (see Table 5). When a relatively dense plume with a 5000 mg/L NaCl source is simulated with this permeability field, and no "user applied" perturbations to flow occur, a small lobe forms on the lower edge of the plume early in the simulation (Figure 60). After 72 hours the small lobe has been smoothed out and the nose of the plume begins a downward trajectory, as it follows the higher permeability zone, in the lower right portion of the permeability field (Figure 61). The time sequence shown in Figure 62 better illustrates the evolution of this perturbation. The lobe was formed early in the simulation as a consequence of the dense plume interacting with a lower permeability lens on downward trajectory. The plume dominantly follows the higher permeability zones, and when it encountered a lower permeability lens, a portion of the plume was essentially deformed around the low permeability zone. This bifurcation of mass around lenses also was observed in flow tank experiments conducted in a lenticular medium by Schincariol and Schwartz (1990). In this simulation it appears that the perturbation was essentially stable, although this may not be the case in other heterogeneous permeability fields.

The feature that is described has the appearance of an instability but differs from the interface instabilities previously
Figure 59. Permeability field realization #4 (μ=5.2x10^{-11} m^2, 
σ_y^2=0.18, λ_x=0.25 m, λ_y=0.05 m).

Figure 60. Concentration shade map for a 5000 mg/L NaCl source, at 
36 hours, simulated with permeability field realization 
#4.
Figure 61. Concentration shade map for a 5000 mg/L NaCl source, at 72 hours, simulated with permeability field realization #4.

Figure 62. Overlay of the $c/c_0=0.1$ concentration contour for a 5000 mg/L NaCl source plume, at various times (t=12, 18, 36, 48 and 72 hours), on the permeability field (realization #4).
described. It is likely that these instability-like features can be expected to develop in more highly heterogeneous permeability fields. These features appear to have a counterpart in immiscible flow in terms of heterogeneous fingering, which has its origins in the heterogeneous structure of the medium rather than classical interfacial instabilities. This is an area of active study, which potentially can be resolved with much larger fields.

These simulations strengthen the hypothesis that it is very small-scale heterogeneities that initiate perturbations to flow and thus instability formation. Natural perturbations developed both due to plume splitting (Figure 60), and very gentle long-wavelength perturbations or undulations developed with the 2000 mg/L simulation, in the finest correlation structure (Figure 45). However, it was not possible with the existing random-field generator to incorporate very small-scale heterogeneity in the permeability field. These features appear to be necessary to create the narrow instabilities observed experimentally in the sand tank (Figures 8 to 11).

Another question that remains to be examined in more detail is how local variability in small-scale heterogeneity and resulting flow conditions work to control the propagation and growth of instabilities. Several of the probabilistic simulations showed that small areas with low-permeability lenses can effectively dampen instability growth, or in the case of only a weakly unstable plume, completely stabilize any perturbations. The longer the correlation among these low permeability lenses, the more effective they are at
dampening the upward and downward fluid motions that are synonymous with instabilities. This result conceptually can be expected from stochastic process theory because as $\lambda_z/\lambda_x$ gets smaller, the medium effectively becomes more anisotropic (Dagan, 1989). Greater variance in the permeability field also can dampen instability growth when local low permeability zones overpower the density-dependent flow forces and instability fluid motions.

Instability propagation, in a mildly heterogeneous medium, is controlled by the balance between the variability of the permeability field and the density difference between the plume and ambient groundwater. The experimental work of Schincariol and Schwartz (1990) found that for their particular lenticular media, which had a permeability range of $3.1 \times 10^{-10}$ to $1.2 \times 10^{-11}$ m$^2$, although instabilities readily formed in a 2000 mg/L NaCl source plume, in a homogeneous and isotropic medium, they did not form in the lenticular media. The lenses acted to inhibit vertical motion and instability development. With a source density increase to 5000 mg/L, the combination of free and forced convection gave rise to much more complicated patterns of spreading. When the density was increased to 10,000 mg/L density driven flow began to overpower the influence of the ambient flow and small lobular instabilities, similar to those observed in the homogeneous medium (Figure 9), formed along the lower upgradient portion of the plume.

