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National Cooperative for the
Disposal of Radioactive Waste

TECHNICAL REPORT 00-02

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Summary

The SANTA (Sensitivity Analysis of Nuclide Transport Aspects) program is a simple box model created to simplify understanding of radionuclide or contaminant transport through a fractured medium. SANTA is a teaching tool and allows scoping calculations, interpretation of migration experiments, sensitivity studies, and assists in the development of conceptual models.

The processes acting upon a contaminant explored by SANTA include advection in the main channel, dispersion in the main channel, linear/non-linear sorption and desorption in the main channel, diffusion into and out of the rock matrix, sorption and desorption in the rock matrix, radioactive decay and any combination of the above processes.

Conceptually SANTA uses an array of identical boxes (both in physical dimensions and geochemical content) to represent a 1-D homogeneous main channel (fracture), with an optional 1-D homogeneous rock matrix, accessed by diffusion, arranged symmetrically about the main channel and represented by arrays of identical boxes. Transport in the main channel is implemented by simple movement of the aqueous phase from one box to the next during a set time, while diffusion into the rock matrix is governed by a discrete approximation of Fick's first law.

The source term, supplying the first box, is limited to a single contaminant input supplied continuously at a fixed concentration, or as a pulse of finite duration. The status in the last box at the end of the fracture is continuously recorded and represents the breakthrough curve.

SANTA contains a built-in grapher to display results such as concentration profiles (fracture and rock matrix) or breakthrough curves, or optionally results can be output to a file.

Code testing focuses on SANTA's implementation of advective flow, diffusion into the rock matrix (within a bounded and unbounded medium), sorption, dispersion and a combined process test, and compares SANTA's results with analytical solutions and results from alternative numerical models. The comparative tests attest sufficient numerical accuracy for the purposes SANTA was designed for.

SANTA was programmed in a combination of FORTRAN and VISUAL BASIC, retaining the proven mathematical ability of FORTRAN, while including the user-friendly Windows environment of VISUAL BASIC, with integral graphing and printing capabilities. The program also features a fully illustrated Help file containing an on-line user manual and reference guide, and comes with a selection of example input files. SANTA runs on the following operating systems: Windows 3.x, Windows 95 and Windows NT.

Zusammenfassung

Das Programm SANTA ("Sensitivity Analysis of Nuclide Transport Aspects") ist ein einfaches Boxmodell, das zum besseren Verständnis des Transports von Radionukliden oder Schadstoffen in einem geklüfteten Medium entwickelt wurde. SANTA ermöglicht als anschauliches Instrument Überschlagsberechnungen, die Interpretation von Migrationsexperimenten sowie Sensitivitätsstudien und ist bei der Entwicklung von konzeptuellen Modellen behilflich.

Dabei berücksichtigt SANTA folgende Prozesse, die auf einen Schadstoff einwirken: Advektion, Dispersion, lineare/nicht-lineare Sorption und Desorption – jeweils entlang des bevorzugten Transportwegs – Diffusion in die und aus der Gesteinsmatrix, Sorption und Desorption in der Gesteinsmatrix, radioaktiver Zerfall sowie jede Kombination dieser Prozesse.

In SANTA wird eine Reihe identischer Boxen (sowohl bezüglich physikalischer Dimensionen als auch geochemischem Inhalt) konzeptionell zur Darstellung eines eindimensionalen bevorzugten Transportwegs (Kluft) verwendet. Als Option kann eine eindimensionale homogene Gesteinsmatrix gewählt werden, die für Diffusion zugänglich und symmetrisch um die Kluft angeordnet ist und durch Reihen identischer Boxen dargestellt wird. Transport in der Hauptkluft wird durch einfache Verschiebung der wässrigen Phase von einer Box zur nächsten während einer bestimmten Zeit durchgeführt, während die Diffusion in die Gesteinsmatrix durch eine diskrete Annäherung an das Erste Fick'sche Gesetz gesteuert wird.

Der Quellterm für die erste Box beschränkt sich auf die Zugabe eines einzigen Schadstoffs und erfolgt kontinuierlich mit einer festgelegten Konzentration oder als Puls einer bestimmten Dauer. Der Zustand in der letzten Box am Ende der Kluft wird kontinuierlich erfasst und entspricht der Durchbruchskurve.

SANTA verfügt über ein integriertes Grafikprogramm, um die Resultate als Konzentrationsprofile (Kluft und Gesteinsmatrix) oder Durchbruchskurven darzustellen, eine weitere Möglichkeit besteht in der Ausgabe der Resultate in einem File.

Der Test des Computercodes richtet sich nach den in SANTA implementierten Prozessen, wie advektivem Fluss, Diffusion in die Gesteinsmatrix (innerhalb eines begrenzten und unbegrenzten Mediums), Sorption, Dispersion sowie einem kombinierten Prozesstest, und vergleicht die Resultate von SANTA mit analytischen Lösungsansätzen und Ergebnissen alternativer numerischer Modelle. Die vergleichenden Tests zeigen eine ausreichende numerische Genauigkeit für die in SANTA vorgesehenen Anwendungen.

SANTA wurde in einer Kombination aus FORTRAN und VISUAL BASICS programmiert und vereint damit die bewährten mathematischen Fähigkeiten von FORTRAN mit dem benutzerfreundlichen Windows-Programm VISUAL BASICS und all dessen integrierten grafischen und Druckmöglichkeiten. Das Programm weist ebenfalls ein vollständig erläuterndes Help-File auf, das on-line ein Benutzer- und Referenzhandbuch mit einer Reihe von Beispielen zu Eingabe-Files enthält. SANTA erfordert folgende Betriebssysteme: Windows 3.x, Windows 95 und Windows NT.

Résumé

Le programme SANTA (Sensitivity Analysis of Nuclide Transport Aspects) est un modèle simple de type boîtes successives destiné à la compréhension du transport de contaminants en milieu fracturé. Il s'agit d'un outil d'enseignement permettant des calculs étendus, l'interprétation d'expériences de migration, des études de sensibilité et l'assistance au développement de modèles conceptuels.

Les processus agissant sur un contaminant et pris en compte par SANTA comprennent la convection dans le conduit principal, la dispersion dans le conduit principal, l'adsorption et la désorption linéaires/non linéaires dans le conduit principal, la diffusion dans et de la matrice rocheuse, l'adsorption et la désorption dans la matrice rocheuse, la désintégration radioactive et toute combinaison des processus mentionnés.

Le principe de SANTA est basé sur l'utilisation d'une série de boîtes identiques (dans leurs dimensions physiques et leur contenu géochimique) pour représenter un conduit principal homogène unidimensionnel (fracture), et de manière optionnelle une matrice rocheuse homogène unidimensionnelle accessible par diffusion; cette matrice est disposée d'une manière symétrique autour du conduit principal et représentée par des séries de boîtes identiques. Le transport dans le conduit principal est dicté par le simple mouvement de la phase aqueuse d'une boîte à la suivante durant un laps de temps donné, tandis que la diffusion dans la matrice rocheuse est régie par une approximation discrète de la première loi de Frick.

Le terme source, alimentant la première boîte, se limite à une injection simple du contaminant de manière continue et à concentration fixe, ou à une impulsion de durée limitée. L'état dans la dernière boîte, à l'autre extrémité de la fracture, est enregistré et représente la courbe de restitution.

SANTA possède un générateur de graphes incorporé pour la représentation des résultats tels que des profils de concentration (dans la fracture et la matrice rocheuse) ou des courbes de restitution; de manière optionnelle, les résultats peuvent être enregistrés dans un fichier.

Le contrôle du programme de SANTA a été focalisé sur la simulation de l'écoulement convectif, de la diffusion dans la matrice rocheuse (milieu limité ou non), de l'adsorption, de la dispersion et de la combinaison de ces processus. Ce contrôle permet de comparer les résultats de SANTA avec les solutions analytiques et les résultats d'autres modèles numériques. Les tests comparatifs ont révélé une précision numérique suffisante pour les utilisations auxquelles SANTA est destinée.

SANTA a été programmé en combinant le FORTRAN avec le VISUAL BASIC, en raison des capacités mathématiques éprouvées du FORTRAN et de l'environnement Windows convivial du VISUAL BASIC, comprenant des graphiques intégrés et des facilités d'impression. Le programme fournit aussi un fichier d'aide abondamment illustré, ainsi qu'un manuel et un guide de référence en ligne ; une série d'exemples de fichiers d'entrée est également fournie. SANTA fonctionne sur les environnements suivants: Windows 3x, Windows 95 et Windows NT.

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1 Introduction

SANTA (Sensitivity Analysis of Nuclide Transport Aspects) was created primarily as a teaching tool to simplify understanding of radionuclide transport through the geosphere, and secondly, as a simple scoping tool to quickly evaluate the effect of a range of retardation mechanisms on contaminant transport. It is intended that SANTA's transparent and clear implementation of the processes will enable the user a basic insight into the calculations not afforded by more complex methods. SANTA is designed to treat a single contaminant species without consideration of complex chemical interaction.

To achieve this, SANTA employs the "box modeling" approach which, very simply, breaks down the ground water flow path into a linked series of identical boxes with the same physical properties (i. e. porosity, rock chemistry etc.). It is inside each of these boxes that the processes causing partitioning of the contaminant between the rock and ground water phases (i.e. sorption) can be simulated in a simple, transparent manner. The process of advection is implemented simply by moving the mobile ground water phase of a box into the next box down stream.

One main advantage of the box modeling approach is the clearly defined physical approach that results in an easily visualised system of boxes and their inter-actions with each other. The user can define all the relevant parameters used in the code. These parameters are fixed physical dimensions and properties of the fracture material being modeled. All other parameters are derived from these simple input parameters. SANTA, therefore does not need the input of a large amount of fit, or constant of proportionality factors. During the testing stages (documented later) any errors or limitations introduced by this box model approach are clearly shown.

This simple approach contrasts strongly with some of the alternative methods, such as solving complex non-linear sets of partial differential equations (PDEs) describing coupled reaction and transport in a multicomponent system by using finite difference techniques. The methods to solve these sets of PDEs themselves introduce discretisation, truncation and stability errors. These errors are usually minimised by carefully selecting the grid spacing and time stepping to be used, but without care an error term can quickly swamp the calculations. This approach, therefore, requires the understanding of mathematical methods unfamiliar to many potential users of the code and, as stated earlier, it is the intention for the user to become involved in the actual methodology employed to solve the problem not simply to find a numerical solution to the problem.

It must be stated that in either case, many of the values used for input terms are themselves subject to much debate and uncertainty. Without a complete examination of the flow system, a conceptual model is used for the internal properties of the system. This limitation must be kept in mind when quoting the apparent accuracy of results produced by numerical codes in general.

To enable the user to avoid the long learning and familiarisation process necessary to use complex models, SANTA was coded to perform simple transport/retardation calculations quickly and easily on a standard PC using the familiar environment offered by Microsoft Windows. SANTA's integrated environment contains its own input files, graphing abilities and output options thus enabling easy, quick desk-top scoping.

2 The Box Model

The aim of SANTA is to model the transport and retardation of a tracer in a fractured rock using a simple box model to represent the ground water flow path. The basic principle of a box model is that this ground water flow path is divided into a number of identical compartments or boxes (Fig. 2.1). Each of these boxes is a simplified representation of the more complex reality, with all boxes in the main fracture having identical dimensions and the same internal properties (i.e. porosity, rock density) and volume. A simple array of these boxes can be constructed to represent a water flowing fracture in one dimension, and, with an additional array of side boxes, a rock matrix can be represented (Fig. 2.2). These boxes contain distinct phases ; namely the ground water and the rock with which it is in contact. The water phase (aqueous species) is the mobile part and can move through the series of boxes carrying with it any tracer, while the rock (solid species) is stationary and remains permanently in a given box, retaining any retarded material. A source supplies the first box of the fracture while the contents of the last box of the fracture leave the system.

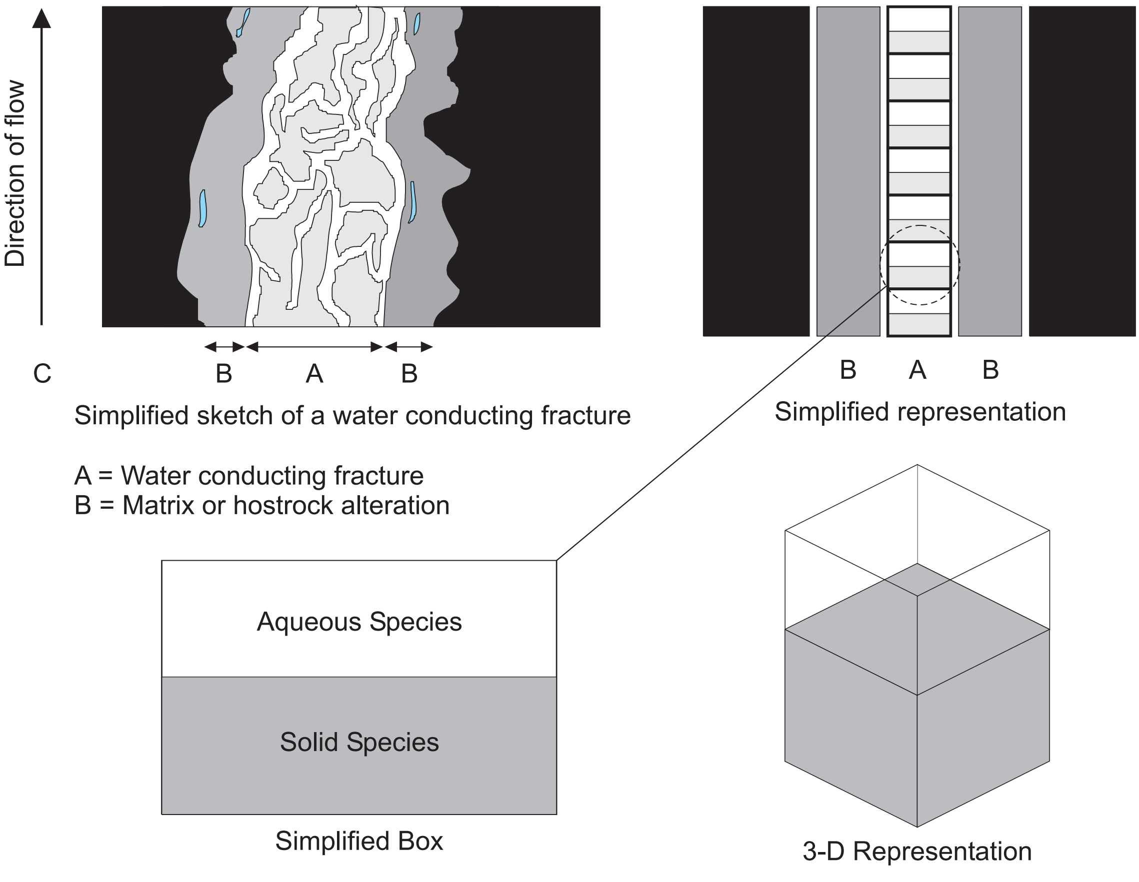

Fig. 2.1: A box derived from a representation of reality

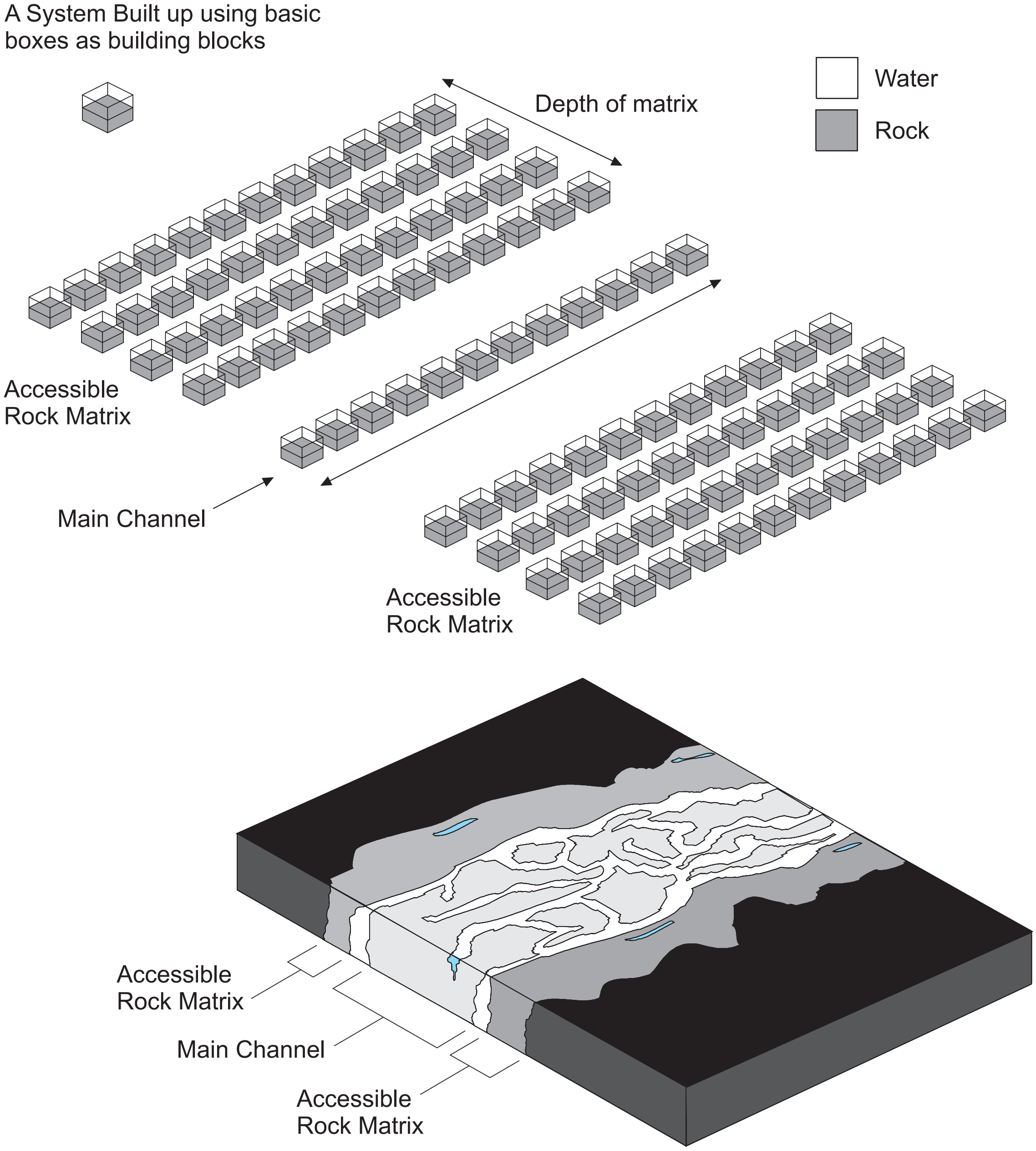

Fig. 2.2: Typical system constructed from boxes and comparative 3-D simplification of reality

In addition to the boxes used to represent the main flow path, the rock matrix adjacent to a fracture can be represented by additional boxes with different internal properties and volume than the fracture to represent rock matrix which is accessible by diffusion from the fracture. A typical setup with an advective channel and a diffusive rock matrix is shown in Fig. 2.2 along with a simplification of a water flowing fracture.

