Web-Based Interactive Simulation of Groundwater Pollutant Fate and Transport

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ABSTRACT: A series of interactive web simulation models were developed to help students understand the coupled physical, chemical, and microbiological processes that affect the transport and fate of pollutants in groundwater. Conventional models that simulate coupled processes are often not effective learning tools because they are too complex, they suffer from cumbersome interfaces, and/or they are difficult to install and run. The web models are fully interactive Java applets that run locally through a web browser. They have graphical user interfaces, straightforward input and output fields, and rapid response times. These features enhance learning because students can rapidly visualize the impact of changes to parameter values and boundary and initial conditions, and explore the effect of different reaction processes. Presently, six different web models have been developed to explore coupled processes such as advection, longitudinal and transverse dispersion, linear or rate limited sorption, and first order decay. A web model was also developed to study the flow patterns caused by multiple pumping wells in two-dimensional steady flow. Several examples of how the models can be used to teach students about coupled processes are discussed. Last, an assessment of the effectiveness of the models to enhance student learning is presented.
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INTRODUCTION

Study of groundwater hydrology and hydraulics has been a traditional part of the curriculum in Civil Engineering and Geology departments. However, the growing importance of contamination and remediation over the past two decades has led to a shifting emphasis toward the study of pollutant fate and transport processes within the groundwater curricula,

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as well as to the development of specialized courses on hazardous waste and contaminant hydrogeology [8,15]. The fate of groundwater pollutants is affected by numerous physical transport, mass transfer, geochemical, and microbiological processes. It is a challenge for an instructor to effectively present these processes and their coupled influence on pollutant behavior.

Mathematical simulation models are invaluable instructional tools for integrating the important underlying physical, chemical, and microbiological processes. These models use mass balance principles as the organizing framework for integrating all the processes into a mathematical representation of pollutant fate and transport. Many recent groundwater texts [3,7,8] emphasize mass balance principles and mathematical modeling, and in fact many textbook figures are direct graphical output of such models. The importance of modeling as a pedagogical tool for groundwater and environmental problems is discussed further by Mohtar and Engel [16] and Kolar and Sabatini [13]. These authors, as well as the general literature on education and teaching improvement [e.g., Davis, 1993], emphasize that computer simulation is an effective teaching tool only if it is interactive and engages students to become active learners.

Despite the pedagogical value of mathematical simulation, the typical engineering instructor has limited access to appropriate models for use at the introductory level. An instructor has the option of purchasing state-of-the-art commercial interfaces, such as Visual MODFLOW (http://www.visual-modflow.com) or the Department of Defense's Groundwater Modeling System (GMS) [12]. These are ''industrial strength'' packages with advanced flexibility and highly sophisticated graphical user interfaces. For an introductory course such flexibility is not necessary and these packages require an excessive amount of learning time for the typical student. Some textbooks describe the use of simulation programs that are included on media that come with the text [e.g., [7,8,9]]. However, the programs are occasionally just presented as supplements for the student, or the codes may lack a friendly and convenient user interface. Several government agencies (e.g., http://water.usgs.gov/nrp/gwsoftware; http://www.epa.gov/ada/csmos.html; http://www.ussl.ars.usda.gov/MODELS/MODELS.HTM) provide a variety of powerful public domain codes that are written in languages such as Fortran and C/C++, however, these codes lack a simple interface and are cumbersome to use for the typical undergraduate student. More recently, spreadsheet-based models have become available. These models are easy to use, but students must either download the application to a computer or the instructor must install the application on a computer network. One of the most widely used spreadsheet models is BIOCHLOR, which solves for three-dimensional contaminant transport with sequential decay. BIOCHLOR is intended to serve as a screening tool for chlorinated solvent natural attenuation; it is described further in the book by Wiedemeier et al. [24] and it is distributed by the US EPA at http://www.epa.gov/ada/csmos/models/biochlor.html.