The importance of the "local" field versus "asymptotic" or full field parameters can be further examined by calculating the
asymptotic longitudinal and transverse dispersivities and macrodispersivities. The theoretical equation, which assumes unidirectional mean flow and an exponential covariance, is provided by Gelhar and Axness (1983):

\[ A_L = \frac{\sigma_L^2 \lambda}{\gamma^2} \]  \hspace{1cm} (17)

where \( A_L \) is the asymptotic longitudinal dispersivity, \( \sigma_L^2 \) is the variance of the log-transformed permeability (i.e. \( Y = \ln k \)), \( \lambda \) is the correlation length in the mean direction of flow, and \( \gamma \) is a flow factor that Dagan (1982) considers equal to one. Therefore, \( A_L \) represents the macroscopic dispersion created by the heterogeneous structure of the porous medium through variability in velocity. The contribution of the local or pore-scale component, dispersivity (\( \sigma_L \)) and diffusion, are accounted for directly with the input parameters to the transport model. The overall longitudinal and transverse asymptotic macrodispersivity (\( A_L^* \) and \( A_T^* \), respectively) can be calculated from:

\[ A_L^* = A_L + \alpha_L + \frac{D_d^*}{v} \]  \hspace{1cm} (18)

\[ A_T^* = \alpha_T + \frac{D_d^*}{v} \]  \hspace{1cm} (19)

where \( D_d^* \) is the bulk diffusion coefficient and \( v \) is the linear groundwater velocity. The transverse asymptotic dispersivity (\( A_T \)) is zero implying that the heterogeneous structure of the porous medium
does not create transverse dispersion (Sudicky, 1986).

Utilizing these equations the asymptotic dispersivities can be calculated (Table 6). Among permeability realizations 1 to 3, the field with the highest asymptotic dispersivity and macrodispersivity is realization #2, whereas realization #1 has the smallest values. Although, if the growth curves for the 3000 mg/L simulations are plotted together (Figure 63), the growth rates for these two fields are very similar. This is in marked contrast to the results of the dispersivity sensitivity simulations in the homogeneous media where smaller differences in the dispersion parameters resulted in very different growth rates. Among these three probabilistic simulations, the greatest difference is with realization #3 where the increased variance in permeability effectively dampened instability growth early in the simulation.

Overall, if the particular geologic environment can create perturbations to flow at wavelengths greater than the critical wavelength, instabilities will begin to grow. If the heterogeneous nature of the porous medium does not overpower the undulating velocity field caused by instabilities, the instabilities will significantly promote contaminant mixing until this mixing reduces the density gradient at which point instabilities will decay. If the natural variations in the flow field and low permeability lenses dampen instability growth significantly the contaminant mixing will be dominated by the geologic nonidealities that generate mechanical dispersion at various scales. As stated previously, a certain
Table 6. Macrodispersivities

<table>
<thead>
<tr>
<th>Realization Number</th>
<th>#1</th>
<th>#2</th>
<th>#3</th>
<th>#4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_L^*$ (m)</td>
<td>3.7x10^{-3}</td>
<td>8.7x10^{-3}</td>
<td>6.7x10^{-3}</td>
<td>4.6x10^{-2}</td>
</tr>
<tr>
<td>$A_L$ (m)</td>
<td>2.5x10^{-3}</td>
<td>7.5x10^{-3}</td>
<td>5.5x10^{-3}</td>
<td>4.5x10^{-2}</td>
</tr>
<tr>
<td>$\alpha_L$ (m)</td>
<td>1.0x10^{-3}</td>
<td>1.0x10^{-3}</td>
<td>1.0x10^{-3}</td>
<td>1.0x10^{-3}</td>
</tr>
<tr>
<td>$D_L*/\nu$ (m)</td>
<td>2.0x10^{-4}</td>
<td>2.0x10^{-4}</td>
<td>2.0x10^{-4}</td>
<td>2.2x10^{-4}</td>
</tr>
<tr>
<td>$A_T^*$ (m)</td>
<td>4.0x10^{-4}</td>
<td>4.0x10^{-4}</td>
<td>4.0x10^{-4}</td>
<td>4.2x10^{-4}</td>
</tr>
<tr>
<td>$\alpha_T$ (m)</td>
<td>2.0x10^{-4}</td>
<td>2.0x10^{-4}</td>
<td>2.0x10^{-4}</td>
<td>2.0x10^{-4}</td>
</tr>
</tbody>
</table>
Figure 63. Growth rate curves for perturbations to a 3000 mg/L NaCl source plume developed in three different permeability field realizations.
balance must exist between the forces of density dependent flow and the variable velocity/permeability field for instabilities to propagate. For plumes of low to moderate density, instabilities would probably most easily propagate in a high permeability, relatively homogeneous, environment. This geologic environment is represented "experimentally" with the flow tank experiments conducted in the "homogeneous/isotropic" media, plumes shown in Figures 8 to 11, and numerically with the small-scale heterogeneous simulations (Figures 46 to 49). As plume density increases, as long as the forces of density dependent flow do not overpower instability propagation, a more heterogeneous, lower permeability media, can also be expected to propagate instabilities.