Note: For reasons of simplicity the rock matrix boxes are shown here with the same dimensions as the main channel boxes. In most cases the rock matrix boxes will have dimensions different than the main channel boxes.

2.1 Overview of the SANTA box model

The geometry outlined above is restricted to the following elements:

- A 1-D homogeneous main-channel (fracture) represented by an array of identical boxes (both in dimension and content).
- A 1-D rock matrix (optional) accessable by diffusion arranged symmetrically about the main channel and represented by arrays of identical boxes (both in dimension and content).

A single tracer source is input to the first main channel box. The source can be:

1. supplied continuously at a fixed (initial) concentration, or
2. supplied as a pulse of finite duration at a fixed concentration.

The processes simulated by SANTA include:

- Advection in the main channel
- Dispersion in the main channel
- Sorption and desorption in the main channel
- Diffusion into and out of the rock matrix
- Sorption and desorption in the rock matrix
- Radioactive decay
- Any combination of the above processes.

3 Advection

SANTA represents advection as the physical movement of a contaminant, in this case using water as the transport medium. In the very simple case of advection along a single flow path, a linear sequence of identical boxes may be used (Fig. 3.1).

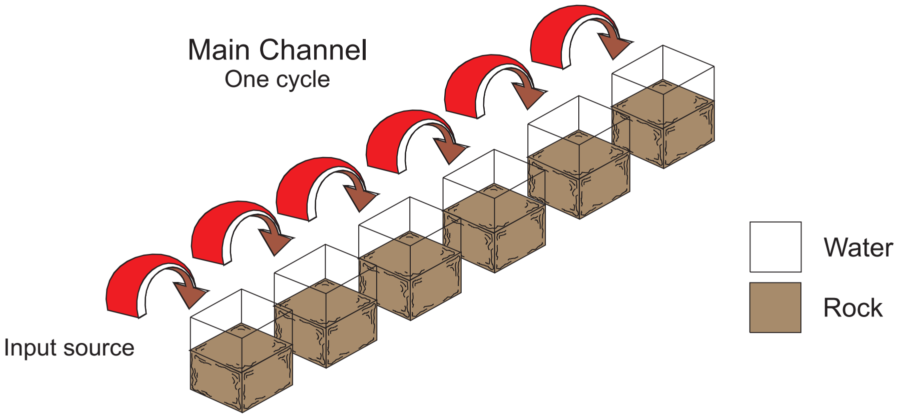

Fig. 3.1: Simple advection system

The SANTA code simulates the movement of water by moving the aqueous contents of box n to box n + 1 (Fig. 3.2). The contents that were in the last box leave the system, while the input to the first box comes from the source term outside the system (being either background water or an injected pollutant). The process of moving water between boxes and subsequent solute redistribution is called a *cycle*, a measurement of time used within SANTA. Thus SANTA transports the water volume in each box to the next box in one of these cycles to simulate advection. The time taken for one of these cycles is the residence time a solute remains in a box and is used in any calculations that are time dependent.

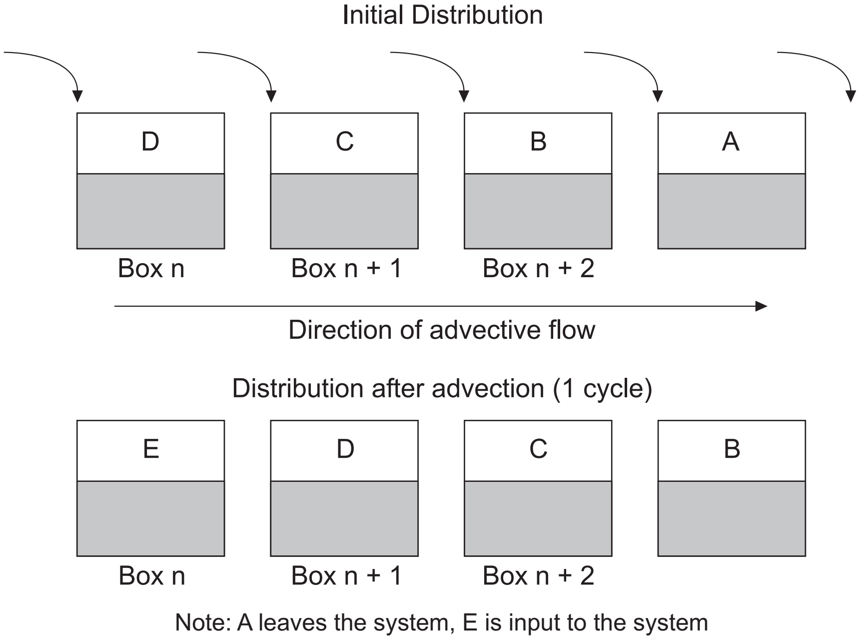

Fig. 3.2: Advective flow

In SANTA's representation of advection the aqueous phase moves forward one box per cycle. With a constant input of tracer and considering only advection (no dispersion, retardation etc.) the development of the predicted distribution profile is shown in Fig. 3.3 after 5 cycles.

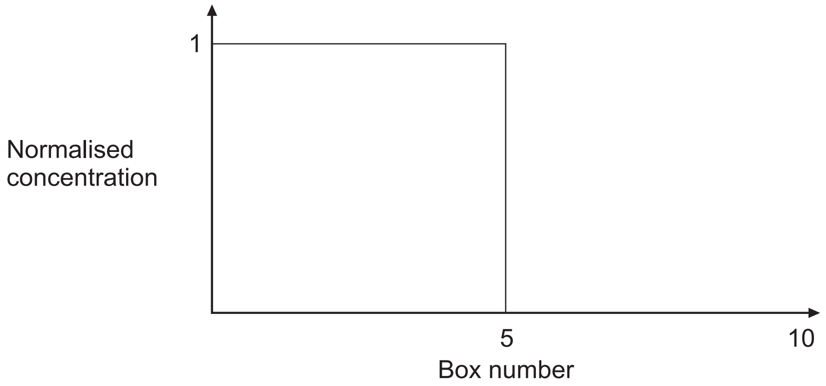

Fig. 3.3: Predicted distribution of contaminant after 5 cycles

The predicted distribution profile is shown in Fig. 3.4 after 10 cycles.

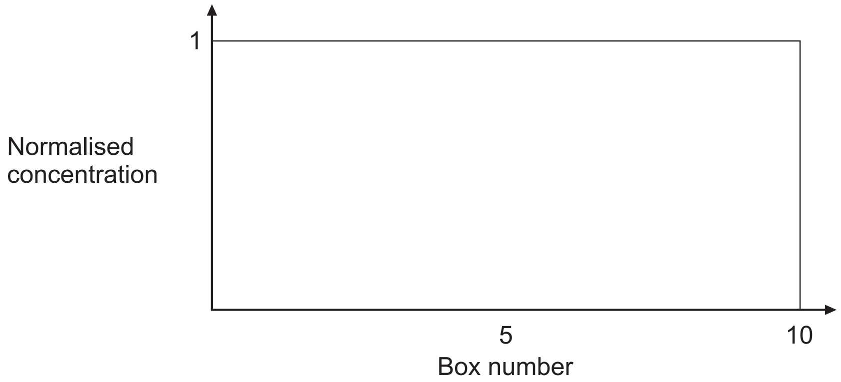

Fig. 3.4: Predicted distribution of contaminant after 10 cycles

If the input of tracer is switched off after the 10th cycle and the process of advection allowed to continue until the 15th cycle the predicted distribution profile would be as illustrated in Fig. 3.5. This type of box model leads to a numerically accurate description of plug flow (square pulse).

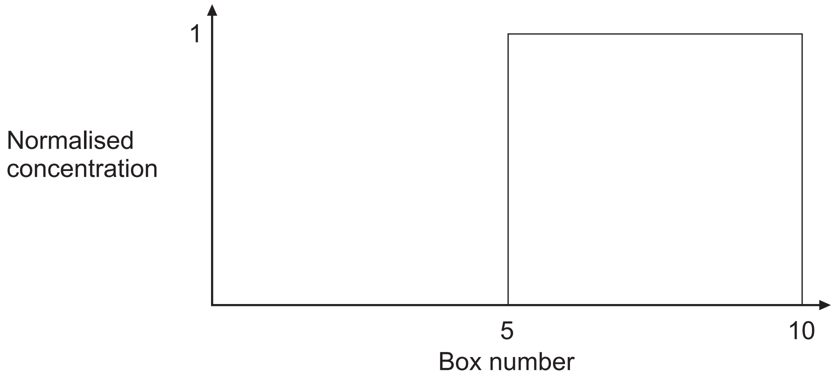

Fig. 3.5: Predicted distribution contaminant after 15 cycles

4 Diffusion

To represent rock matrix diffusion SANTA uses an array of boxes extending perpendicularly in the horizontal plane, adjacent to the main channel. This is illustrated in Fig. 4.1 below (with a depth of diffusion of 2 boxes) and with the rock matrix boxes having the same proportions as the main channel boxes for clarity only (i. e. this need not be so). Diffusion in the main channel is omitted (it is assumed that advection will dominate transport in the main channel). In general, the boxes of the rock matrix will usually be much smaller than the main channel boxes due to the shorter distance the diffusive flux can achieve within a cycle compared to the advective flow.

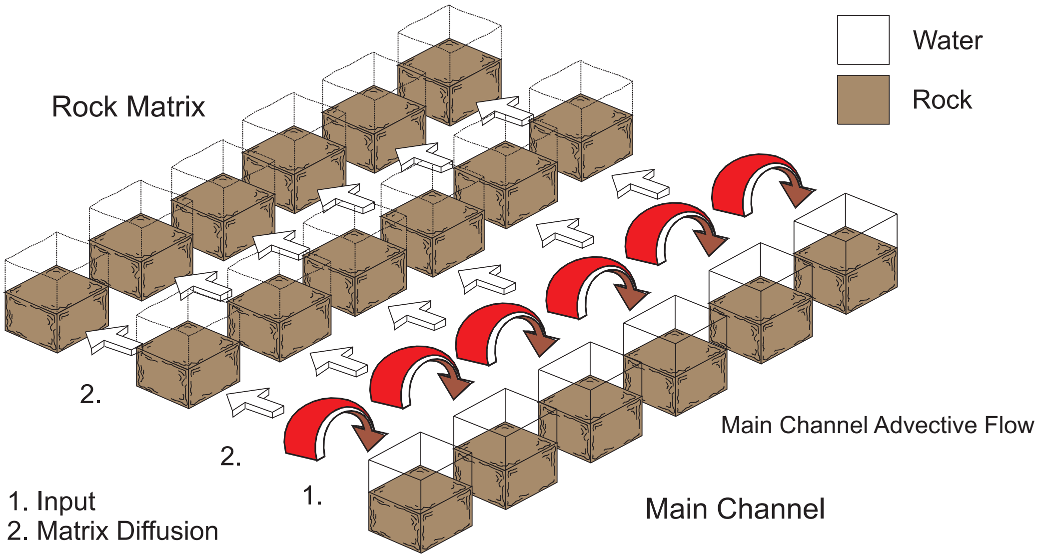

Fig. 4.1: Representation of diffusion in the rock matrix

Diffusive transport into the rock matrix boxes is represented by Fick's first law (CRANK et al. 1981):

$$Flux = -\frac{dC}{dx}D \qquad \text{(Eq. 4.1)}$$

where D is the coefficient of diffusion and $\frac{dC}{dx}$ is the concentration (C) gradient in the x direction. If this gradient is over a layer of thickness l, then:

$$Flux = D\frac{C1 - C2}{l} \qquad \text{(Eq. 4.2)}$$

where flux is defined from box I to box II (which lie perpendicular to the main channel) with concentrations $C1$ and $C2$ respectively, and positive towards lower concentration.

For the mass balance equation, the mass transferred between boxes (**MT**) is defined:

$$\boldsymbol{MT} = Flux\ A\ \phi\ t_c \qquad \text{(Eq. 4.3)}$$

where A is the contact area (area of rock matrix box parallel to main channel), ϕ is the porosity of the medium in which diffusion occurs and t_c the time of one cycle.

To calculate the diffusion length l, the following equation was used: $l = 2\sqrt{D \cdot t_c}$

At time t_c, 90 % of the mass of the tracer will be contained in the matrix from depth 0 to depth l (Fig. 4.2). Therefore the full depth of the rock matrix will be l times the number of rock matrix boxes (l • NoSideBoxes).

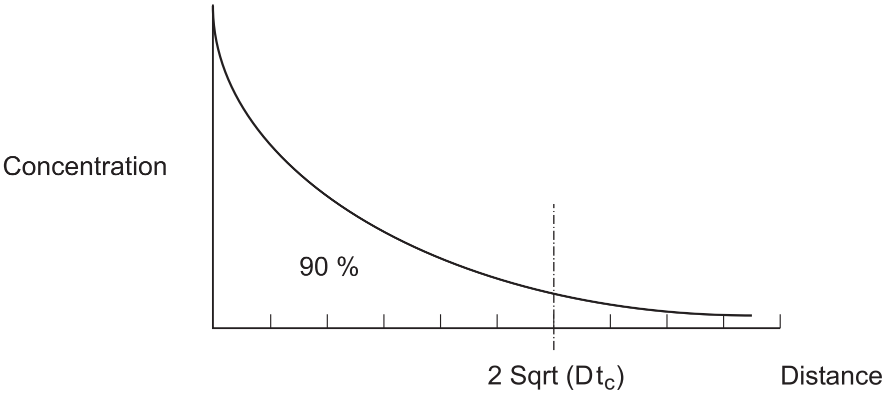

Fig. 4.2: Definition of diffusion length

NOTE: At present the code defaults to the depth of 10 rock matrix boxes. This can be modified to more rock matrix boxes, i.e., enable longer run times. As the diffusion length is proportional to the root of time, and the duration of the injection pulse is usually small compared to the duration of advective flow, it might be possible to fix the maximum number of rock matrix boxes at a number << 100. At present the maximum number of rock matrix boxes allowed by the code is 20.

With the $Flux = D\dfrac{C1 - C2}{l}$

and Mass Transfer (MT) = $D\dfrac{C1 - C2}{l} A \cdot t_c \cdot \phi$,

this gives:

$$MT = \frac{D \cdot A \cdot \phi \cdot t_c \cdot (C1 - C2)}{2 \cdot \sqrt{D \cdot t_c}} \quad \text{for a cycle} \qquad \text{(Eq. 4.4)}$$

As all the factors except $C1$ and $C2$ will be constant throughout a run, Equation 4.4 may be formulated as:

$$MT = KDiff(C1 - C2); \quad \text{with } KDiff = \frac{D \cdot A \cdot \phi \cdot t_c}{2\sqrt{D \cdot t_c}}$$

With the mass transfer known for a cycle, the concentrations $C1$ and $C2$ can be updated accordingly. Care must be taken when moving a mass of contaminant to, or from, a main channel box to a rock matrix box due to the possible different volumes of these boxes. If $C1$ is the concentration in the main channel box (1), and $C2$ is the concentration in the first rock matrix box (I), the updated concentrations can be calculated as follows:

With $C1 > C2$;

$$C1 = \frac{C1 \cdot MBWaterVolume - KDiff \cdot (C1 - C2)}{MBWaterVolume} \qquad \text{(Eq. 4.5)}$$

$$C2 = \frac{C2 \cdot RMWaterVolume + KDiff \cdot (C1 - C2)}{RMWaterVolume} \qquad \text{(Eq. 4.6)}$$

where $MBWaterVolume$ is the volume of water in the fracture box and $RMWaterVolume$ is the volume of water in the rock matrix box.

In representing diffusion the code assumes that the initial incoming pulse to the first rock matrix box (I) off the first main channel box (1) can only travel the distance of one box per cycle. Thus, with a constant injection, the tracer will reach the second rock matrix box (II) in the second cycle (illustrated below, Fig. 4.3, with a depth of diffusion of 6 boxes). This prevents a pulse reaching the furthest rock matrix box in the first cycle. The code, at this stage, does not consider diffusion between different rock matrix columns, i. e. no diffusion occurs between any rock matrix boxes adjacent to Box 1 and any rock matrix boxes adjacent to Box 2. Diffusion occurs perpendicular to the main channel.