Web-based technology has the potential to overcome many of the difficulties noted above. Students are comfortable using web browsers for a variety of purposes and thus they are eager to use this same interface for simulation modeling. The web is an ideal vehicle for interactive modeling since students can query the model or modify data and parameters and receive nearly instantaneous response. These advantages have been noted by others working in the educational software field [e.g., 10,17]. There are two different ways the web can be used for interactive simulation. In the first approach, the web serves as an interface to a simulation model that resides on a remote server; students use their web browser to create input files that are sent to the model and the model results are then sent as web pages back to the student. An advantage of this approach is that a powerful central server is able to run computationally intensive models that may require access to large databases; however, communication between the student and the server can be slow depending upon network traffic and quality. Mohtar and Engel [16] provide an example of this approach, where they use the web as an interface to existing large-scale water quality models that require input from weather and GIS databases. In the second approach, fully interactive simulation models can be programmed as Java applets that run locally through a web browser. In this approach communication bottlenecks are avoided, allowing students to rapidly visualize the impact of changes to parameter values and boundary and initial conditions, and to explore the effect of different types of reaction processes. Because of their rapid response time, interactive Java applets are ideal for use during lectures or class demonstrations. Although in this approach complex models cannot be used due to excessive Java execution times, this will become less of a drawback as computer processor speed continues to increase. The purpose of this paper is to describe a series of interactive web simulation models that we have developed and to demonstrate how these models can be used to improve student understanding of pollutant fate and transport. Detailed examples of specific class assignments incorporating these applets are given in Reference [21].

DESCRIPTION OF MODELS

The processes controlling the fate of dissolved contaminants in groundwater systems can be categorized as physical, chemical, and biological. Physical processes include advection (transport with the average flow velocity), molecular diffusion, and mechanical dispersion (the spreading caused by deviations of the local velocity from its average value). There are a wide variety of chemical and biological processes that can affect pollutant behavior. Some of the more significant processes include adsorption and desorption, radioactive decay, and biological transformation. These processes are described in greater detail in groundwater texts [e.g. 7,8]. In our classes we place significant emphasis on understanding each of these processes, and then we use the mass balance principle to develop mathematical models that integrate and couple these processes.

These models often take the form of multi-dimensional partial differential equations, which in general need to be solved by numerical techniques such as the finite difference or finite element method. Although it is certainly possible to program simple finite difference or finite element models as Java applets, for introductory level courses it is often suitable to adopt certain assumptions (i.e., the aquifer is homogeneous and the reactions are linear) so that it becomes possible to develop analytical solutions to the models. Often these solutions involve simple functions (e.g., the error function) that are easily computed. However, in some cases these solutions can be difficult to evaluate since they are in the form of complicated integrals that must be approximated numerically. Before the development of the web models, we were simply not able to consider any of these more complex cases in our classes, which forced us to neglect important processes such as multi-dimensional dispersion, rate-limited mass transfer, and sequential biological transformation.

Table 1 lists the models that we have developed to date. All of these Java applets are accessible at the following web site: www.cee.uiuc.edu/transport. Each applet has links that fully describe the user interface and the model theory. We found it important for students to find the user interface attractive, simple, and flexible. Specific examples illustrating the user interface and model applications are presented in the next section. A typical user interface is presented in Figure 1. As shown, the student has several ways to observe and query the model results: (a) graphical display, (b) display of numerical values via ‘‘sliders’’ that are operated by the mouse, and (c) display of the raw numerical output in a separate window. The last option gives students the flexibility of pasting the results into other programs like Excel to produce additional plots if necessary. This proved particularly useful for graduate students in an advanced numerical

Table 1 Description of Interactive Web Simulation Models

Model	Processes	Reference
Diffusive transport	Diffusion into an empty sphere, diffusion out of uniformly and non-uniformly contaminated spheres	[4]
One-dimensional transport with decay and equilibrium sorption	Advection, longitudinal dispersion, linear equilibrium sorption, first order decay reaction; instantaneous, finite-duration pulse or continuous input of pollutant; first-order decay of source zone concentration; user can input observed concentration data for trial-and-error curve fitting	[11,23]
One-dimensional transport with decay and rate-limited sorption	Advection, longitudinal dispersion, sorption divided into an instantaneous fraction (linear equilibrium) and rate-limited fraction (linear reversible rate), first order decay of dissolved and sorbed solute, finite-duration pulse or continuous input of pollutant	[20]
One-dimensional transport of multiple species with sequential chain decay	Advection and longitudinal dispersion of up to four species undergoing sequential first-order reaction, linear equilibrium sorption, finite-duration pulse or continuous input of pollutant	[22]
Two- and three-dimensional transport with decay and equilibrium sorption	Advection, longitudinal dispersion, transverse dispersion, linear equilibrium sorption, first-order decay, continuous input of solute	[2,6,14]
Two-dimensional steady flow with wells and particle tracking	Superposition of uniform regional flow and injection/extraction wells for homogeneous aquifers; tracking of streamlines and particle paths	[11]