It is the balance between the variability in the permeability field, and the forces of density dependent flow and ambient groundwater flow, which precludes expressing plume density quantitatively in the preceding statements. Essentially, the complexity of instability growth and propagation in a "plume" environment necessitates a numerical modeling approach to assess whether or not instabilities will form.
CHAPTER V
SUMMARY AND CONCLUSIONS

The major findings of this study are summarized in the following sections in relation to the major thrusts of the research, namely (i) image processing and validation data sets, and (ii) instabilities in variable-density flow.

Image Processing and Validation Data Sets

Image processing techniques provide an excellent way to obtain concentration distributions in flow-tank experiments where the dye can be observed through a glass or plexiglas wall. The technique is noninvasive, does not disturb plume dynamics, and provides detailed concentration data over the whole plume, as observed at the tank wall. Concentration data were obtained on a 1.3 x 1.3 mm grid, which represents approximately \(4.4 \times 10^2\) measuring points, with a maximum error of approximately 7 to 10%. Most of this error was due to the background subtraction and other correction techniques that were used to correct for the lighting nonuniformities inherent in the original data. At the time the original experiments were run, the requirements for rigorous lighting control were not appreciated. Overall, one should (1) avoid uneven lighting, (2) maintain a
spectrally consistent light source (exclude sunlight from the room), (3) avoid reflections on the tank face of other fixtures around the room, (4) surround the tank with 18% gray cards to assess lighting nonuniformity, (5) have the same gray scale present in all photographs within a calibrated group, (6) clearly mark fiducial points on tank or photographic subject, and (7) maintain consistent film type, exposure, and development techniques. If care is taken with the photographic setup to control room lighting and a broad range of dye concentrations are run for the optical density-concentration calibration curve, the maximum error should be less than a few percent. For additional calibration, point samples can be taken with a syringe through septa ports at known locations. These concentrations can then be compared to the concentrations resulting from image analysis.

**Instabilities in Variable-Density Flow**

(1). In simulations of density stratified systems, instabilities may develop when perturbations to flow occur. These perturbations may occur by themselves in cases where numerical spatial oscillations develop in the solution or may be created by a mathematical perturbation of the interface, at the source, with care taken to assure essentially no numerical errors. Perturbations created through the propagation of numerical errors are virtually uncontrollable because the magnitude and location of the error varies during the simulation. The character of the resulting instabilities,
for this same reason, is different than one would see in experiments, and those generated by perturbing the interface with a specified mathematical function. Similarly, among a series of simulations, small alterations to the dispersion parameters, model grid or time stepping scheme, which alter the grid Courant and Peclet numbers, can cause different styles of instabilities to form. It is, therefore, inappropriate to rely on numerical errors within a code to create perturbations to the plume.

Given that numerical errors may grow to become instabilities, one must control numerical errors to a much greater extent than with linear transport problems. The often cited guidelines to minimize numerical errors in finite-difference and finite-element codes (Pe< 2; Cr< 1), with linear basis and weighting functions, appear to be a useful reference point. In practice, however, the appropriate criteria for a given problem should be established through sensitivity analysis. For the most common finite-difference and finite-element schemes, controlling numerical errors appropriately, in cases where dispersion is small, leads to large model grids and small time steps.