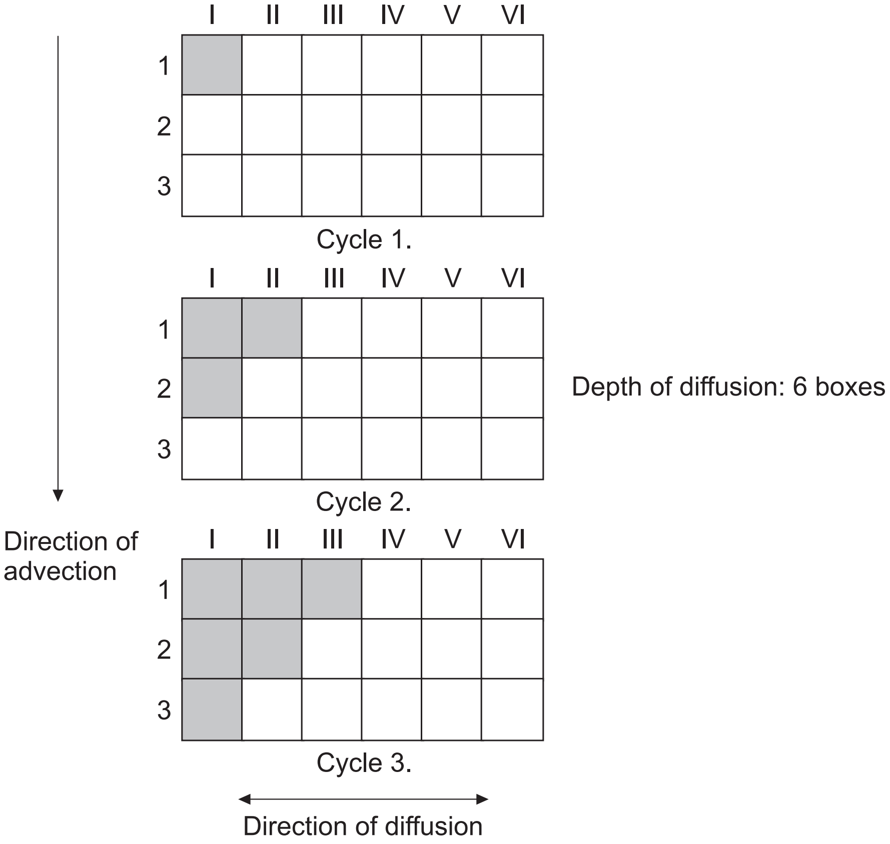

Fig. 4.3: Consecutive build-up diffusing contaminant in the rock matrix

5 Sorption

The process of sorption can occur in every box in the system and is the first process that SANTA calculates in a box on the incoming fluid (followed by diffusion into the rock matrix, if selected). The concept underpinning the sequence of events relies on sorption being relatively fast compared to diffusion. This is outlined in Fig. 5.1 below, with the (possible) order of events:

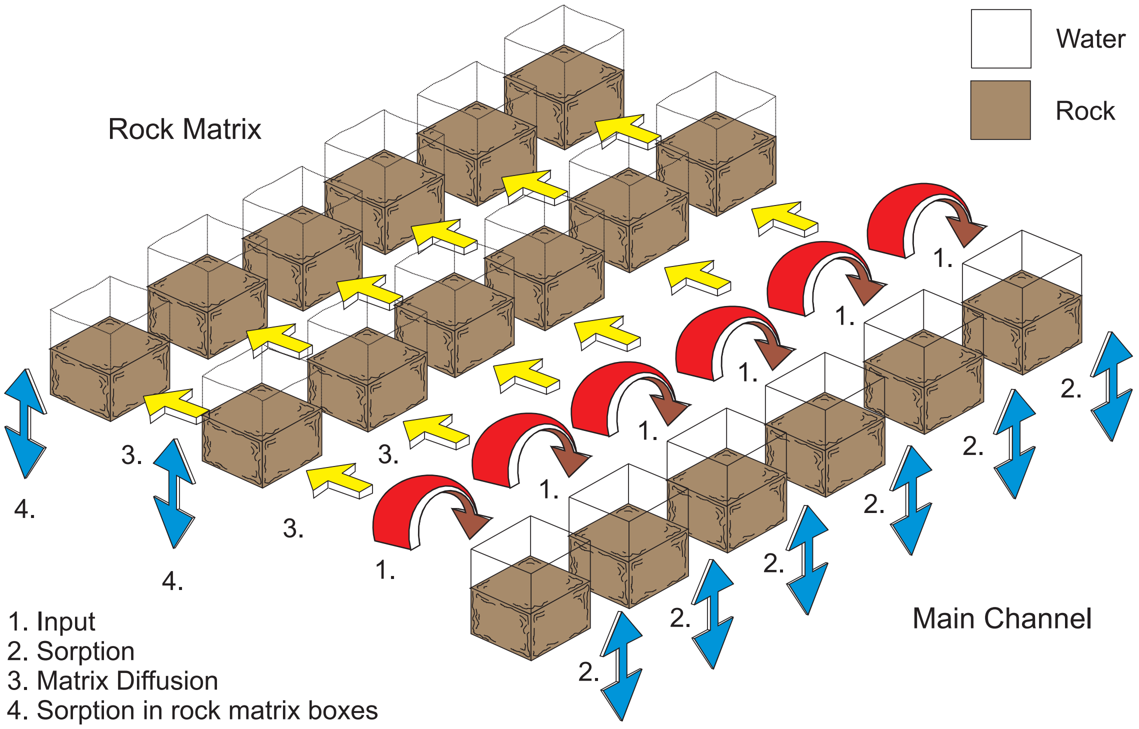

Fig. 5.1: Representation of sorption in the box model

In the model sorption is described by the general Freundlich equation (APPELO & POSTMA 1993):

$$C_r = \alpha \cdot C_w^{\beta} \qquad \text{(Eq. 5.1)}$$

where:

C_r: Concentration in the rock [kg/kg]
C_w: Concentration in the water [kg/m^3]
α: Freundlich alpha for sorption [m^3/kg]
β: Freundlich beta for sorption [-]

This equation describes the relationship between the concentration in the rock and the concentration in the water for a contaminant, while α and β are known parameters whose values have been previously derived experimentally. Therefore the concentrations in the water and rock can be determined with Equation 5.1. For most cases in natural environments β is smaller than one.

Initially an inventory of the mass of contaminant in the box is taken as follows:

$$INV = WaterVolume \cdot C_w + Rockmass \cdot C_r \qquad \text{(Eq. 5.2)}$$

Replacing C_r;

$$INV = WaterVolume \cdot C_w + RockMass \cdot \alpha \cdot C_w^{\beta} \qquad \text{(Eq. 5.3)}$$

It is now possible to solve for C_w. There are three methods to solve Equation 5.3 depending on the value of β. The first case is if $\beta = 1$, producing a linear relationship between C_w and C_r. For this case $\alpha = Kd$ and Equation 5.3 becomes:

$$INV = WaterVolume \cdot C_w + RockMass \cdot Kd \cdot C_w \qquad \text{(Eq. 5.4)}$$

Making C_w the subject of the equation results in:

$$C_w = \frac{INV}{WaterVolume + RockMass \cdot Kd} \qquad \text{(Eq. 5.5)}$$

Equation 5.5 is now immediately solvable as all the parameters are known. By back substitution into Equation 5.1, the new value for C_r can be calculated. The updated value for concentration in the water is the value that is now available to control diffusion into the rock matrix, where the process of sorption occurs again.

The remaining methods are used if $\beta \neq 1$. In this case Equation 5.3 is non-linear and requires a different approach. One such approach is the use of the Newton-Raphson one-dimensional root-finding method. This method enables the honing in on the root, or numerical solution, to Equation 5.5 to a desired accuracy. Algebraically, the method derives from the standard Taylor series expansion of a function in the neighbourhood of a point:

$$f(x+\delta) \approx f(x) + f'(x) \cdot \delta + \frac{f''(x)}{2} \cdot \delta^2 + ... \qquad \text{(Eq. 5.6)}$$

For small enough values of δ, and for well behaved functions, the terms beyond the linear term can be ignored, hence:

$$f(x+\delta) = 0 \text{ implies } \delta = -\frac{f(x)}{f'(x)} \text{ with an overall error of } \approx \frac{f''(x)}{2} \cdot \delta^2$$

This gives rise to the Newton-Raphson formula:

$$x_{i+1} = x_i - \frac{f(x_i)}{f''(x_i)} \quad \text{where } x_i = \text{initial guess, and } x_{i+1} = \text{improved estimate}$$

This Newton-Raphson formula can now be used iteratively until some defined accuracy is obtained. In the SANTA code this accuracy is input by the user. If the relative accuracy is defined to be 0.01, then if $x_i - x_{i+1} \leq \pm 0.01 \times x_{i+1}$ the iterative process is halted and the value of C_w is taken to be x_{i+1}.

Re-arranging Equation 5.1 to make C_w the subject:

$$C_w = \left(\frac{C_r}{\alpha} \right)^{\frac{1}{\beta}} \qquad \text{(Eq. 5.7)}$$

Defining $A = \left(\frac{1}{\alpha} \right)^{\frac{1}{\beta}}$ and $B = \frac{1}{\beta}$ Equation 5.4 becomes:

$$INV = WaterVolume \cdot A \cdot C_r^B + RockMass \cdot C_r \qquad \text{(Eq. 5.8)}$$

which is equivalent to:

$$f(C_r) = WaterVolume \cdot A \cdot C_r{}^B + RockMass \cdot C_r - INV = 0 \qquad \text{(Eq. 5.9)}$$

The first derivative becomes:

$$f'(C_r) = B \cdot WaterVolume \cdot A \cdot C_r{}^{B-1} + RockMass \qquad \text{(Eq. 5.10)}$$

By putting B = 1 in Equation 5.9 an initial estimate of C_r can be obtained. Once this starting point and the desired accuracy are known a new value of C_r is solved iteratively by the Newton-Raphson method outlined above. Again with this new value of C_r known, by back substitution into Equation 5.1 the value of C_w can be obtained.

5.1 Diffusion with Sorption in the rock matrix

Sorption is implemented in the rock matrix in exactly the same manner as for the main channel boxes (outlined above). An incoming tracer can react with the rock according to the Freundlich equation (Equation 5.1). The only difference is that the tracer flow into or out of a box is controlled by diffusion and not by advection as in the main channel. In most common applications for rock matrix sorption the value for β will remain at 1.0 due to the lack of experimental data to define β. The actual number and dimensions of the rock matrix boxes remain unaltered from those defined in Chapter 4.

6 Dispersion

The effect of purposely induced numerical dispersion is used to implement physical dispersion in the main channel in combination with retardation due to sorption. Up until now it is assumed that the entire contents of a box moves into the subsequent box during the time step of a cycle. This conforms to the equation:

$$v\Delta t = \Delta x \qquad \text{(Eq. 6.1)}$$

Where v is the average ground water velocity, Δt the cycle time step, and Δx the box length. If this was the case each content of a box would be moved from one box to next with the box concentrations moving neatly with the box boundaries and remaining sharp (plug flow).

The sharpness is blurred when the front transfer and box boundaries do not correspond ($v\Delta t \neq \Delta x$). In this case the mixing of old and new concentrations in a box leads to a gradual smoothening of the transitions, an effect termed numerical dispersion.

Numerical dispersion can be used to represent physical dispersion by choosing the cycle time (Δt) in relation to box length (Δx) in such a way that numerical dispersion is equal to the desired physical dispersion. Physical dispersion is the result of uneven path lengths traveled by solutes in a porous medium combined with the effect of diffusion of solutes in the aqueous phase. With this approach it is not possible to represent the process of dispersion by itself. The method outlined here is closely linked with retardation caused by sorption.

Numerical dispersion can be calculated as follows (APPELO & POSTMA 1993):

$$\alpha_{num} = \frac{\Delta x}{2} - \frac{v\Delta t}{2R} \qquad \text{(Eq. 6.2)}$$

R is the retardation factor and defined as:

$$R = \left(1 + \frac{\rho_B}{\phi} \cdot Kd\right) \qquad \text{(Eq. 6.3)}$$

where

ρ_B = the bulk density of the rock, not including the pore spaces filled with water (= rock density · (1 – porosity))
ϕ = the porosity of the main channel
Kd = Kd for sorption (when $\beta = 1$, $\alpha = Kd$, Equation 5.1)

To determine the total number of boxes needed to represent a fixed dispersion value the following approach is taken.

Noting that:

$$\Delta x = \frac{PthL}{NoB}\ ,\ \Delta t = \frac{Tt}{NoB}\ \text{ and }\ v = \frac{PthL}{Tt}\ ,$$

where $PthL$, NoB and Tt are the path length, number of main channel boxes and transit time respectively. Thus substituting back into Equation 6.2:

$$\alpha_{num} = \frac{\frac{PthL}{NoB}}{2} - \frac{\frac{PthL}{Tt}\frac{Tt}{NoB}}{2R} \qquad \text{(Eq. 6.4)}$$

$$= \frac{\frac{PthL}{NoB}}{2} - \frac{\frac{PthL}{NoB}}{2R} \qquad \text{(Eq. 6.5)}$$

$$= \frac{PthL}{2NoB}\left(1 - \frac{1}{R}\right) \qquad \text{(Eq. 6.6)}$$

$$NoB = \frac{PthL}{2\alpha_{num}}\left(1 - \frac{1}{R}\right) \qquad \text{(Eq. 6.7)}$$

Therefore by introducing a dispersivity of α_{num} to represent the actual field dispersivity, it is now possible to determine the number of boxes (NoB) in the main channel necessary to produce this dispersivity using Equation 6.7, and hence, travel time and the number of boxes cannot be chosen independently.

Addendum

The above method is implemented in the code at present but has a simple limitation: there must be some amount of sorption in the main channel in order to simulate any dispersion (the number of boxes approaches 0 at $R = 1$ in Equation 6.7). A simple continuation of this theme results in a method to model dispersion when no sorption processes are defined in the main channel. In the simplest case defined below, just enough sorption to introduce a numerical dispersion (equivalent to the physical dispersion) is used and an increased average linear velocity (u) is used to offset the resultant retardation (R').

Following from Equation 6.1: $u = \frac{\Delta x}{\Delta t}$; $\frac{v}{R} = \frac{u}{R'}$

where u is the corrected migration velocity (i.e. the effective velocity (v) is unchanged).

Using $$R' = \frac{1}{1 - \frac{(2a_L NoB)}{PthL}} \qquad \text{(Eq. 6.8)}$$

Which has been defined to have the following property:

$$a_L = \frac{1}{2}\left(\Delta x - \frac{u}{R'}\Delta t\right) \qquad \text{(Eq. 6.9)}$$

$$a_L = \frac{\Delta x}{2}\left(1 - \left(1 - \frac{2a_L Nob}{PthL}\right)\right) \qquad \text{(Eq. 6.10)}$$

$$a_L = \frac{1}{2} \cdot \frac{\Delta x}{PthL} \cdot 2a_L NoB = a_L \qquad \text{(Eq. 6.11)}$$

With R' defined as a virtual retardation factor that is used to define the numerical dispersion to simulate a desired physical dispersion (a_L). From this R' value a virtual Kd' can be derived and thus, by using the existing code for sorption with this Kd' value, it is possible to induce the defined dispersion even when no effects of sorption are wanted by the user.

Further $$u = \frac{v}{R} R' = \frac{v}{R}\left(1 - \frac{PthL}{2a_L NoB}\right) \qquad \text{(Eq. 6.12)}$$

For stability $R' \geq 1$, i. e. $NoB \leq \frac{PthL}{2a_L}$

As can be seen this method can also be combined with the user's defined sorption data in Equation 6.12 to produce a new modified Kd' that includes a dispersion effect.

7 Code Testing

At present the code simulates advection, diffusion, dispersion and retardation by sorption. As these aspects of solute transfer are fundamental in migration experiments, it is essential that they can be proven to be working as they were defined in the model. It was in order to demonstrate confidence in the basic mechanics of the code that the following testing strategies were carried out. A set of test cases were constructed which enabled a close examination of any one or a combination of processes. Due to the focus being on the mechanics of the code, the input parameters might not necessarily represent any geological reality. All results were plotted using Excel for direct comparison with generated analytical results.

7.1 Advective flow

To check that the advective process was operating correctly this first test was constructed which did not activate the routines for sorption, dispersion or diffusion. The aim was to follow an input pulse as it traveled through the system. A set of test dimensions were selected to input a tracer pulse lasting exactly one cycle, and watch this pulse for 6 cycles. The dimensions used were as follows:

SETUP PARAMETERS

No. of Boxes:	5	
Transit Time:	1 hour	
Duration of a run:	1 hour 12 minutes – 1.2 hours (6 cycles)	
Duration of input pulse:	0.2 hours	
Input Elemental concentration:	10 kg m^{-3}	Totally arbitrary number
Dispersion:	"n"	Switched off
Accuracy:	0.01	Not used by this version

MAIN CHANNEL

Path Length:	5 m	
Channel Width:	1 m	
Aperture of Fracture:	1 m	
Fracture Porosity:	0.5	Not used by this version

These figures result in each box having unit dimensions.

ROCK MATRIX
Rock matrix is not used in this test.

SORPTION VALUES – switched off
None of the values for sorption are used in this test.