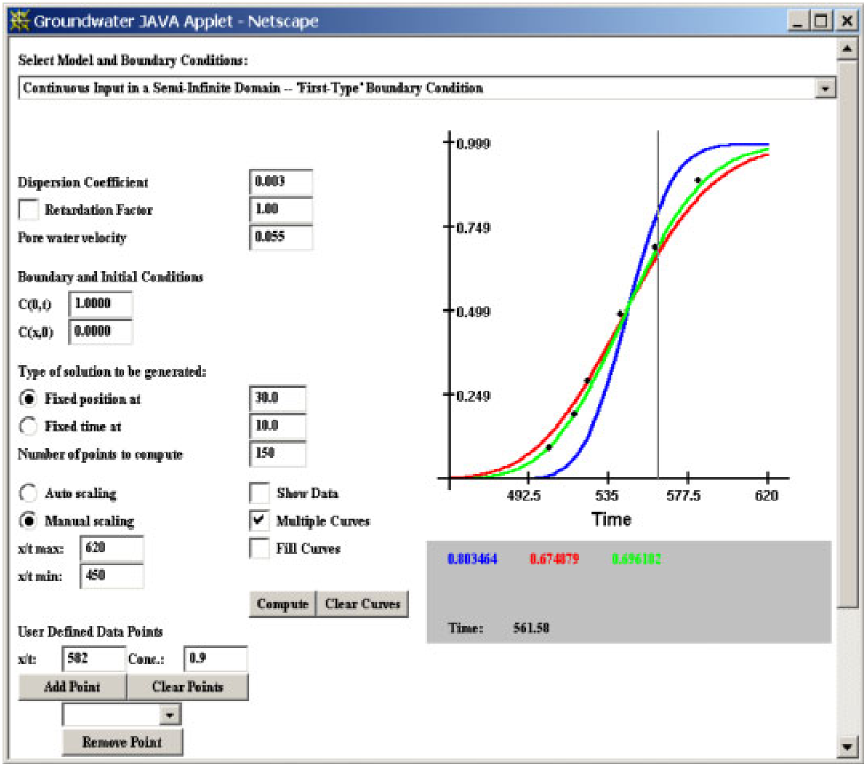

Figure 1 Example of the ‘‘One-Dimensional Transport With Decay and Equilibrium Sorption’’ applet. Results show the concentration breakthrough curve for various values of the dispersion coefficient. Data from a laboratory breakthrough experiment have been added by the user in order to estimate the dispersion parameter. [Color figure can be viewed in the online issue, which is avaliable at www.interscience.wiley.com.]

modeling class, as it enabled them to use the interactive web models to compute analytical solutions that were then plotted for direct comparison with the output from their numerical codes.

EXAMPLES OF HOW THE MODELS CAN BE USED

In this section, we describe a few of the applets in Table 1 and describe how they may be used to illustrate reactive transport processes. We do not describe any of the details about the governing equations or the form of the solution, as that information is available in the applet tutorials and in the references listed in Table 1.