(2). The concept of a critical wavelength (List, 1965; Marle, 1981) extends to the flow and transport problem considered here. As List (1965) suggests, all variable-density problems with a more dense fluid overlying a less dense fluid are potentially unstable. What is required to create instabilities, within the spectrum of potential
perturbations, is for the perturbation to be above the critical wavelength. The analyses presented here have shown that below concentrations of about 1000 to 2000 mg/L NaCl the critical wavelength will begin to increase dramatically. However, these concentrations will vary depending upon the problem parameters.

Practically, it becomes harder and harder to cause stratified systems with diminishing density contrasts to become unstable. Perturbations with very long wavelengths cannot be propagated because the length of time is so great that dispersion/diffusion smooths out the perturbation before it has time to develop one wavelength or grow. Ideally, one would probably need a system with no dispersive capabilities to demonstrate instability at small density contrasts.

(3). There are other ways in which the propagation of instabilities depend upon the dispersive characteristics of any system. List’s (1965) work, and this work, have shown that instabilities tend to develop most easily in weakly dispersive systems. Within a particular simulation, the effects of dispersion will ultimately spread the mass and cause the instabilities to begin to breakdown. This behavior is reflected by a leveling off or gradual decline in the rate of growth of instabilities.

(4). The inverse relationship between the critical wavelength and density explains the observation that in porous media the greater the density difference the more likely that instabilities will occur.
Experiments normally depend upon the medium alone to perturb the interface. An isotropic/homogeneous medium can likely only create interface perturbations up to a maximum wavelength. Thus, there will appear to be some density difference at which apparent stability of the system is achieved. However, the system would again be unstable once a perturbing function of the appropriate wavelength is applied at the source. Eventually, the dispersive tendencies of the system would defeat any long-wavelength perturbation.

These observations and theoretical arguments would suggest that the simple Rayleigh stability criterion, developed for problems of free convection in a box, should not be generally applicable to the instability problem studied here. One can at best speculate about the nature of the stability criterion. Clearly some parameters would remain (e.g., apparent diffusivity) but others would be required such as the wavelength of the perturbing function.

(5). Through sensitivity analyses with the deterministic conceptualization, the growth/decay of instabilities was examined with respect to the dispersive characteristics of the medium, the average linear flow velocity, and the permeability. These simulation results identified the hydrogeologic conditions that appear to promote the growth of instabilities in variable-density flow. Instabilities grow most easily in higher permeability zones with the effect of increasing permeability, at least initially, being approximately equal to the effect of increasing the density of the
plume. Instability growth/decay is highly sensitive to changes in dispersivity. Reducing dispersivities promotes instability growth, whereas small increases can readily dampen perturbations to the plume interface so that instabilities never form. The velocity of the ambient flow field exhibits a similar effect, although one slightly less sensitive, with a slow velocity field promoting instability growth.

(6). The probabilistic simulations allowed more realistic geologic environments or permeability fields to be examined, and illustrated the role played by small-scale heterogeneities in controlling instability growth. These simulations show that low permeability lenses can effectively dampen instability growth or, in the case of only a weakly unstable plume, completely stabilize any perturbations. The longer the correlation among these low permeability lenses, the more effective they are at dampening the upward and downward fluid motions that are required for instability growth. Essentially the more anisotropic or heterogeneous a permeability field is, the greater the dampening of instability growth.

Although heterogeneities tend to dampen instability growth, a comparison of a deterministic and the probabilistic simulations of instability propagation in an anisotropic permeability field ($k_x/k_z > 1$) illustrates that it is the heterogeneous nature of porous media that allows vertical fluid exchange and instability propagation.
This conceptualization also illustrates the importance, in modeling variable-density flow, that realistic representations of the heterogeneous and anisotropic nature of the porous media be incorporated into the permeability field.

(7). The probabilistic simulations also illustrate that in heterogeneous media it is likely that one will encounter at least two types of instabilities. There will be those that form due to the growth of small fluctuations of the density interface, and those that form due to bifurcation of mass around lenses. The former type will occur predominately with plumes of low to moderate density and relatively homogeneous permeability fields, whereas the latter in a more variable or heterogeneous media with more dense plumes.