With this setup it can be seen that the concentration in the boxes at each cycle (0.2 hours) should be as follows:

Cycle	**Box 1.**	**Box 2.**	**Box 3.**	**Box 4.**	**Box 5.**
Cycle 1 (0.2 hours)	10.0	0.0	0.0	0.0	0.0
Cycle 2 (0.4 hours)	0.0	10.0	0.0	0.0	0.0
Cycle 3 (0.6 hours)	0.0	0.0	10.0	0.0	0.0
Cycle 4 (0.8 hours)	0.0	0.0	0.0	10.0	0.0
Cycle 5 (1.0 hours)	0.0	0.0	0.0	0.0	10.0
Cycle 6 (1.2 hours)	0.0	0.0	0.0	0.0	0.0

When the code was run the following data was output (all concentrations in kg m^{-3}):

```
   TEST.OUT DATA RUN
****** ADVECTION TESTS *******

Cycle no        1
incoming concentration to system =      10.000000000000000
conc in this box         1 =     10.000000000000000
conc in this box         2 =   0.000000000000000E+000
conc in this box         3 =   0.000000000000000E+000
conc in this box         4 =   0.000000000000000E+000
conc in this box         5 =   0.000000000000000E+000

Cycle no        2
incoming concentration to system =   0.000000000000000E+000
conc in this box         1 =   0.000000000000000E+000
conc in this box         2 =      10.000000000000000
conc in this box         3 =   0.000000000000000E+000
conc in this box         4 =   0.000000000000000E+000
conc in this box         5 =   0.000000000000000E+000

Cycle no        3
incoming concentration to system =  0.000000000000000E+000
conc in this box         1 =   0.000000000000000E+000
conc in this box         2 =   0.000000000000000E+000
conc in this box         3 =      10.000000000000000
conc in this box         4 =   0.000000000000000E+000
conc in this box         5 =   0.000000000000000E+000
```

```
Cycle no        4
incoming concentration to system =  0.000000000000000E+000
conc in this box        1 =  0.000000000000000E+000
conc in this box        2 =  0.000000000000000E+000
conc in this box        3 =  0.000000000000000E+000
conc in this box        4 =     10.0000000000000000
conc in this box        5 =  0.000000000000000E+000

Cycle no        5
incoming concentration to system =  0.000000000000000E+000
conc in this box        1 =  0.000000000000000E+000
conc in this box        2 =  0.000000000000000E+000
conc in this box        3 =  0.000000000000000E+000
conc in this box        4 =  0.000000000000000E+000
conc in this box        5 =     10.0000000000000000

Cycle no        6
incoming concentration to system =  0.000000000000000E+000
conc in this box        1 =  0.000000000000000E+000
conc in this box        2 =  0.000000000000000E+000
conc in this box        3 =  0.000000000000000E+000
conc in this box        4 =  0.000000000000000E+000
conc in this box        5 =  0.000000000000000E+000
```

The computed results are identical to the expected results. This confirms that the algorithm employed by the code to transport the contents of one box to another during a cycle (without diffusion, sorption or dispersion) is performing correctly.

7.2 Diffusion

The testing of the representation of diffusion in and out of the rock matrix was broken down into several parts, each of which examines a different aspect of diffusion. The following tests look closely at the representation of diffusion into an unbounded and bounded medium with a continuous input (or tracer supply), and at the diffusion from this medium into the main channel when the input is switched off. SANTA is treating the rock matrix accessable to diffusion as a bounded medium with an impermeable boundary set at a depth equivalent to the number of boxes considered for diffusion. The impermeable boundary may be a feature wanted or unwanted by the modeler. The following tests attempt to establish the limit to which the de-facto bounded geometry can mimic an unbounded geometry.

7.2.1 Diffusion into the Rock Matrix from the Main Channel

The system was set up using the following parameters to investigate diffusion into the side matrix, and the subsequent build up of tracer in each of the side boxes:

SETUP PARAMETERS
No. of Boxes: 10
Transit Time: 0.5 hours
Duration of a run: 1 hour (= 20 cycles, 1 cycle = 0.05 hours)
Duration of input pulse: 1 hour
Input Elemental concentration: 5E-05 kg m^{-3}
Dispersion: "n" Switched off.
Accuracy: 0.01

MAIN CHANNEL
Channel Width: 0.5 m
Path Length: 2.0 m
Aperture of Fracture: 1E-04 m
Fracture Porosity: 0.99

ROCK MATRIX
Depth of rock matrix (boxes): 10
Value of effective Diffusivity: 0.1E-11 $m^2 s^{-1}$
Rock matrix zone porosity: 0.05

SORPTION VALUES – switched off
None of the values for sorption are used for this test. Sorption is switched off.

With these chosen values, a constant input of 5E-05 kg m^{-3} enters the first box. With this constant condition in box 1, the effect of diffusion could be analysed at every cycle (every 0.05 hours). The code writes to a special file the record of the concentration in each of the Rock Matrix boxes adjacent to the first Main Channel box. Also included in this file was a running total of the transfer of mass through the Main Channel / Rock Matrix boundary which enabled a check of the mass transfer per cycle to be made against the analytical results.

To calculate the mass entering the first Rock Matrix box on the first cycle Equation 4.4 is used:

$$MT = \frac{1E-12 \times 0.1 \times 0.05 \times 0.05 \times 3600 \times 5E-5}{2\sqrt{1E-12 \times 0.05 \times 3600}} = 1.677050983\text{E-12 kg} \qquad \text{(Eq. 7.1)}$$

Thus the updated values of concentration for the first Main Channel and Rock Matrix boxes are obtained using Equations 4.5 and 4.6.

In this case $KDiff \cdot (C1 - C2) = 1.677050983\text{E-12}$;

$$C1 = \frac{5E-5 \times 9.89999984E-6 - 1.677050983E-12}{9.89999984E-6} = 4.983060091\text{E-5 kg m}^{-3} \qquad \text{(Eq. 7.2)}$$

and

$$C2 = \frac{0.0 \times 1.34164076E-7 + 1.677050983E-12}{1.34164076E-7} = 1.25\text{E-5 kg m}^{-3} \qquad \text{(Eq. 7.3)}$$

The code recorded to the special file (*Diff.out*) the details for the first Main Channel box and its associated Rock Matrix boxes for every cycle. Only the first few cycles (and to a depth of only 5 Rock Matrix boxes) are listed below. The Mass transfer value is a running total of mass transferred into the Rock Matrix. Also of note is the adherence to the pattern outlined in Fig. 4.3.

```
Main Channel Matrix 1      Matrix 2     Matrix 3     Matrix 4     Matrix 5

Equations 7.2 and 7.3
.498306E-04  .125000E-04  .000000E+00  .000000E+00  .000000E+00  .000000E+00
.498729E-04  .164063E-04  .546875E-05  .000000E+00  .000000E+00  .000000E+00
.498862E-04  .199707E-04  .772705E-05  .257568E-05  .000000E+00  .000000E+00
.498983E-04  .225403E-04  .101425E-04  .382347E-05  .127449E-05  .000000E+00

Mass Transfer:  cycle 1=  1.677050999883405E-012           Equation  7.1
Mass Transfer:  cycle 2=  2.934839228456907E-012
Mass Transfer:  cycle 3=  4.061607854332973E-012
Mass Transfer:  cycle 4=  5.068821086245884E-012
```

The file *Diff.out* (including data for all cycles and Rock Matrix boxes off main channel box 1) produced the graph in Fig. 7.1 for the time period 0.05 to 1 hour. This shows the development of the concentration profile for each time step for the Rock Matrix adjacent to Box 1 of the Main Channel.

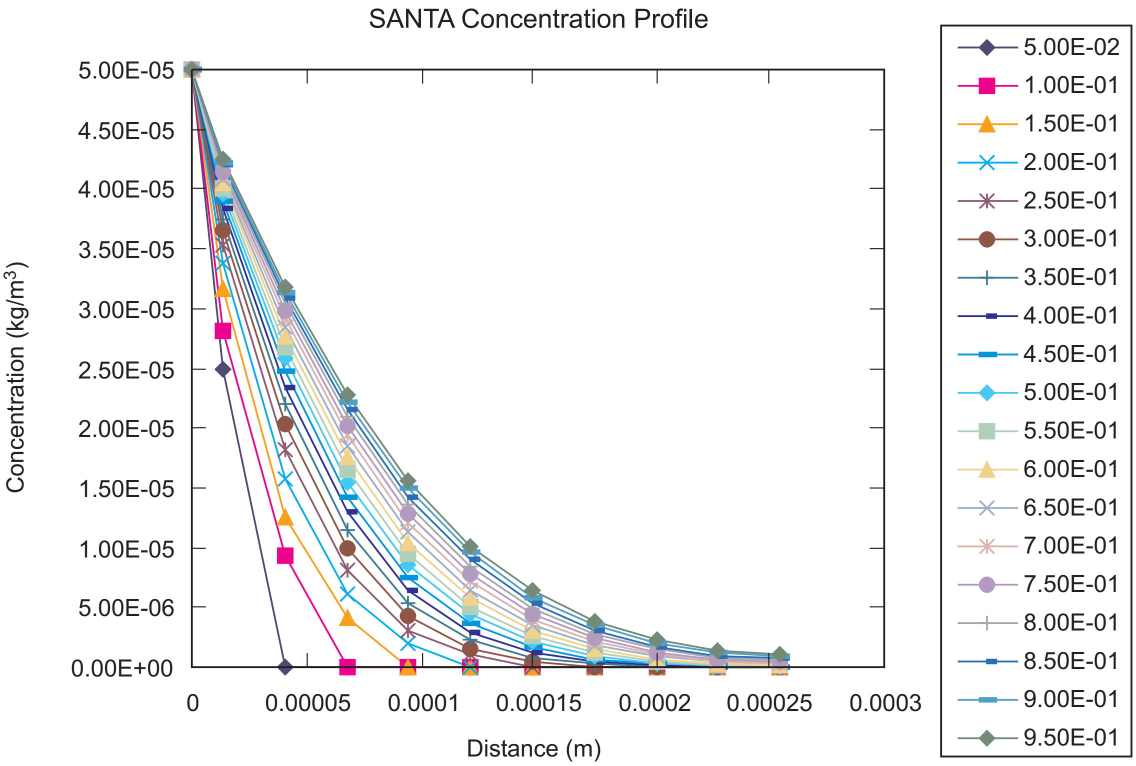

Fig. 7.1: Development of SANTA concentration profile for the rock matrix adjacent to main channel box 1 (time period 0.05 to 1 hour)

This profile can be checked directly against the analytical profile generated by using the following equation to define the concentration at a specific time (t) and distance (x):

$$C(t,x) = C_S \cdot erfc\left(\frac{x}{2\sqrt{Dt}}\right) \qquad \text{(Eq. 7.4)}$$

Equation 7.4 is the 1-D analytical solution to the transient diffusion equation

(Ficks 2nd law; $\frac{dC}{dt} = D\frac{d^2C}{dx^2}$, CRANK et al. 1981)

for the case of an infinite half-space, initially at 0 concentration, with a fixed concentration, C_s, at $x = 0$ (CARSLAW & JAEGER 1959).

Using this equation a set of values can be calculated using the same time steps as those used by SANTA, and at distances equivalent to Rock Matrix boxes. The graph obtained is shown in Fig. 7.2, again from 0.05 to 1 hour. As the scales used on both graphs are the same, direct comparisons can be made.

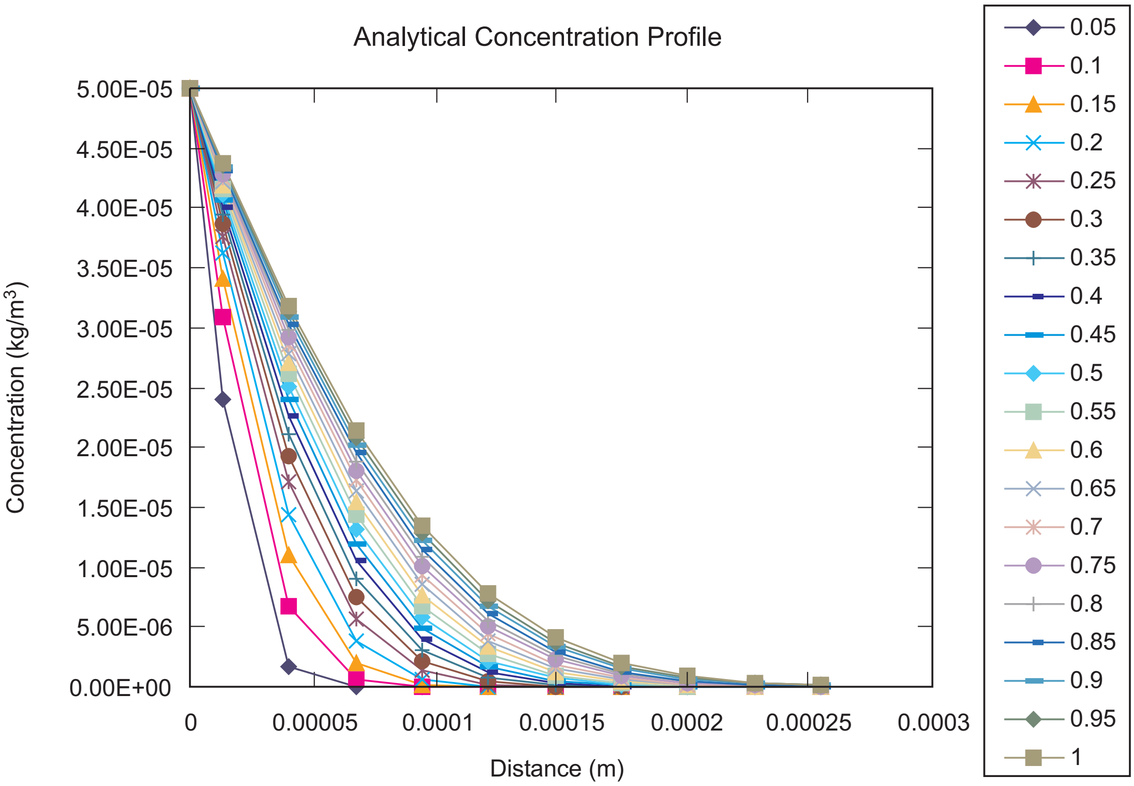

Fig. 7.2: Development of analytical concentration profile for the rock matrix adjacent to main channel box 1 (time period 0.05 to 1 hour)

While this shows the very close matching of the analytical results with those produced by the SANTA code a more informative comparison can be made by analysing the flux of mass across the Main Channel / Rock Matrix interface per cycle. The code already outputs a record of the mass transfer, and this was plotted along with the analytical result generated from the following equation (for time integrated flux; CARSLAW & JAEGER 1959):

$$Q = \int_0^1 q(t, x=0)\,dt = \frac{2\cdot D\cdot C_S\cdot t\cdot A\cdot\phi}{\sqrt{\pi\cdot D\cdot t}} \qquad \text{(Eq. 7.5)}$$

Fig. 7.3 shows the cumulative mass transported into the Rock Matrix at the end of each time step (0.05 hours) by the code, and the analytical solution over the same time period.

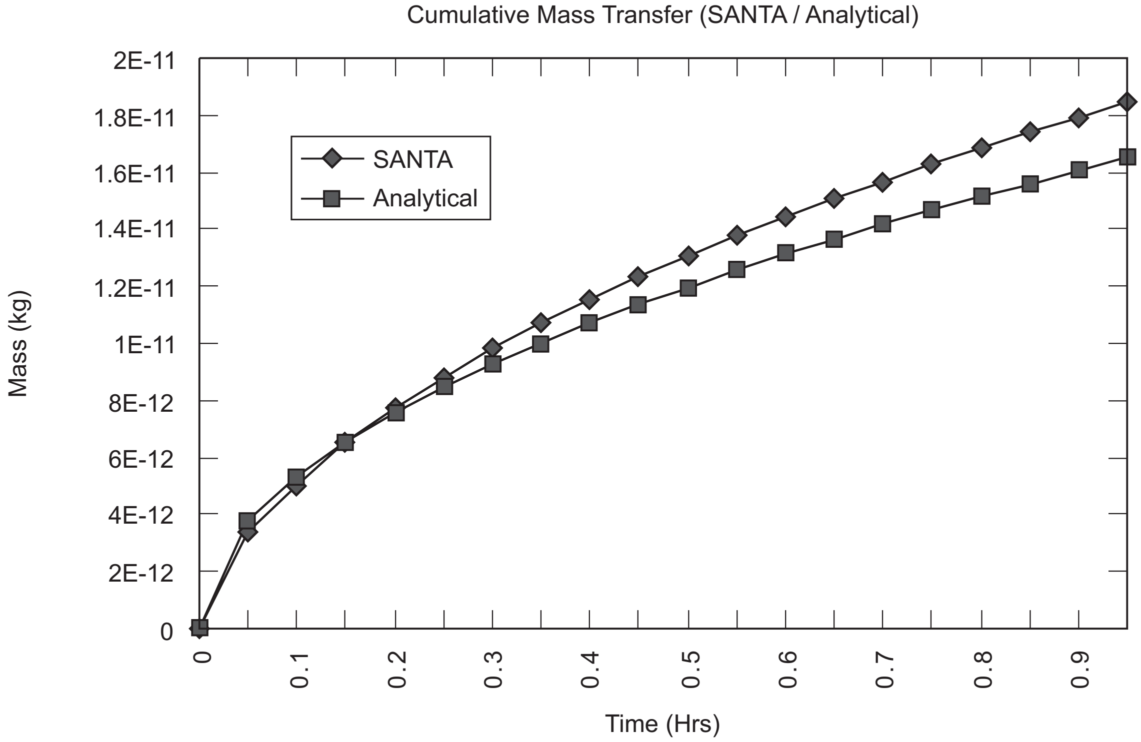

Fig. 7.3: Cumulative mass transfer into the rock matrix at the end of each time step (0.05 hours), produced with SANTA and analytical solution

As can be seen, the flux of mass calculated by the code is very similar to that predicted by the analytical solution. A further analysis was made of the incremental mass transfer per time step. This examined the calculated mass transfer per time step with that predicted by the analytical solution. Fig. 7.4 shows these values and the absolute difference between these results:

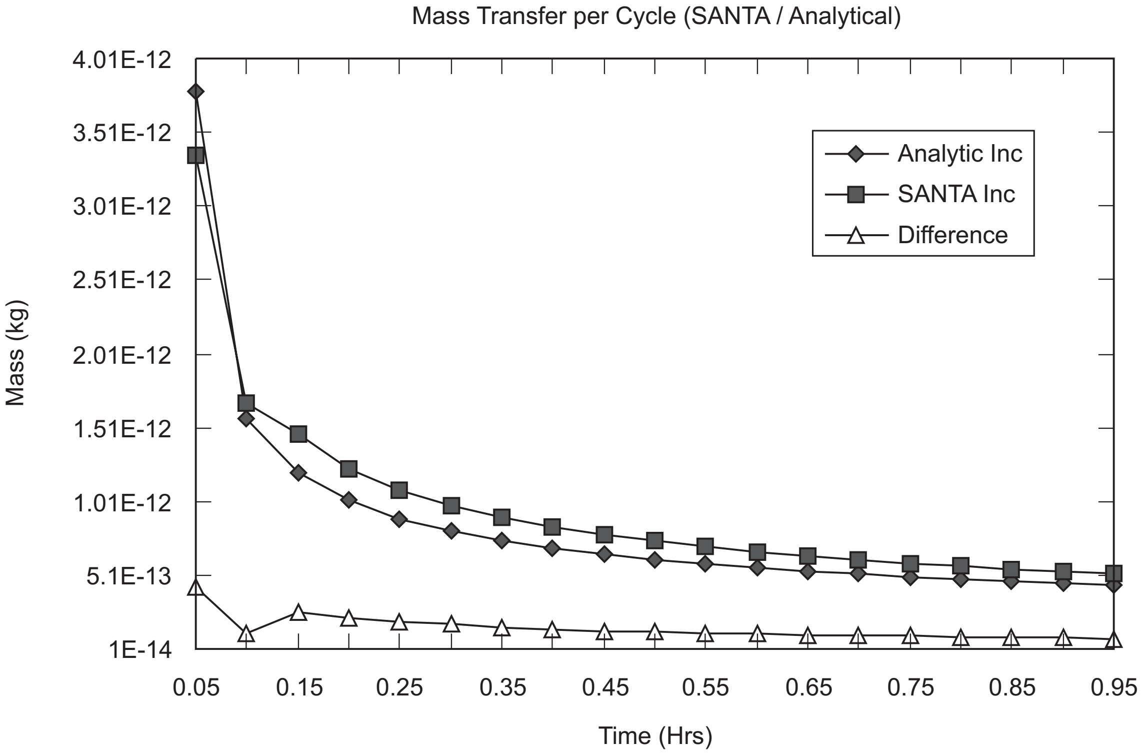

Fig. 7.4: Incremental mass transfer per time step calculated by SANTA and predicted by analytical solution

Of particular interest in Fig. 7.4 is the curve for the absolute difference (labeled Difference) between the analytical solution and the results output by SANTA. Initially, due to the starting conditions of maximum concentration in the main box and 0 concentration in the first side box, the biggest error occurs. This is due to the manner that SANTA approximates the concentration gradient ($\frac{dc}{dx}$), in Equation 4.1, by $(C1 - C2) / l$. After this initial error the absolute error settles down and stabilises to a near straight line. The error present will stay within known bounds, and at acceptably low values.