One-Dimensional Transport With Decay and Equilibrium Sorption

This is one of the more simple applets in Table 1, incorporating the processes of advection, longitudinal dispersion, linear equilibrium sorption, and first-order decay. A variety of boundary conditions and contaminant input scenarios can be selected by the user. The analytical solutions for this model are well-known and consist of exponential and error functions [e.g., 11,23]. The sample model output shown in Figure 1 displays the non-reactive contaminant breakthrough curve at a fixed distance (equal to 30 cm in this example). As noted previously, Figure 1 illustrates that the model results are presented graphically but that the student can also display numerical values via a ‘‘slider’’ that is operated by the mouse and obtain a table of the raw numerical output in a separate window by clicking the ‘‘Show Data’’ box. Figure 1 also illustrates how the student can use the model to do simple curve-fitting to estimate transport parameters. The output shown is the result for a class assignment where the students must fit a longitudinal dispersion coefficient to the results of a laboratory column experiment reported by Pickens and Grisak [18]. The students examine the paper by Pickens and Grisak [18] and enter the data from the breakthrough curve obtained in the laboratory experiment by using the "User Defined Data Points" feature of the model. Then they use trial-and-error and run the model with different dispersion coefficients; the results in Figure 1 indicate that a value of $D = 0.003$ cm^2/min seems to provide the best fit to the data.

One-Dimensional Transport With Decay and Rate-Limited Sorption

This model is still restricted to one-dimensional transport but the sorption reaction follows a more complex and realistic "two-site" model with a fraction (f) of the available sorption sites governed by linear local equilibrium while the remaining sites are governed by linear rate-limited mass transfer. As developed by Torride et al. [20] the solution requires numerical evaluation of an integrand containing exponential, error and Bessel functions. A FORTRAN code provided by Toride was used to develop the Java applet.

Figure 2 shows an example output from this more sophisticated model. The results show the aqueous and sorbed phase concentration profiles in space at a fixed time (equal to 500 days in this example) for different mass transfer coefficients (α). Figure 2 is for the case where all the sites are rate limited ($f = 0$) and dramatically illustrates the impact of slow mass transfer. For a large value of α, sorption is nearly at equilibrium so the aqueous and sorbed phase profiles are identical. As the mass-transfer coefficient decreases, the sorbed phase profile lags behind the aqueous phase profile and the slowly desorbing mass results in a highly skewed aqueous profile with a long tail. Note that in the limit as the mass-transfer coefficient goes to zero there is no sorption and the aqueous profile peak would be located at the advective front distance of 5 m (equal to the velocity of 0.01 multiplied by 500 days). The tailing caused by slow desorption is generally regarded as a significant factor limiting the performance of many aquifer remediation strategies, and, as can be seen from Figure 2, this applet is a highly effective tool for students to explore how various processes and parameters influence this tailing phenomenon.