Overall, if the particular geologic environment can create unstable perturbations to the flow, and the heterogeneous nature of the porous medium does not overpower the undulating velocity field caused by instabilities, the instabilities will significantly promote contaminant mixing until this mixing reduces the density gradient, at which point instabilities will decay. With this conceptualization it can be expected, in a natural geologic setting, that the role of instabilities in promoting contaminant mixing will be most important close to the contaminant source.
APPENDIX A

CODE VERIFICATION - Theis
- 1-D Transport
CODE VERIFICATION

As discussed previously in Chapter III the VapourT numerical model has been verified and validated. After porting and compiling the source code for VapourT to the various computer systems where it was to be used (Cray Y-MPA/864, HP 9000/750, and DECSystem 5400), the code was verified against example data sets provided in the VapourT users manual. All simulations agreed with example data sets. Code modifications were then made to VapourT so that saturated zone transport could be simulated. The modified code was then verified against several analytical models testing various characteristics of the code. This model testing is discussed below.

Thesis Verification

The original VapourT code only accounted for fluid (gas) compressibility in the specific storage calculations since gas compressibilities are much larger than the compressibility of the rock matrix. When considering saturated flow both the fluid and matrix compressibilities are important. Thus the code was modified to include both the aquifer and fluid compressibility in the specific storage formulation. Verification of the fluid flow portion of the code was accomplished by comparing drawdown versus time data to that
generated from the Theis equation. Drawdown versus time data were
generated for close, intermediate and distant points from the pumping
well. In all cases model drawdowns were within 1% of drawdown
calculated from the Theis equation (Table 7). In addition the
steady-state drawdowns calculated by the numerical model were
compared to the analytical values as computed from the Theis
equation. The differences in drawdown between several pairs of wells
were within 0.5% of the values calculated from the Theis equation
(Table 8).

Solute Transport

The transport solution generated from VapourT for a ideal tracer
(no density difference or sorption) was compared with an analytical
solution (Wexler, 1989) generated for the one-dimensional solute-
transport equation. A first-type (or Dirichlet) boundary condition
is specified at the inflow end, such that:

\[ c = c_0, \ x = 0 \]  \hspace{1cm} (20)

The analytical solution used in the comparison assumes the system can
be treated as semi-infinite and therefore a first-type or second-type
(Neuman) boundary condition can be specified at the outflow boundary,
such that:

\[ c = 0, \ \frac{dc}{dx} = 0, \ x = \infty \]  \hspace{1cm} (21)
Table 7. Theis Verification Data

<table>
<thead>
<tr>
<th>Radius (m)</th>
<th>Time (s)</th>
<th>Drawdown (m)</th>
<th>Drawdown (m) Vapour</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>720</td>
<td>0.0227</td>
<td>0.0221</td>
<td>2.6</td>
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<td>2160</td>
<td>0.0419</td>
<td>0.0417</td>
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<td>10</td>
<td>7200</td>
<td>0.0649</td>
<td>0.0649</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>21600</td>
<td>0.0866</td>
<td>0.0866</td>
<td>0.2</td>
</tr>
<tr>
<td>10</td>
<td>72000</td>
<td>0.1106</td>
<td>0.1106</td>
<td>0.3</td>
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<tr>
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<td>216000</td>
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<td>0.1325</td>
<td>0.3</td>
</tr>
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<td>7200</td>
<td>0.000396</td>
<td>0.000403</td>
<td>1.8</td>
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<tr>
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<td>21600</td>
<td>0.00526</td>
<td>0.00525</td>
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<tr>
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<td>72000</td>
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<td>0.01977</td>
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<td>0.06129</td>
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<td>0.000709</td>
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<td>720000</td>
<td>0.007908</td>
<td>0.007898</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Input Parameters