7.2.2 Diffusion into the Rock Matrix (with fixed boundary) from the Main Channel

As can be seen from Fig.s 7.1 and 7.2 the diffusion profile in the previous calculations does not significantly reach the furthest box in the Rock Matrix. To investigate the effects of a fixed boundary at the end of box 10, the code was run with the parameters listed below. The time of a run was extended to 26 hours (520 Cycles) with a constant input during this time.

SETUP PARAMETERS

No. of Boxes:	10	
Transit Time:	0.5 hours	
Duration of a run:	**26 hours (= 520 cycles, 1 cycle = 0.05 hours)**	
Duration of input pulse:	**26 hours**	
Input Elemental concentration:	5.0E-5 kg m^{-3}	
Dispersion:	"n"	Switched off.
Accuracy:	0.01	Not used in this test.

In this case due to the large number of cycles the code recorded data on only every 12th cycle. Again, the code output data for the concentration profile (every 12th cycle). This concentration profile can be compared directly with the analytical concentration profile generated using the following equation (CARSLAW & JAEGER 1959):

$$c(x,t) = C_0 \sum_{n=1}^{\infty} (-1)^n \left\{ erfc\left(\frac{(2n+1)l + x}{2\sqrt{Dt}} \right) + erfc\left(\frac{(2n+1)l - x}{2\sqrt{Dt}} \right) \right\} \qquad \text{(Eq. 7.6)}$$

giving the solution to the problem of zero initial concentration, and the surface at $x = -l$ maintained at a constant concentration C_0, and a fixed barrier at $x = 0$.

The concentration profiles generated analytically for the unbounded half-space (Fig. 7.5), and a bounded geometry (Fig. 7.6) and by SANTA (Fig. 7.7), for a select number of cycles (after 0.05, 12.05 and 23.45 hours) are shown below. SANTA output resembles that of the analytical solution to the bounded geometry. Deviations between the infinite half-space and the bounded geometry become increasingly larger with time.

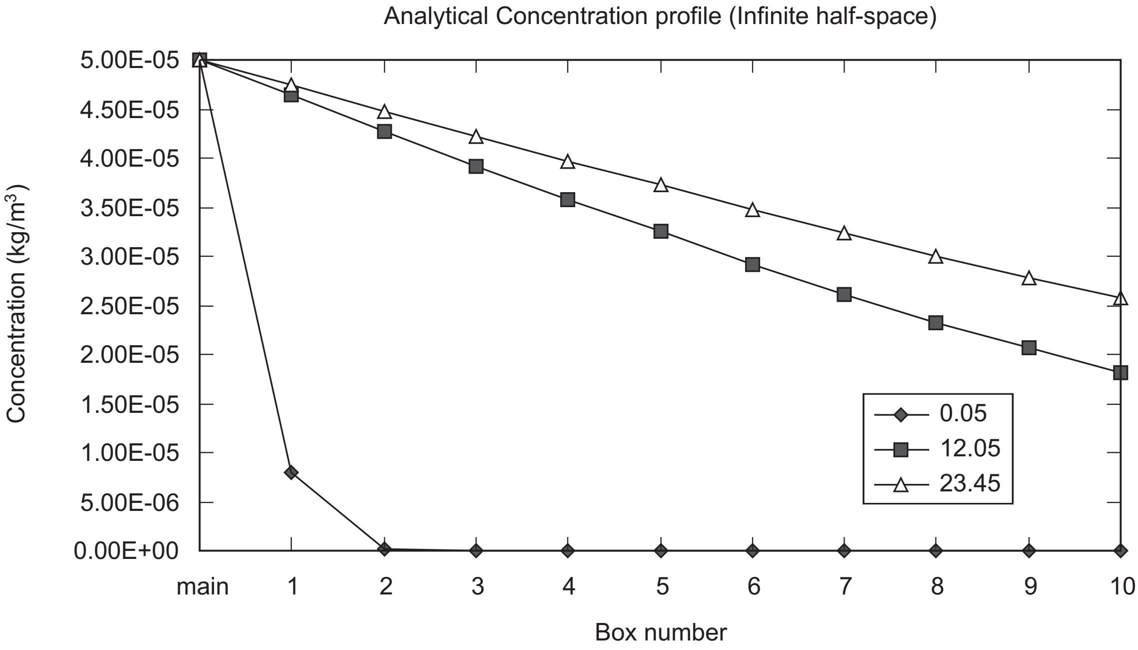

Fig. 7.5: Analytical concentration profile for the unbounded infinite half-space (after 0.05, 12.05 and 23.45 hours)

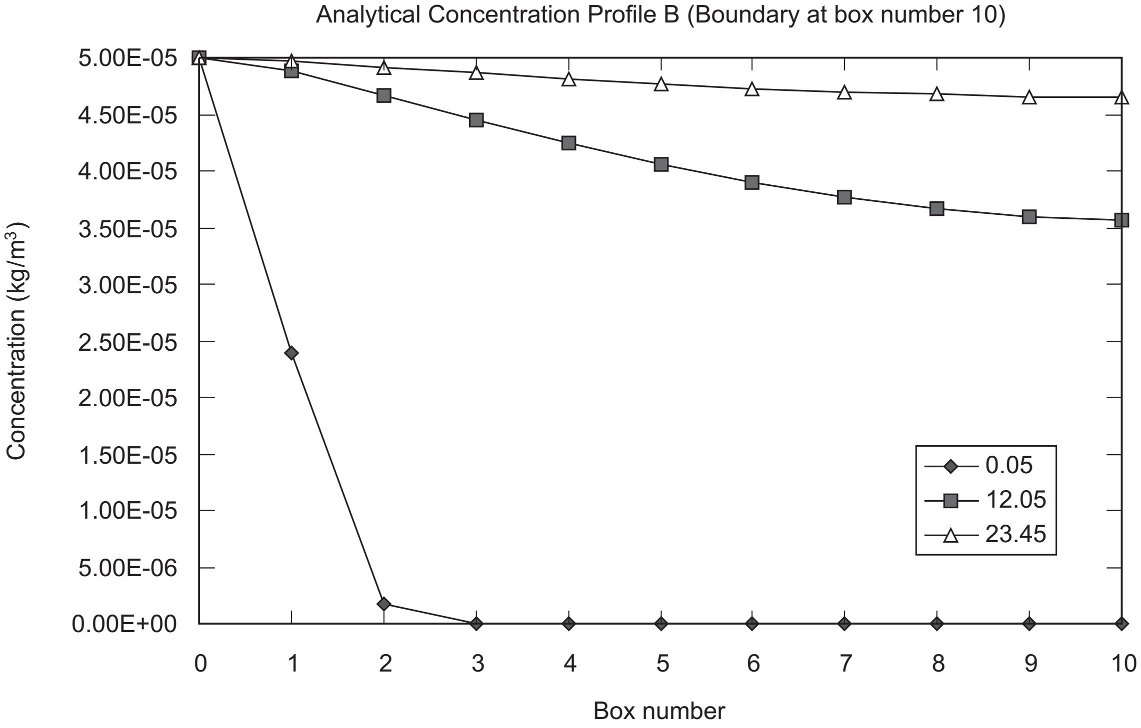

Fig. 7.6: Analytical concentration profile for a bounded system with a boundary after the 10th box (after 0.05, 12.05 and 23.45 hours)

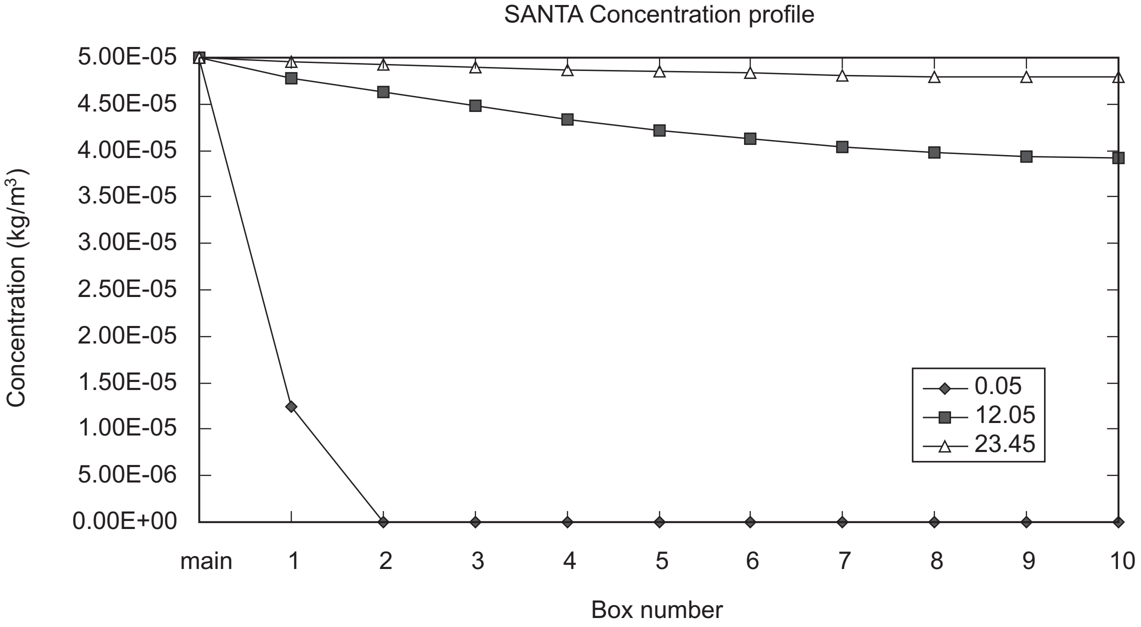

Fig. 7.7: Concentration profile calculated by SANTA (after 0.05, 12.05 and 23.45 hours)

The mass transfer per 12 cycles was recorded by SANTA, and this compared against the analytical results obtained from using the following equation (CARSLAW & JAEGER 1959) for the bounded geometry:

$$M(t) = lC_0 \left\{ 2\left(\frac{Dt}{\pi l^2}\right)^{\frac{1}{2}} \left\{ 1 + 2\sum_{n=1}^{\infty} -1^n e^{\frac{-n^2 l^2}{Dt}} \right\} - 4\sum_{n=1}^{\infty} -1^n n \cdot erfc \frac{nl}{\sqrt{Dt}} \right\} \qquad \text{(Eq. 7.7)}$$

First, the cumulative flux of mass across the Main Channel/Rock Matrix interface was analysed. In this case the analytical solution with a boundary (Analytic B) and SANTA data were plotted along with the analytical solution for the infinite half-space (Analytic A). The results are plotted every 12 cycles, and are shown in Fig. 7.8.

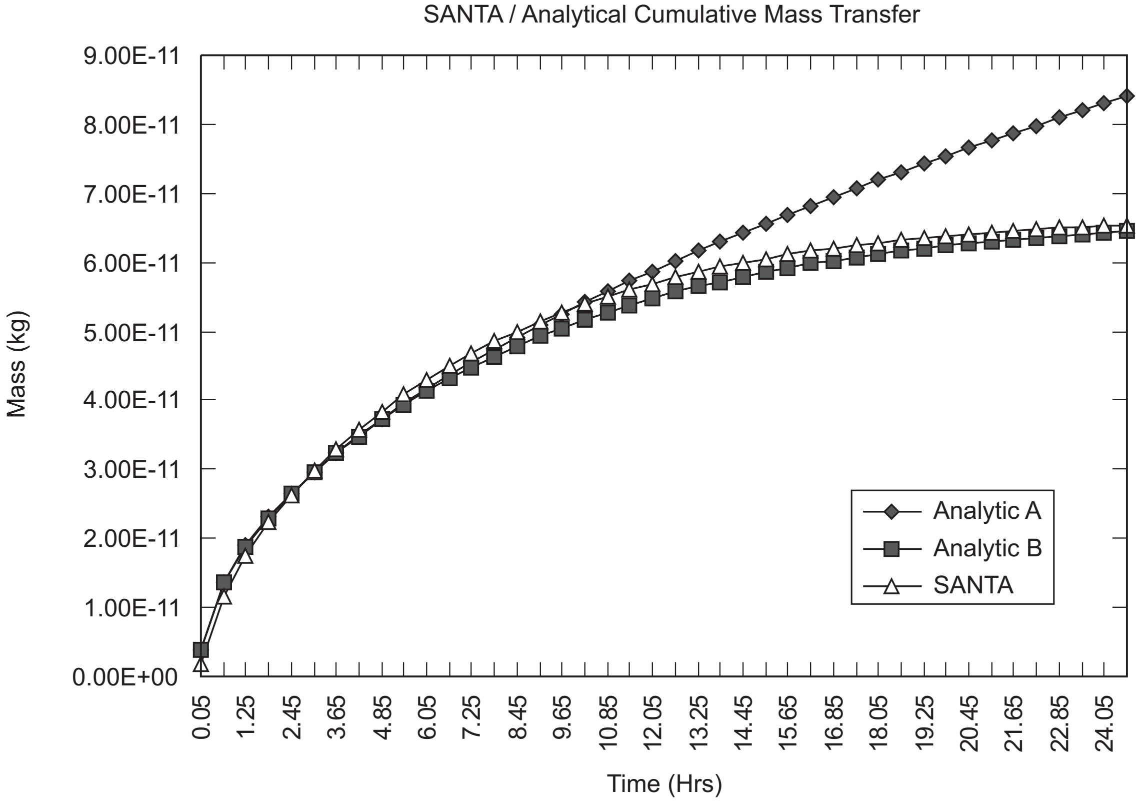

Fig. 7.8: Cumulative mass transfer across the main channel/rock matrix interface plotted every 12 cycles; Analytic A: analytical solution for the infinite half-space, Analytic B: analytical solution with a boundary after the 10th box and SANTA data

Fig. 7.8 shows clearly that as time increases, less mass is transferred into the Rock Matrix when a barrier is present after the 10th Box compared to the infinite half-space. The Rock Matrix is approaching equilibrium with the Main Channel box concentration when an impermeable boundary is present, whereas for the case of the infinite half-space diffusion into the Rock Matrix continues.

The mass transfer per 12 cycles for the analytical solution for the infinite half-space, the bounded geometry and SANTA is shown below (Fig. 7.9). The difference between the analytical solution with a boundary after the 10th box and the results from SANTA are labeled "Difference (SANTA – Analytic B)".