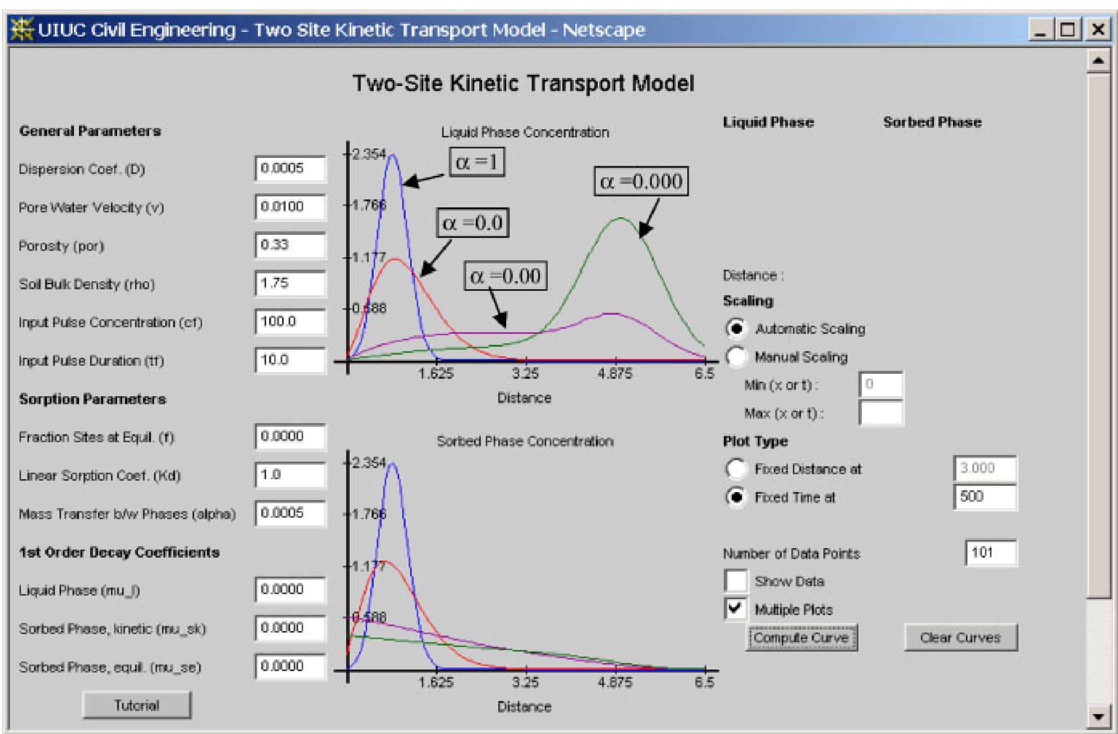

Figure 2 Example of the "One-Dimensional Transport with Decay and Rate-Limited Sorption" applet. Results display the aqueous and sorbed phase concentration profiles, demonstrating how slow mass transfer (decreasing α) affects tailing behavior. [Color figure can be viewed in the online issue, which is avaliable at www.interscience.wiley.com.]

Three-Dimensional Transport With Decay and Equilibrium Sorption

We present this case as an example of a multi-dimensional dispersion model. The contaminant is input as a constant concentration rectangular source in the (y, z) plane at $x = 0$. The transport processes are advection at uniform velocity along the x-axis, longitudinal dispersion, and horizontal and vertical transverse dispersion. The approximate analytical solution for this model is given by Domenico [6] and involves exponential and error functions. Figure 3 is a sample output that shows the spatial distribution of concentration along a horizontal slice of the (x, y) plane located at $z = 0$. Some notable features of the output interface are the flexibility to control the contour levels for the concentration plume display and the ability to examine concentration plots along horizontal and transverse cross sections through the plume using the mouse as a ‘‘slider.’’ Using this latter feature, students are able to visualize the impact of transverse dispersion and decay upon the longitudinal and vertical extent of the plume.

Two-Dimensional Steady Flow With Wells and Particle Tracking

This final example differs from those presented above because it considers non-uniform flow with purely advective transport. Potential flow theory applies to two-dimensional steady flow in a homogeneous aquifer, so that superposition of elementary solutions can be used [1,19]. We have implemented uniform regional flow with sources and sinks to represent injection and extraction wells; our model is based upon the presentation in Reference [11]. After superposition is used to compute the velocity field, tagged particles can be tracked to draw flowpaths and streamlines. An example is shown in Figure 4 for the classical case of an injection-extraction well doublet in a uniform regional flow field; the injection well is on the left and the extraction well is on the right. Attractive features of the interface include: (a) the regional flow direction and magnitude can be easily changed; (b) wells can be added or removed by pointing and clicking; (c) existing wells can be moved by selecting and dragging the mouse; (d) tagged particles used for streamline