- \( Q = 5 \times 10^{-4} \text{ m}^3 \text{ s}^{-1} \)
- \( K = 1.9997 \times 10^{-3} \text{ m} \text{ s}^{-1} \)
- \( D = 1 \text{ m} \)
- \( T = 1.9997 \times 10^{-3} \text{ m}^2 \text{ s}^{-1} \)
- \( \alpha = 1.299 \times 10^{-6} \text{ m}^2 \text{ s}^{-1} \)
- \( \beta = 4.40 \times 10^{-10} \text{ m}^2 \text{ s}^{-1} \)
- \( n = 0.2 \)
- \( S = 0.0127168 \)

Equations

- \( u = \frac{r_2^2 - r_1^2}{4T} \)
- \( s = \frac{Q \sqrt{r_2 - r_1}}{4\pi T} \)
- \( Q = \frac{2\pi KD (s_{m2} - s_{m1})}{2.301 \log(r_2/r_1)} \)

Table 8. Thiem Verification Data

<table>
<thead>
<tr>
<th>( r_2(\text{m}) )</th>
<th>( r_1(\text{m}) )</th>
<th>( s_{m1} - s_{m2} ) Thiem</th>
<th>( s_{m1} - s_{m2} ) Vapour</th>
<th>Percent Difference</th>
</tr>
</thead>
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<td>0.04369</td>
<td>0.04389</td>
<td>0.5</td>
</tr>
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<td>0.5</td>
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<td>0.5</td>
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<tr>
<td>1510</td>
<td>10</td>
<td>0.19954</td>
<td>0.20046</td>
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<td>0.03385</td>
<td>0.5</td>
</tr>
<tr>
<td>470</td>
<td>30</td>
<td>0.10943</td>
<td>0.10994</td>
<td>0.5</td>
</tr>
</tbody>
</table>
A semi-infinite system assumes the outflow boundary of the system being simulated is far enough away from the source such that the boundary will not affect the solute concentrations within the area of interest (Wexler, 1989).

The finite-element grid consisted of 502 nodes defining 500 triangular elements on a one-dimensional grid. The nodal spacing was 0.00635 m (0.25 inches) and the time step was a constant 0.05 hours. The grid Peclet and Courant accuracy and stability numbers were kept well below the established criteria for linear problems [Daw et al., (1985), Pes2 and CrsFe/2]. The second-order accurate centered-in-time (Crank-Nicolson) scheme is used for the flow and transport equations to minimize smearing. As can be seen in Figure 64 points generated from the analytical solution fall almost exactly on the concentration vs. distance curve computed with the VapourT transport algorithm. The model input parameters can be seen in Table 9.
Figure 64. Comparison of VapourT transport algorithm to analytical solution by Wexler (1989).

Table 9. Input Parameters for Solute Transport Problem

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>average linear groundwater velocity</td>
<td>$4.233 \times 10^{-8} \text{ m s}^{-1}$</td>
</tr>
<tr>
<td></td>
<td>(0.6 in h$^{-1}$)</td>
</tr>
<tr>
<td>longitudinal dispersion coefficient</td>
<td>$1.075 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$</td>
</tr>
<tr>
<td></td>
<td>(0.6 in$^2$ h$^{-1}$)</td>
</tr>
<tr>
<td>solute concentration at inflow boundary</td>
<td>1.0 mg L$^{-1}$</td>
</tr>
</tbody>
</table>
APPENDIX B

COMPARISON WITH LABORATORY EXPERIMENTS TO ASSESS DISPERSION PARAMETERS

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Comparison With Laboratory Experiment

The laboratory apparatus, illustrated in Figure 65, is 116.8 cm long, 71.0 cm wide, and 5 cm deep, and was constructed of 1.8 cm Plexiglas. Most flow-tank/porous media parameters needed for the numerical modeling were known from previous studies (Table 3). The dispersion parameters, though, had to be determined through model fitting using concentration data from tracer studies conducted in the flow tank by Schincariol (1989).

Black and white negatives of a 500 mg/L Rhodamine WT solution added to the injection chamber were image processed as discussed in Chapter II. Concentration versus distance plots then were generated along the centerline of the plume and along various transverse sections. Similar plots generated from numerical modeling studies using VapourT then could be compared to the experimental dataset until a fit of the dispersion parameters was obtained.