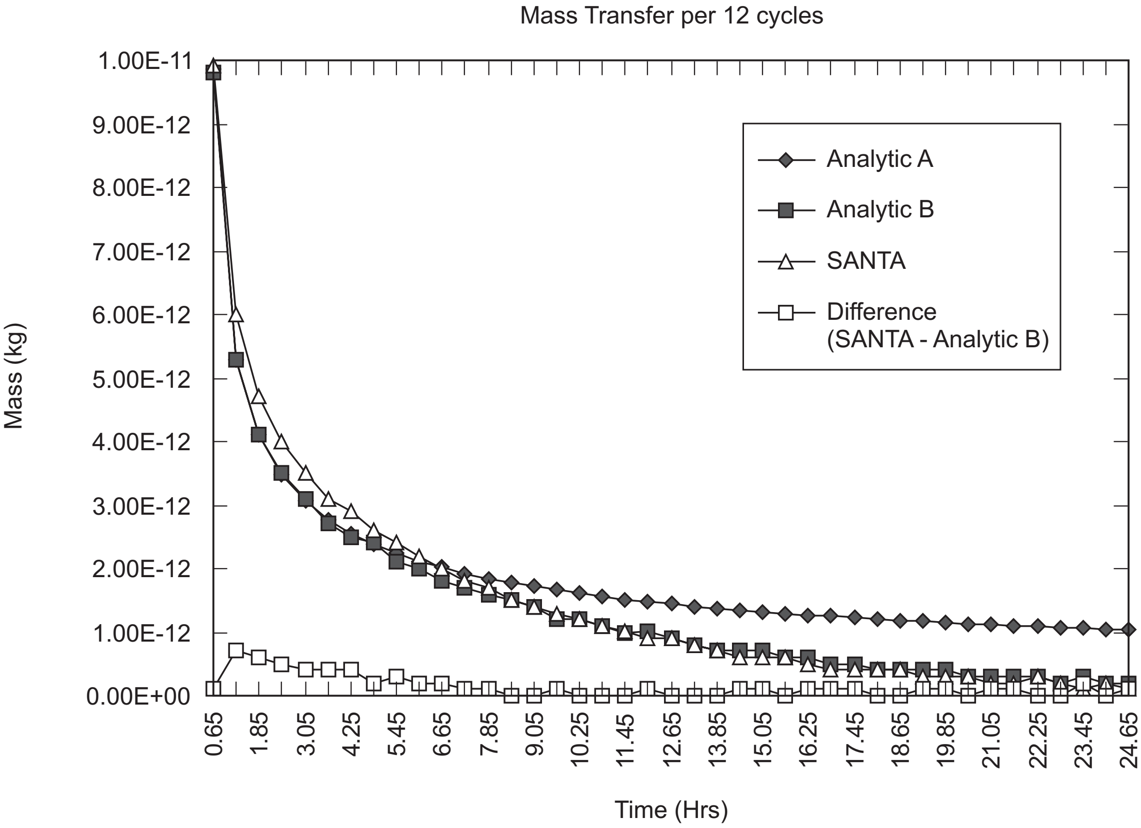

Fig. 7.9: Mass transfer across the main channel/rock matrix interface plotted every 12 cycles; Analytic A: analytical solution for the infinite half-space, Analytic B: analytical solution with a boundary after the 10th box, SANTA data and Difference between SANTA and Analytic B

Fig. 7.9 shows the close matching of the SANTA results with those of the analytical solution for the case of an impermeable boundary. The error present remains stable, within known bounds, and at acceptably low values.

The development of concentration profiles and fluxes become distinctly different for the bounded geometry (10 boxes) and the infinite half-space after about 10 hours. For the SANTA calculations this is equivalent to 200 cycles, which is equivalent to a characteristic diffusion depth of $\sqrt{200}$ (14) boxes. The restriction of a bounded geometry imposed on SANTA can therefore be expected to mimic the infinite half-space without significant error to at least twice the theoretical limit of the square of the number of Rock Matrix boxes.

7.2.3 Diffusion into the Main Channel from the Rock Matrix

The next step in investigating the codes handling of diffusion takes into account that a tracer can move out, as well as into, the Rock Matrix. To investigate this the code was set up with the previous values, except that the run was for 2 hours (Parameters shown below), with the duration of the input pulse remaining at 1 hour. This would mean that after 1 hour the main channel concentration in Box 1 would become 0, and so flow of tracer would be from the Rock Matrix into the Main Channel. The equations that govern the mass transfer in the SANTA code are identical to those quoted previously, except that in this case there will be a negative gradient, and hence an opposite direction of mass transfer.

SETUP PARAMETERS

No. of Boxes:	10	
Transit Time:	0.5 hour	
Duration of a run:	**2 hours (= 40 cycles, 1 cycle = 0.05 hours)**	
Duration of input pulse:	1 hour	
Input Elemental concentration:	5.0E-5 $kg\,m^{-3}$	
Dispersion:	"n"	Switched off.
Accuracy:	0.01	Not used in this test.

As the concentration profiles generated up to 1 hour are identical to those discussed in the earlier chapter, these will be omitted from the graphs. Therefore the time of interest is from 1 to 2 hours (10th to 20th cycle). The output concentration profile generated by SANTA is shown below (Fig. 7.10) for the concentration in each of the 10 Rock Matrix boxes off the Main Channel box no. 1, for each cycle.

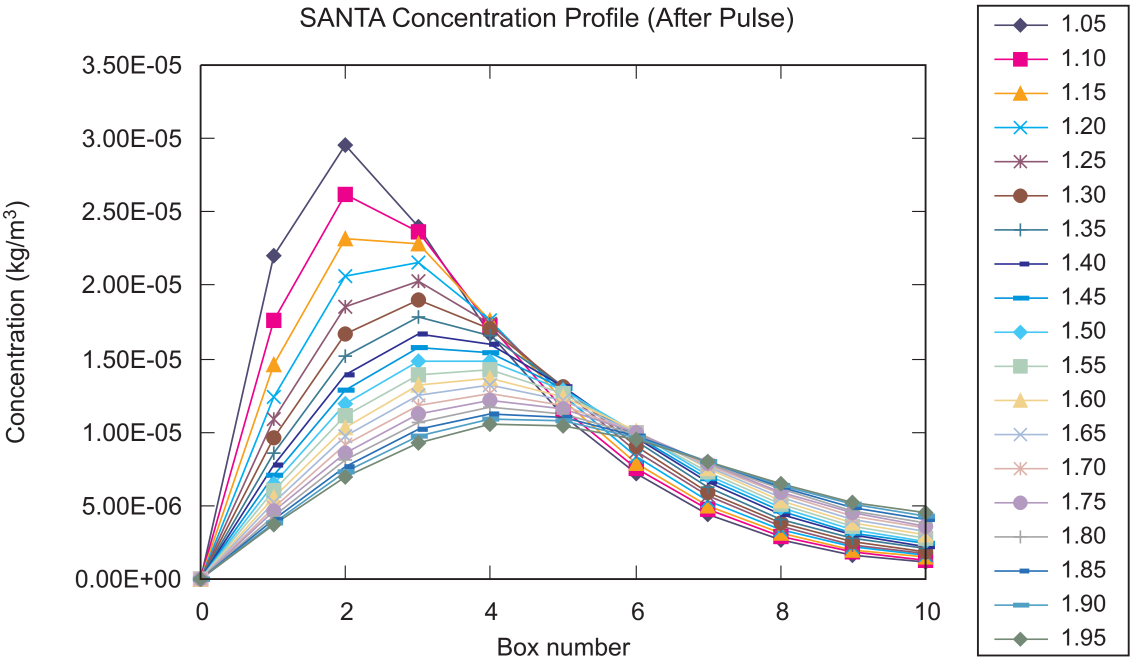

Fig. 7.10: SANTA concentration profile (after pulse)

Again, this can be checked directly against the analytical profile generated by using the following equation (Eq. 7.8) to define the concentration at a specific time (t) and distance (x), after a concentration profile has developed up to time t_p (CARSLAW & JAEGER 1959).

using Equation 7.4:

$$c(x) = C_S \cdot erfc\left(\frac{x}{2\sqrt{Dt}}\right)$$

setting $t = t_p = 1$ hour;

$$C\left(x,t'\right) = \frac{1}{2\sqrt{\pi D t'}} \int_0^\infty C(u)\left[e^{\frac{-(x-u)^2}{4Dt'}} - e^{\frac{-(x+u)^2}{4Dt'}}\right] \qquad \text{where } t' = t - t_p \qquad \text{(Eq. 7.8)}$$

The function $C(u)$ is required in this case to define the concentration profile present in the Rock Matrix that has been created prior to the main channel concentration dropping to 0.

The resultant analytical concentration profiles are shown below in Fig. 7.11, again for the period 1 to 2 hours.

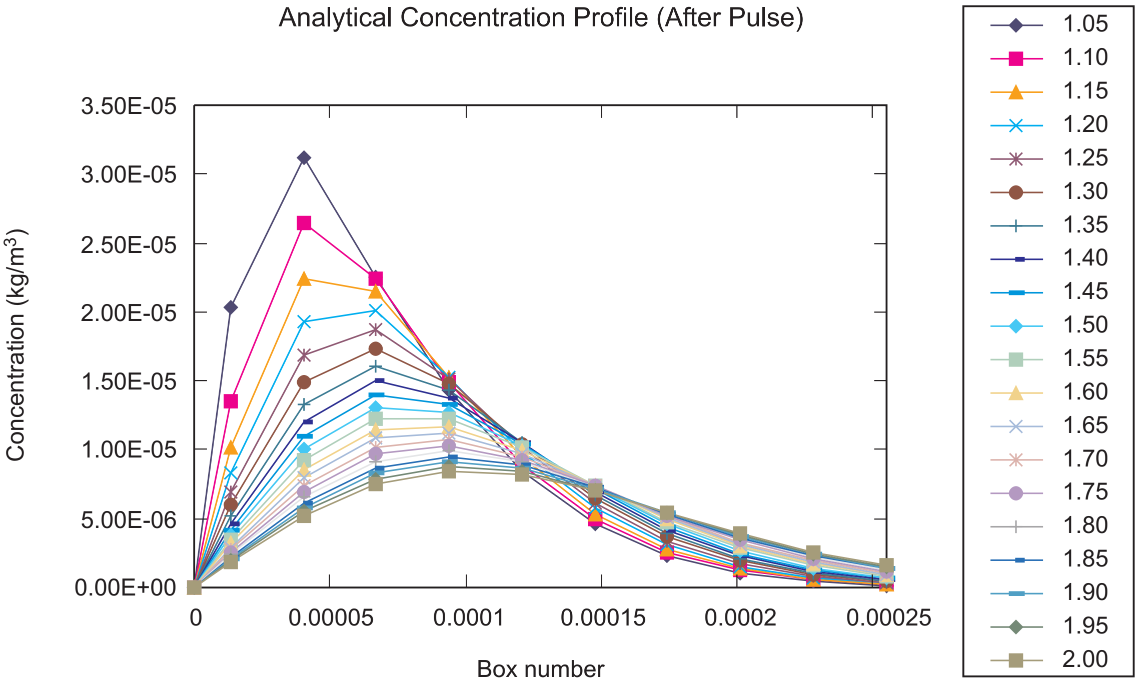

Fig. 7.11: Analytical concentration profile (after pulse)

Again, a check was made on the mass flux through the Main Channel/Rock Matrix interface. As previously, the code recorded the mass transfer but a different approach was taken to analytically calculate the flux. Using Equation 7.8 to calculate the concentration at 80 separate points in each time period, a more accurate set of concentration profiles was obtained. With the aid of a small program, and using the trapezoidal rule, the area under each curve could be approximated. From this the mass of tracer in the Rock Matrix could be calculated. Any change in the mass contained in the Rock Matrix between time periods would be due to a flux across the Main Channel / Rock Matrix interface. Thus, the values of mass flux were calculated for all the time periods. These results, for the analytical and SANTA outputs, are shown in Fig. 7.12.

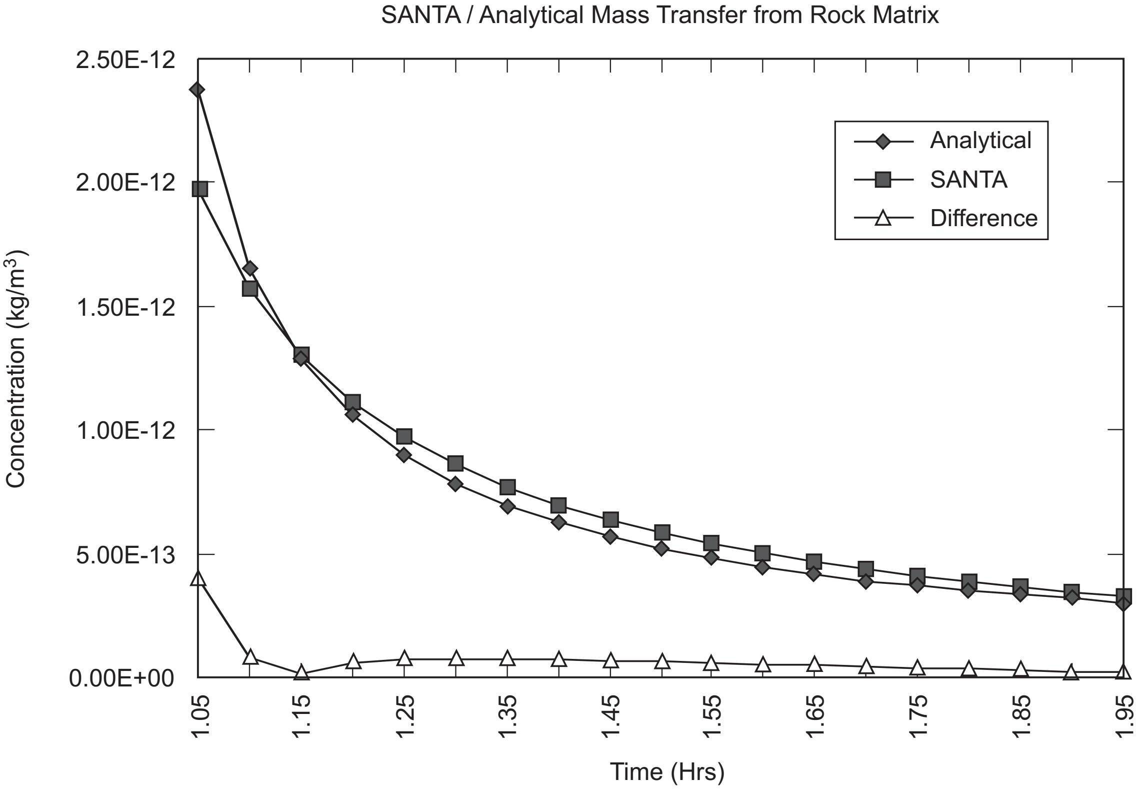

Fig. 7.12: SANTA / Analytical mass transfer from rock matrix

As can be seen in Fig. 7.12 the curve for the absolute difference (labeled Difference) between the analytical solution and the results output by SANTA follows the same pattern as before. Again, in the first time step after the pulse has passed through, the largest concentration difference will be present. As before, the absolute error settles down and stabilises to a near straight line. The error present when mass transfer occurs into the Main Channel will stay within known bounds, and at acceptably low values.

7.3 Sorption/Dispersion

The implementation of dispersion into SANTA is closely linked to retardation caused by sorption (see Chapter 6). The testing for the effect of dispersion also double checks the implementation of linear sorption. Thus, for a fixed dispersivity (set arbitrarily to 0.015 m), a selection of Kd values (Freundlich α, $\beta = 1$) were used to investigate the combined effects of dispersion and linear sorption.

The Kd values used were 0.1, 0.01 and 6.6E-3, and in order to see more clearly the development of the concentration profile the system was run for 8 cycles. The code calculated automatically the number of main channel boxes required for the retardation caused by the different Kd values which meant that different run times had to be used to get to 8 cycles for each Kd value. The set of input values used are listed below:

SETUP PARAMETERS

No. of Boxes:	45, 13, 10 respectively for Kd values	
Transit Time:	0.6 hours	
Duration of a run:	0.11, 0.4, 0.5 hours	
Duration of input pulse:	1 hour	
Input Elemental concentration:	5E-6 kg m^{-3}	
Dispersion:	"n"	Switched off.
Accuracy:	0.00001	

MAIN CHANNEL

Channel Width:	0.5 m
Path Length:	1.8 m
Aperture of Fracture:	1E-4 m
Fracture Porosity:	0.99

ROCK MATRIX

All of the values for the Rock Matrix are not used by this version. The depth of diffusion is set to 0 boxes. Diffusion is switched off.

SORPTION VALUES

Value of Alpha for sorption:	0.1, 0.01 and 6.6E-3 respectively
Value of Beta for sorption:	1.0

Thus three runs were performed by SANTA for the three Kd values. The outputs from SANTA were checked against the analytical result generated from the following equation (APPELO & POSTMA 1993):

$$C(x,t) = C_i + 0.5\left(C_0 - C_i\right) erfc\left(\frac{x - \frac{vt}{R}}{\sqrt{\frac{4D_L t}{R}}}\right) \qquad \text{(Eq. 7.9)}$$

With the following boundary conditions:

$C(x,t) = C_i$ for $x > 0; t = 0$ = 0 in this test case.
$C(x,t) = C_o$ for $x = 0; t > 0$ = input concentration.
$C(x,t) = C_i$ for $x = \infty; t > 0$ = 0 in this test case.

The results from SANTA were plotted along with the analytical results from Equation 7.9. These are illustrated below, each recorded after 8 cycles (see Fig. 7.13 – 7.15).