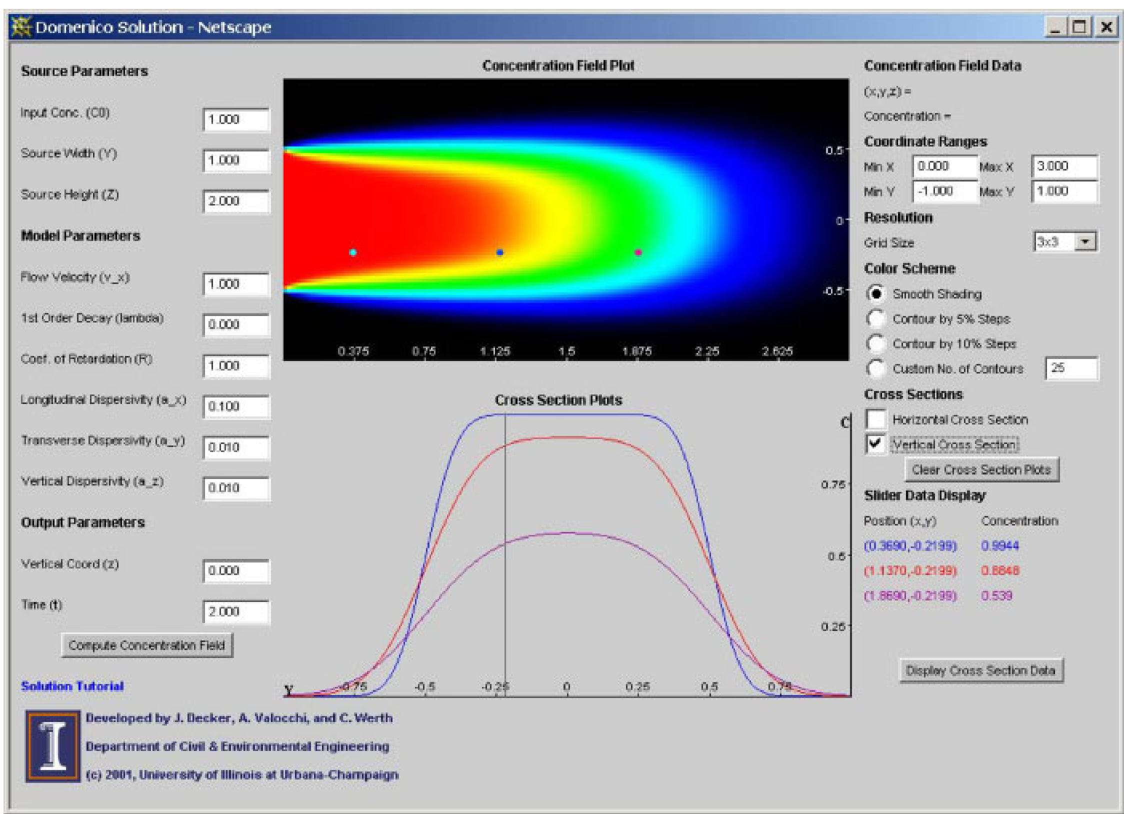

Figure 3 Example of ‘‘Three-Dimensional Transport with Decay and Equilibrium Sorption’’ applet. Results show the spatial profile for horizontal two-dimensional slice in the (x, y) plane along $z = 0$. Also shown are transverse cross-sections at three different positions along the flow direction. [Color figure can be viewed in the online issue, which is avaliable at www.interscience.wiley.com.]

tracing can be marked with different colors or shapes, and in particular particles emanating from injection wells can be distinguished from those in the regional flow. This latter feature is utilized in Figure 4 where the ambient regional groundwater is colored blue and the injected water is colored red. The left panel shows the classic flow pattern resulting from an injection-extraction well doublet in a uniform regional flow field; the well pair forms a separate flow system that is isolated from the regional flow and all of the injected water is captured by the extraction well. The right panel demonstrates that changing the direction of the regional flow causes some of the injected water to ‘‘escape’’ down-gradient while some of the up-gradient ambient groundwater is captured by the pumping well. This applet is highly effective for rapid visualization of these flow patterns, which is important since wells are commonly used in practice to control flow patterns for groundwater remediation and other purposes. The interaction among wells and uniform flow is also a classic topic in groundwater hydraulics and most textbooks will contain figures similar to Figure 4. Student understanding of this topic is greatly enhanced by the interactive applet because they can rapidly try different well patterns and flow rates.

ASSESSING THE EFFECTIVENESS OF THE INTERACTIVE MODELS

From our perspective as instructors these models have dramatically enhanced our courses. We have used the interactive applets directly during lectures (for lecture facilities equipped with a computer and internet connection); students are asked to predict the impact of changing certain process parameter values and the results can be instantly displayed in class. The class then discusses why the computed results did or did not match their expectations. The models have also allowed us to give homework and project assignments that are much more complex, realistic, and interesting than was possible previously. For example, in class the students are introduced to the effects of wells on groundwater flow, and to the use of extraction wells to design capture zones for contaminated aquifers. Although there is a well-known analytical solution for the optimal pumping rate for a single extraction well [e.g., 7], the web models allow the students to go beyond this classical case and to design more realistic multiple-well capture systems that are effective even when there is uncertainty regarding the direction and magnitude of the regional groundwater flow (see Fig. 4). The interactive models have also