The model domain and boundary conditions for the laboratory experiments are illustrated in Figure 15. The left and right boundaries are modeled as specified pressure (Dirichlet conditions) and not specified flow (Neumann conditions) as VapourT does not support a Neumann condition for the transport equation if the input concentration is non-zero. The upper and lower boundaries are no-flow boundaries. In order to maximize memory and CPU time
Figure 65. Laboratory apparatus - flow tank.
constraints the tank's upper no-flow boundary was moved to 12.25 cm above the injection chamber. Model studies show that this boundary does not affect the transport or flow processes within the modeled domain.

Multiple grid sizes were used in the dispersion parameter matching process. It soon became evident that the small value of the dispersion parameters necessitated using the finest grid that the DECSYSTEM 5400 (upgraded to the maximum, 64 megabytes of RAM) was capable of handling due to memory constraints. The finite-element grid consisted of 83,626 nodes defining 170,000 triangular elements. The resulting grid uses 200 spaces of 2.5 mm vertically and 425 spaces of 2.5 mm horizontally. An equidimensional spacing was chosen so that grid Peclet and Courant numbers for the x and z directions would be approximately equal when the 2000 mg/L NaCl studies were simulated. The time step was constant at 0.25 hours. The second-order accurate center-in-time (Crank-Nicolson) scheme is used for the flow and transport equation.

Hydrodynamic dispersion occurs as a consequence of two very different processes - diffusion and mechanical dispersion. These two contributions to hydrodynamic dispersion are represented mathematically as (Domenico and Schwartz, 1990):

\[ D = D' + D'_e \]  

(22)

where \( D \) is the coefficient of hydrodynamic dispersion, \( D' \) is the coefficient of mechanical dispersion, and \( D'_e \) is the bulk diffusion coefficient. The coefficient of mechanical dispersion can be defined
parallel and perpendicular to the direction of flow in a homogeneous and isotropic medium (Domenico and Schwartz, 1990):

\[ D'_l = \alpha_L v \quad D'_t = \alpha_T v \]  

(23)

where \( v \) is the linear groundwater velocity in the direction of flow and \( \alpha_L \) and \( \alpha_T \) are the longitudinal and transverse dispersivities of the medium. The bulk diffusion coefficient accounts for the affect of the porous medium's tortuosity. This can be expressed mathematically as (Bear, 1988):

\[ D'_b = \tau D_d \]  

(24)

where \( D_d \) is the free-solution diffusion coefficient.

Initially a value for the tortuosity (\( \tau \)) of the porous media was calculated using the empirical equation developed by Millington and Quirk (1961) and assuming 100% saturation:

\[ \tau = \frac{(\mu_{saturated})^2}{(\mu_{total})^2} \]  

(25)

This resulted in \( \tau = 0.72 \) for the porous medium. This tortuosity value also agreed well with the value of 0.75 found by Sudicky et al. (1985) in their modeling of a laboratory flow tank containing natural sand. Simulations using \( \tau = 0.72 \) resulted in a value of \( 1.16 \times 10^{-9} \) m² s⁻¹ for the bulk diffusion coefficient. The free-solution diffusion coefficient for a dilute NaCl solution is \( 1.61 \times 10^{-9} \) m² s⁻¹ (Robinson and Stokes, 1970). Figures 66, 67, and 68 compare concentration versus distance curves transverse and along the centerline of the plume for the image processed laboratory data and the numerical
Figure 66. Plot of concentration vs. distance for a vertical transect (x=249 mm) through a 500 mg/L Rhodamine WT plume at 54 hours - experimental data and numerical simulation ($\alpha_x=0.45$ mm, $\alpha_y=0.0$ mm, $\tau=0.72$).