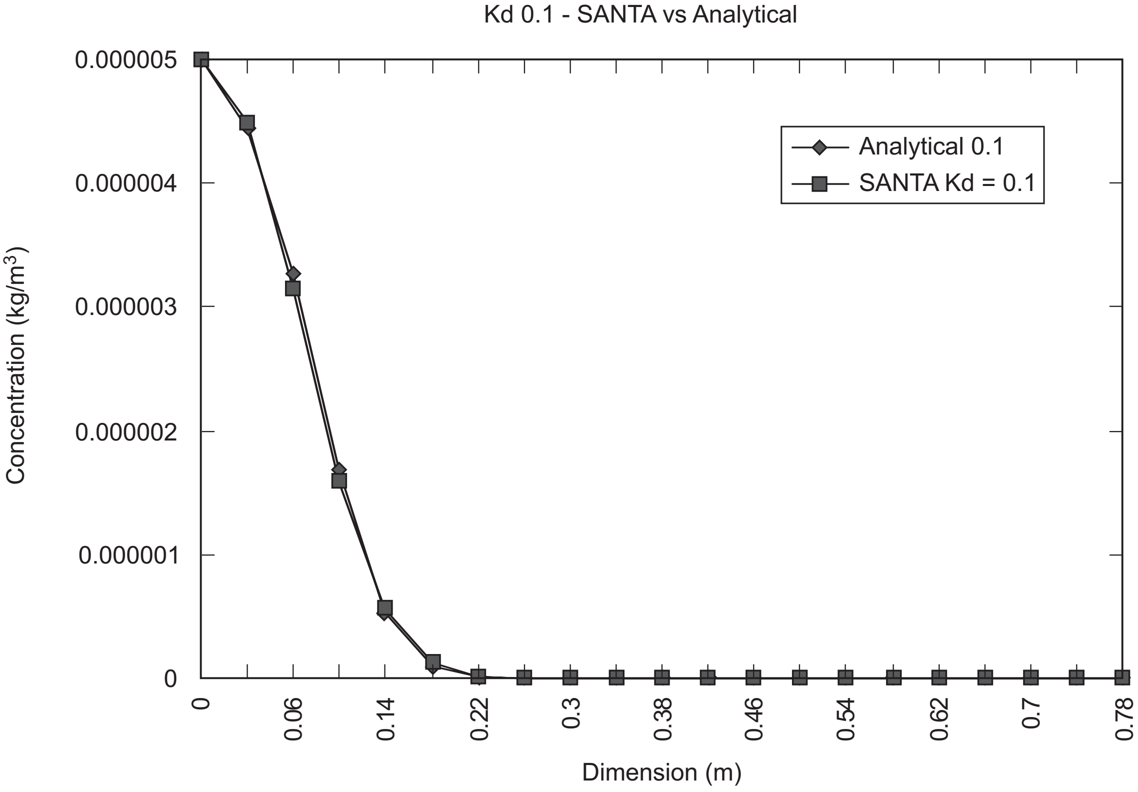

Fig. 7.13: SANTA /Analytical concentration profile (for Kd = 0.1 with 45 boxes)

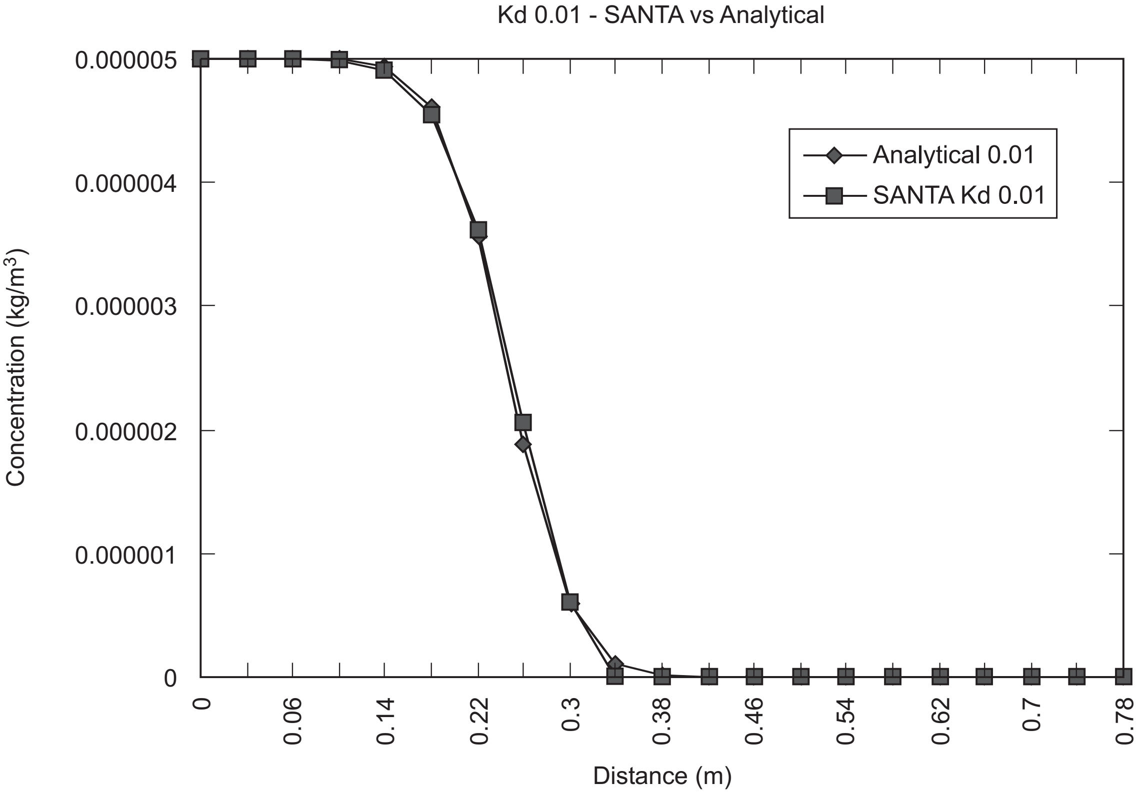

Fig. 7.14: SANTA / Analytical concentration profile (for Kd = 0.1 with 13 boxes)

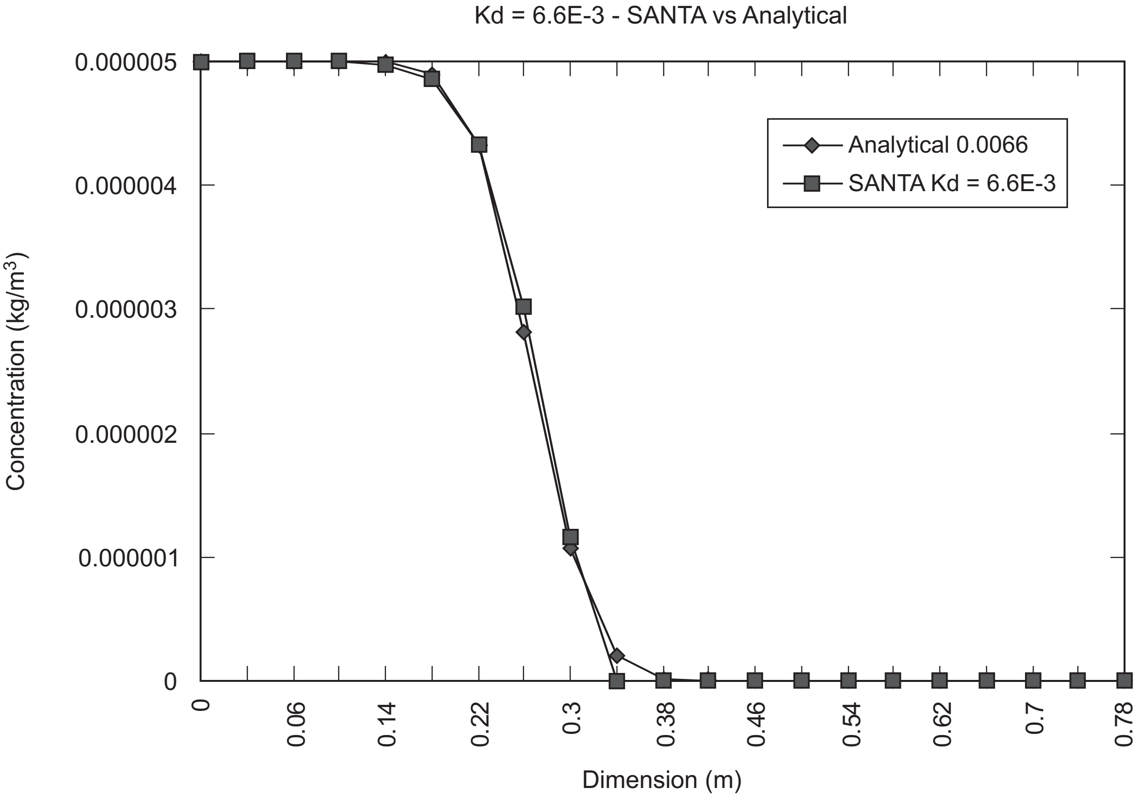

Fig. 7.15: SANTA / Analytical concentration profile (for Kd = 6.6E-3 with 10 boxes)

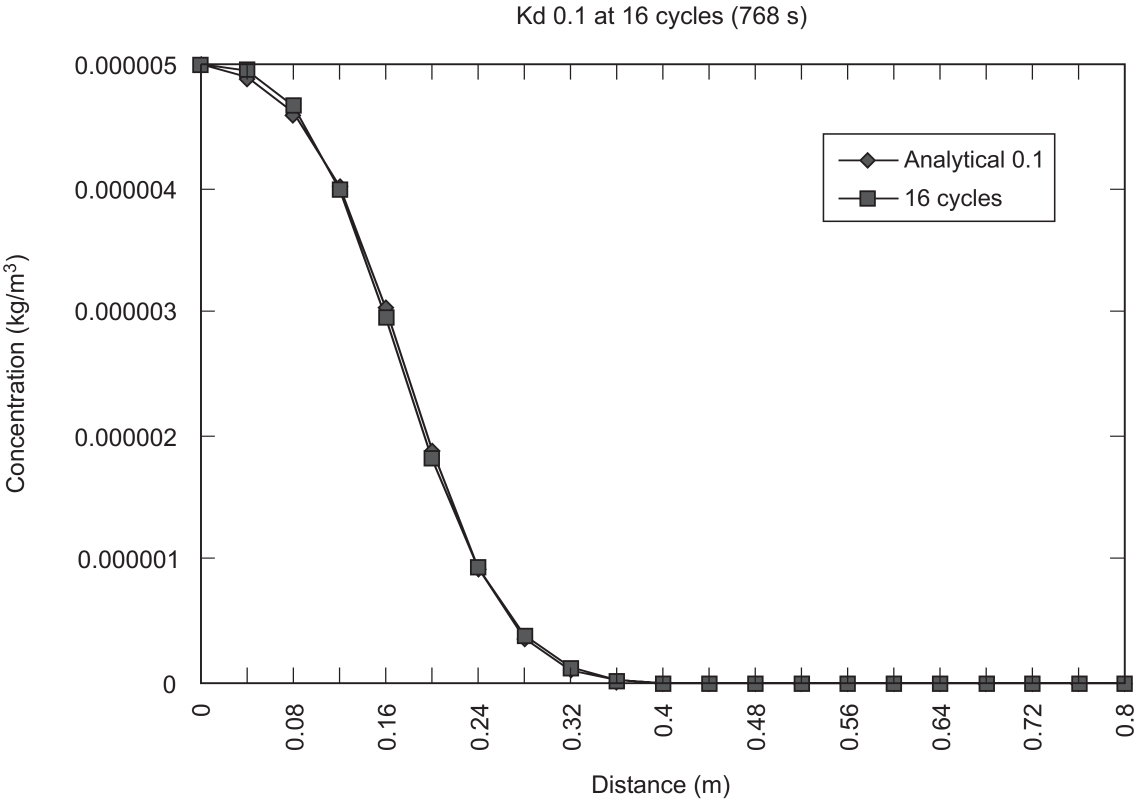

Fig. 7.16: SANTA / Analytical concentration profile at 16 cycles (Kd = 0.1)

As a further test, an investigation into the development of the concentration profile was examined at different time intervals. The value of Kd was set at 0.1 (using 45 boxes) and SANTA produced output files at 16 and 50 cycles (in addition to the previously recorded output at 8 cycles). These were plotted with the analytical results and are shown in Fig.7.16 and 7.17.

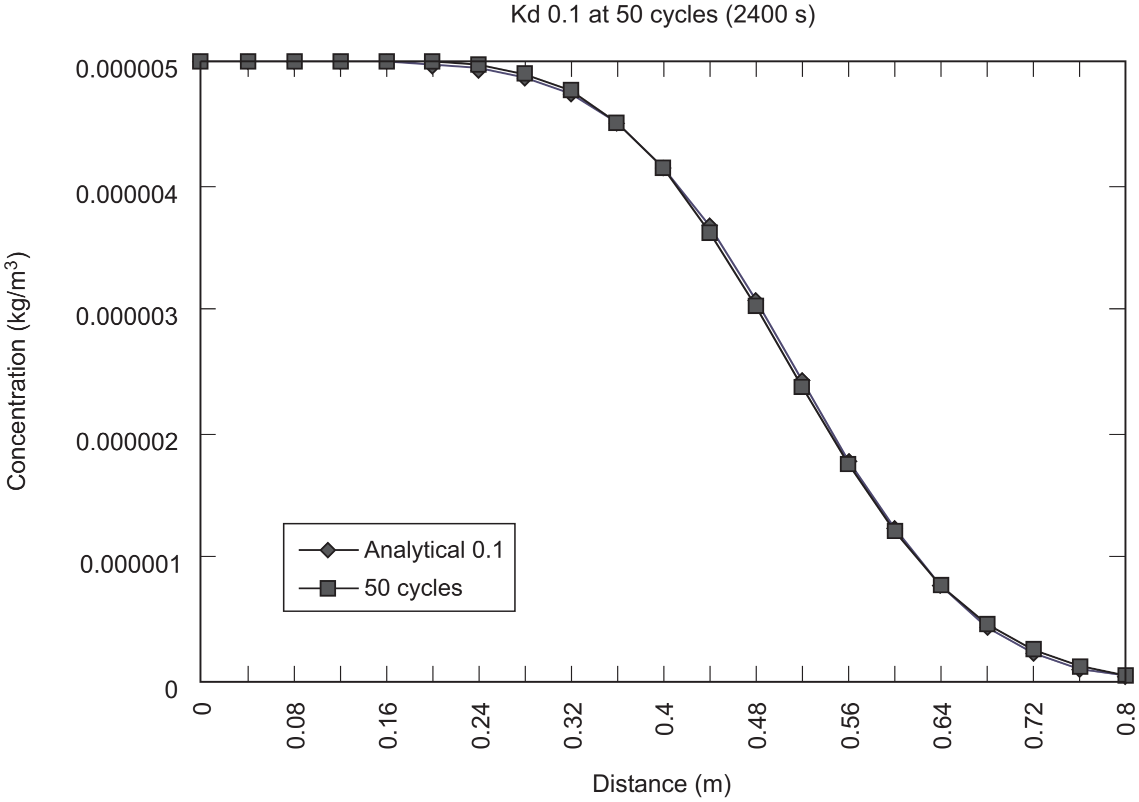

Fig. 7.17: SANTA / Analytical concentration profile at 50 cycles (Kd = 0.1)

Errors are marginal and well within acceptable bounds in all test cases. The input files to repeat the above runs are included on the installation disk (santex1.sin, santex1b.sin, santex1c.sin, santex2.sin, santex3.sin, santex4.sin, santex5.sin).

The coupled implementation of dispersion and retardation (sorption) is numerically exact for linear sorption. Results for weakly non-linear sorption (β close to 1) are also expected to be within acceptable error bounds for scoping calculations. Strongly non-linear sorption ($\beta << 1, \beta >> 1$) will still be modeled correctly in a qualitative way, but results are expected to suffer from numerical imprecision.

7.4 Diffusion with Sorption

Sorption is implemented for the Rock Matrix in exactly the same way as the main channel boxes, although in this case the transport of a contaminant is controlled by diffusion rather than advection. An incoming tracer can react with the rock according to the Freundlich equation thus retarding the transport of the contaminant (when compared with purely diffusive flux). To test the implementation of sorption in the Rock Matrix the code was set up as outlined below and the results recorded. These were then compared with an analytical solution for the same process.

SETUP PARAMETERS

No. of Boxes:	39
Transit Time:	0.6 hour
Duration of a run:	8.86 hours
Duration of input pulse:	8.86 hours
Input Elemental concentration:	1E-5 kg m^{-3}
Dispersivity:	0.015
Accuracy:	0.01

MAIN CHANNEL

Channel Width:	0.3 m
Path Length:	1.8m
Aperture of Fracture:	1E-4 m
Fracture Porosity:	0.99

SIDE MATRIX

Effective Diffusivity:	1.0E-12
Matrix porosity:	0.05
Limit of Diffusion (Boxes):	10

SORPTION VALUES

No values were entered for sorption in the main channel.
The option for sorption was switched off.

ADDITIONAL OPTIONS

Rock Matrix Sorption

Rock Matrix Alpha for sorption:	0.0001
giving retardation factor of:	6.7
Rock Matrix Beta for sorption:	1.0

The above setup is stored in the file "santex6.sin", included on the installation disk.

When the above set of data was run, SANTA output the following results (Fig. 7.18) for the development of contaminant concentration into the rock matrix at the different times shown. All times are in seconds.

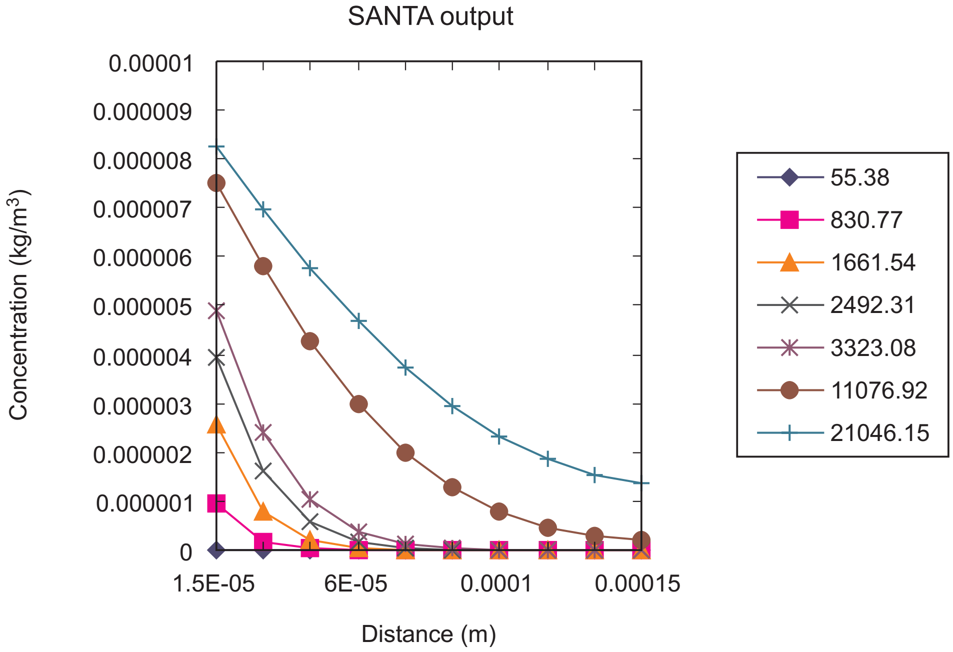

Fig. 7.18: SANTA concentration profile for contaminant

The corresponding chart for the analytical profile is shown below.