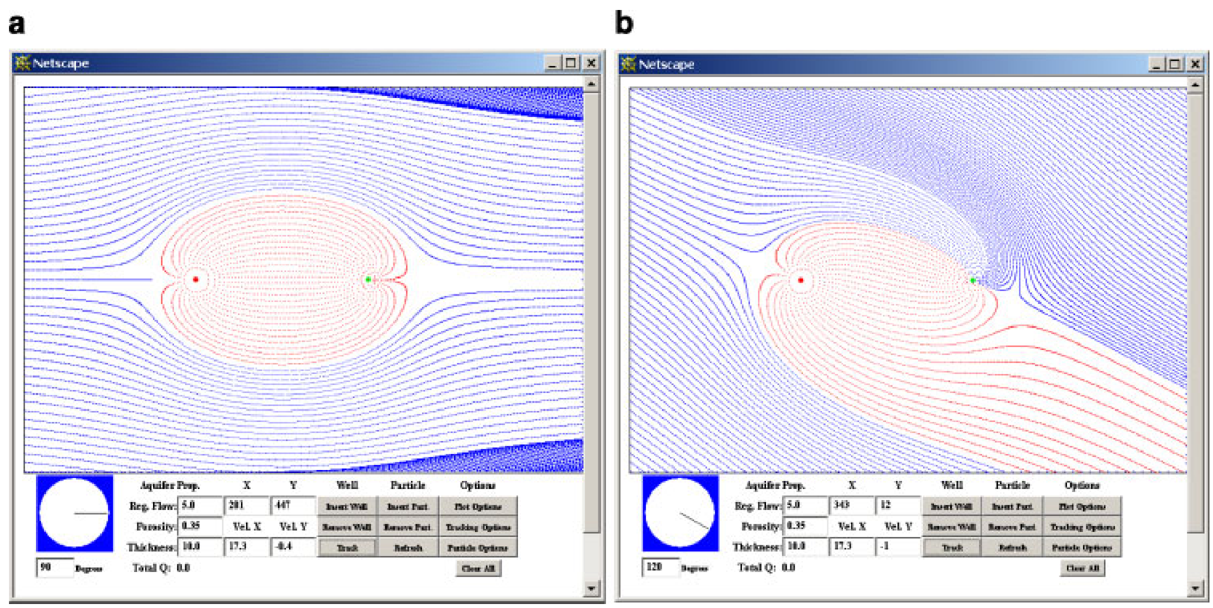

Figure 4 Example of ‘‘Two-Dimensional Steady Flow with Wells and Particle Tracking’’ applet. Results show the effect of the uniform regional flow direction on the flow pattern for an injection-extraction well doublet. The red well on the left is injection, and the green well on the right is extraction; the regional flow direction is indicated by the line on the circular compass on the bottom left. Fluid particles coming into the domain with the regional flow are tagged blue, while particles entering through the injection well are tagged red. [Color figure can be viewed in the online issue, which is avaliable at www.interscience.wiley.com.]

enabled us to analyze quantitatively a wider range of processes than was possible previously.

On the official course evaluations that are completed at the end of each semester, we have added an open-ended question requesting the students to evaluate specifically the value of the interactive simulation models. Student responses have been nearly unanimous in praising the value of the applets. The course evaluations also have an ''other teaching aids'' category that the students evaluate on a scale from 1 (exceptionally low) to 5 (exceptionally high). In a Remediation Design course in the Fall of 2000, 42% of the students ranked this category exceptionally high. In an introductory groundwater course, this category was ranked exceptionally high by 50% of the students during the Fall of 2000, but only by 25% of the students during the Fall of 1997, which was prior to development of the Java applets.

SUMMARY AND CONCLUSIONS

Although computer simulation has a long tradition in the groundwater field, most available software packages are too cumbersome for use in introductory-level courses. We have developed a series of interactive simulation models that are implemented as Java applets that can be executed over any web browser. The models cover a variety of processes relevant to reactive pollutant transport in groundwater, and hence should be useful to instructors in civil and environmental engineering, earth science, geology, and natural resources. As noted above, students can use the interactive models to enhance their quantitative understanding of how pollutant behavior is influenced by coupling among the processes of advection, diffusion, longitudinal, and transverse dispersion, sorption, and decay. Students can also use the interactive models as tools in broader design projects.

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