Figure 67. Plot of concentration vs. distance for a vertical transect (x=455 mm) through a 500 mg/L Rhodamine WT plume at 54 hours - experimental data and numerical simulation ($\alpha_x=0.45$ mm, $\alpha_y=0.0$ mm, $\tau=0.72$).
Figure 68. Plot of concentration vs. distance through centerline of a 500 mg/L Rhodamine WT plume at 54 hours - experimental data and numerical simulation ($\alpha_L=0.45$ mm, $\alpha_T=0.0$ mm, $\tau=0.72$).
simulations. The transverse dispersivity was assigned a value equal to zero and the longitudinal dispersivity was assigned a value of 0.45 mm. Several studies such as Grane and Gardner (1961) have shown that transverse dispersion is dominated by molecular diffusion at average linear groundwater velocities less than about 1.0 m/day. As illustrated in Figures 66 and 67 the numerical simulation has far too much transverse dispersion. The vertical transects are slightly offset as the plume in the flowtank did not follow a perfect horizontal path as occurs in the numerical simulation. Because the transverse dispersivity was set equal to zero this indicates a much too large bulk diffusion coefficient or tortuosity. Numerical dispersion is not considered to be a problem due to Crank-Nicolson time stepping and the fine grid. Maximum Peclet numbers were about 2.96 in the x direction and 0.32 in the z direction. Courant/Peclet ratio was 0.36 in the x direction and 0.17 in the z direction.

Bear (1988) defines tortuosity as:

\[ \tau = \left( \frac{L}{L_w} \right)^2 \]  

(26)

where \( L \) is the length of the porous medium sample and \( L_w \) is the length of the flow channel for a fluid particle. Values of \( (L/L_w)^2 \) are always less than one. Bear (1988) states that values of \( L/L_w \) vary in the range 0.56 to 0.8. This would then give values of tortuosity \( (L/L_w)^2 \) of 0.56² to 0.8² or 0.31 to 0.64. Successive simulations employing lower values of tortuosity (each taking approximately 60 CPU hours @ 1.6 Mflops for a simulation time of 72
hours) resulted in a good fit of experimental data for parameter values of:

- tortuosity ($\tau$) = 0.35
- bulk diffusion coefficient ($D_q^*$) = $5.635 \times 10^{-10}$ m$^2$ s$^{-1}$
- longitudinal dispersivity ($\alpha_L$) = $3.0 \times 10^{-4}$ m
- transverse dispersivity ($\alpha_T$) = 0.0 m

The resultant transverse and longitudinal dispersion coefficients are:

- $D_L = 3.00 \times 10^{-4} + 2.75 \times 10^{-6} + 5.635 \times 10^{-10}$ m$^2$ s$^{-1}$
- $D_T = 8.25 \times 10^{-10} + 5.635 \times 10^{-10}$ m$^2$ s$^{-1}$
- $D_T = 1.389 \times 10^{-8}$ m$^2$ s$^{-1}$

- $D_T = 0.0 \times 2.75 \times 10^{-6} + 5.635 \times 10^{-10}$ m$^2$ s$^{-1}$
- $D_T = 5.635 \times 10^{-10}$ m$^2$ s$^{-1}$

Concentration versus distance plots, at 54 hours, are illustrated in Figures 69, 70, and 71. Maximum Peclet numbers were about 5.07 in the x direction and 0.65 in the z direction. Courant/Peclet ratio was 0.21 in the x direction and 0.08 in the z direction. Exceeding the Peclet criteria could not be avoided because we are at the maximum grid size that the DRCS system 5400 can handle. Exceeding the Peclet criteria resulted in early time (t=3 hrs) concentration overshoots of a maximum of 4% (C/C$_0$=1.04). These oscillations progressively reduced in time. After 54 hours maximum overshoots were less than C/C$_0$=1.000002.
Figure 69. Plot of concentration vs. distance for a vertical transect ($x=249$ mm) through a 500 mg/L Rhodamine WT plume at 54 hours - experimental data and numerical simulation ($\alpha_x=0.3$ mm, $\alpha_t=0.0$ mm, $r=0.35$).

Figure 70. Plot of concentration vs. distance for a vertical transect ($x=455$ mm) through a 500 mg/L Rhodamine WT plume at 54 hours - experimental data and numerical simulation ($\alpha_x=0.3$ mm, $\alpha_t=0.0$ mm, $r=0.35$).
Figure 71. Plot of concentration vs. distance through centerline of a 500 mg/L Rhodamine WT plume at 54 hours - experimental data and numerical simulation ($\alpha_w=0.3$ mm, $\alpha_t=0.0$ mm, $\tau=0.35$).
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