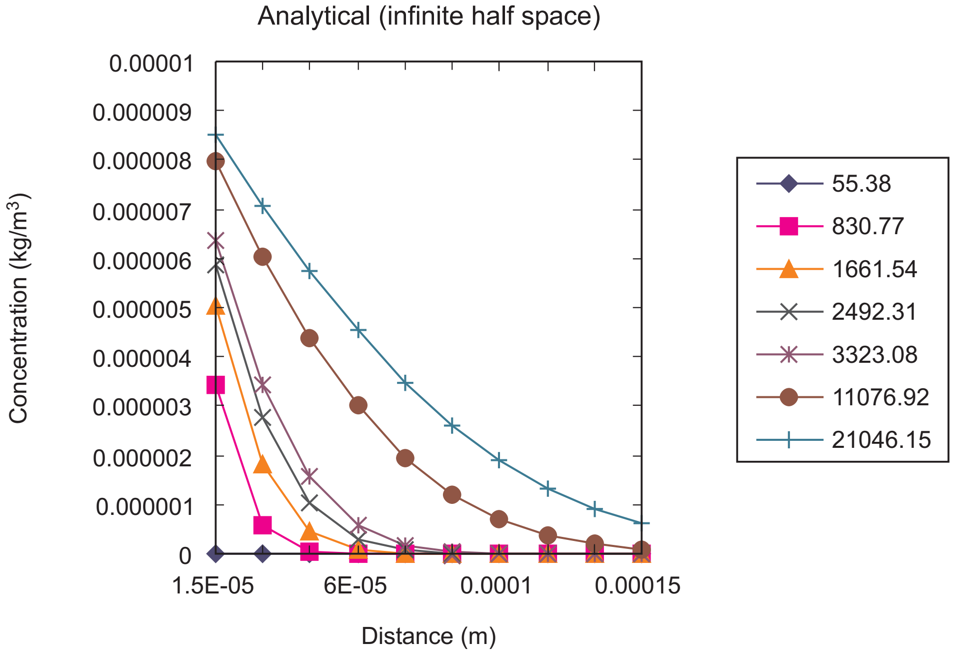

Fig. 7.19: Analytical profile

This shows that the results generated by SANTA follow the analytical solution to an acceptable degree. It must be noted that the analytical solution used above was for a pulse into an unbounded rock matrix, whereas SANTA was calculating for a fixed boundary rock matrix.

Therefore the tail of the SANTA profile will be slightly at a higher concentration than that of the unbounded profile (Fig. 7.20). Also of note is the possible presence of any cumulative error associated with SANTA's implementation of sorption and diffusion.

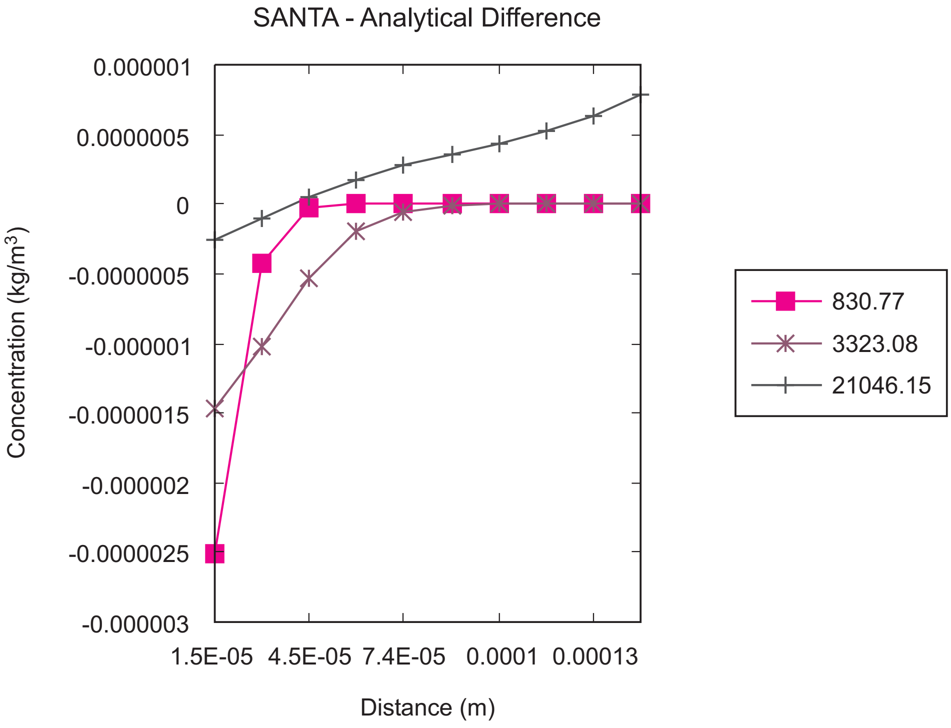

Fig. 7.20: Analytical difference

7.5 Sorption, dispersion and radioactive decay

This example file is based upon the Kristallin-I reference case that is fully documented in NTB 93-22 (NAGRA 1994). All data except the half-life and retardation factor were taken from this report.

This reference case concentrates on the geosphere modeling region. It describes the network of water-conducting features which extend throughout the crystalline basement of Northern Switzerland. The parameters defined below were used for input.

INPUT DATA

The following input data is contained in the SANTA input file "santex7.sin" As a comparison the PICNIC code (BARTEN & ROBINSON 1996) was run with identical parameters.

SETUP PARAMETERS

No. of Boxes:	10
Transit Time:	159272.73 hours
Duration of run:	127418184 hours
Duration of input pulse:	521888954.391 hours
Input Elemental concentration:	1 kg m^{-3}

MAIN CHANNEL

Channel Width: 1 m
Path Length: 200 m
Fracture Aperture: 0.001 m
Fracture Porosity: 0.99
Density: 3000 kg m^{-3}

ROCK MATRIX

No values used in this example.

SORPTION PARAMETERS

Freundlich Alpha: 5 m^3 kg^{-1}
Freundlich Beta: 1

MISC. SETTINGS

Dispersivity: 10 m
Accuracy: 0.0001

In addition the half-life for radioactive decay was set to 1000 years.

RESULTS FROM RUN

The following graphs plot the output from SANTA along with the output from the PICNIC code for comparison.

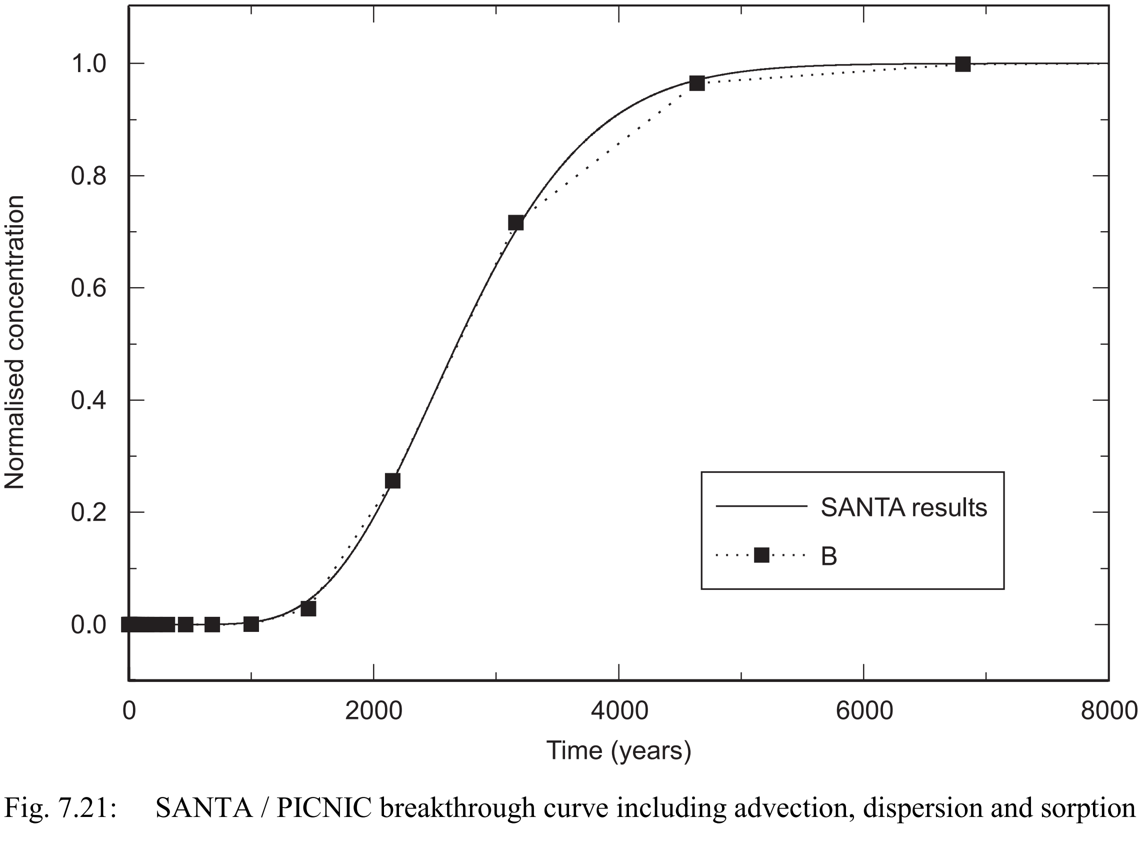

Fig. 7.21: SANTA / PICNIC breakthrough curve including advection, dispersion and sorption

Processes included in Fig. 7.21 – advection, dispersion, sorption. B indicates results calculated using PICNIC version II.

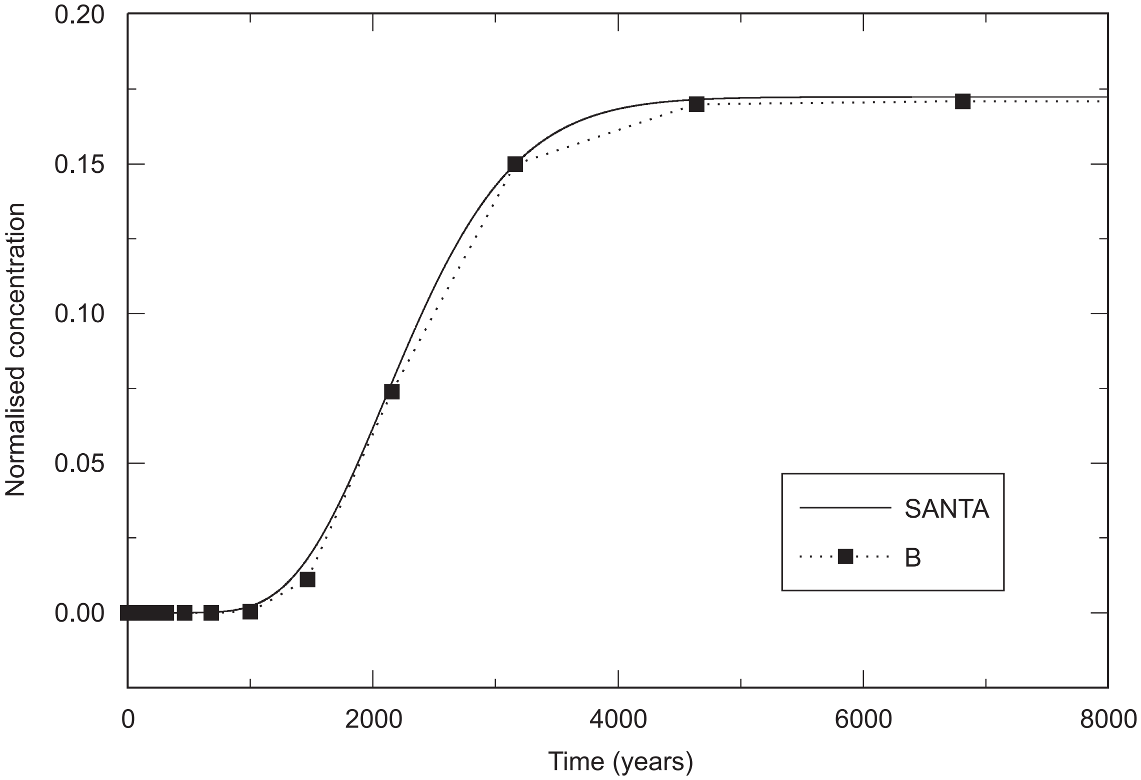

Fig. 7.22: SANTA / PICNIC (B) breakthrough curve including advection, dispersion, sorption and decay

The processes included in Fig. 7.22 – advection, dispersion, sorption + DECAY with a half-life of 1000 years. B indicates results calculated using PICNIC version II.

The output shows SANTA predicting the breakthrough curve almost identically to the PICNIC code prediction.

8 Worked Example

This section outlines the creation of a simple example file and then further modifies the input data to include more of the available options. All the example files created in this chapter are also contained in the SANTA directory (wrkex1.sin, wrkex2.sin, wrkex3.sin and wrkex4.sin) for reference and will be installed automatically by the installation program.

8.1 Worked example 1, advection

Load SANTA by double clicking on the santa icon (or start from the menu in Win95 / NT). The SANTA main screen will be displayed. Click on the button labeled "Create/Load/Update" to access the input screen. This is the main screen for entering the setup parameters of SANTA. There are already a few fields filled with data. These are default values and should be left as they are for the moment. Starting with the "Main Channel Geometry" section enter the following numbers (tip: use the TAB button to move to the next field):

Channel Width [m]:	0.5
Path Length [m]:	1.8
Fracture Aperture [m]:	0.0001
Fracture Porosity:	0.99

Use the default value for Density which is already set at 2700 $kg\,m^{-3}$.

In the "Boxes and Cycles" section enter the following:

No. of Boxes:	45 (replace the value 10)
Transit Time [Hrs]:	1.6
Duration of run [Hrs]:	20
Duration of input pulse [Hrs]:	0.8
Input Elemental concentration [$kg\,m^{-3}$]:	0.00001

In the "Misc Settings:" section leave the "Accuracy" setting at 0.0001. This is the relative error setting for the Newton-Raphson solving algorithms used by SANTA. If greater accuracy is required make this number smaller

Note: The smaller the "Accuracy" number the more calculations SANTA will have to make.

In the comments box enter a text description of the file. In this case it is an example file using only the advection option.

Click on the "Save" button and save as "testex1.sin". This will save all the data to a file on your hard drive (this data is already contained in the file "wrkex1.sin").

Now click on the "Use Values" button. This will return you to the Main screen again (if any errors are present in data entry a warning will be displayed at this time), with the text "- Values successfully loaded -" displayed in the window to the right of the "Start" button in the Process Data section.

Press the "Start" button. SANTA will now start to run. While the calculations are being carried out the upper bar marked "processed" will fill up to show you how far the code has progressed in the calculations. The bar marked "Box 1" indicates the concentration of aqueous tracer existing, at that precise moment, in box 1. Similarly, the bar marked "Box 45" indicates the aqueous concentration for the 45th (last box) in the main channel.

When the calculations are completed the window to the right of the "Start" button will display the message "Run Completed in xx.xx.xx", where xx.xx.xx indicates the time taken for the calculations in hours.minutes.seconds – this will vary depending on computer specification and complexity of the simulation.

It is now possible to access the "Grapher" button. Click on this button to access the built in graphing window. This window is divided into several sections. At the moment only the sections labeled "Distribution" and "Break-thru" are available (There is, at present, no "Diffusion" data to plot).

First click on the "Plot" button in the "Distribution" section. Nothing appears to happen. It is actually plotting the aqueous concentration in all the main channel boxes and, as shown, there is no tracer in any of the boxes at the end of the run – all the tracer has passed through and exited the system. Next, click on the "Plot" button in the "Break-thru" section. This may take a few moments as the code plots the aqueous concentration history for the first (blue) box and the last (green) box (no 45). If desired any of the options marked "Log Conc" or "Log Hours" can be selected and the "Plot" button clicked again, although in this case the differences will not be great – later examples will highlight the usefulness of these buttons.

That is the simplest example of a run completed, next we will add the process of sorption.

8.2 Worked example 2, advection/dispersion and sorption

Return to the main window and again select "Create/Load/Update". The previously entered data will still be displayed. In the section labeled "Main Options" in the top left of the window click on the check box titled "Sorption in Main Channel". The section labeled "Sorption Parameters" should now become active (It was previously ghosted out and unavailable). Leave the value for dispersion (in the "Main Options" section adjacent to the "Sorption in the main Channel" check box) at the default 0.015 m and enter into the "Sorption Parameters" section the following values:

Freundlich Alpha [$m^3 kg^{-1}$]:	0.1
Freundlich Beta:	1

Click on the "Save" button and save as "testex2.sin". This will save all the data to a file on your hard drive. Remember to update your comments in the comments box (this data is already contained in the file "wrkex2.sin").

Now click on "Use Values" to return to the main screen. In the section labeled "Setup of run" the text "-> Main Channel Sorption" should now be visible. This section displays the basic setup of a run. Again, the text box to the right of the "Start" button will display the text "- Values successfully loaded -". Click on the "Start" button.

This time you notice that the displays indicating the concentration in the first and last box show a more smoothly fluctuating value - they no longer rise and fall suddenly. Once this has been completed click on the "Grapher" button.

Once in the Graphing screen click on the "Plot" button in the "Distribution" section. This time there is still some tracer in the system, although only a very small amount (< 1E-28 kg m^{-3}).

Next, click on the "Plot" button in the "Break-thru" section. This illustrates the effect of sorption on the tracer as it passes through the system. The blue line indicates the concentration level in the first box, which rises more slowly to the value of the input source and then tails off when the input pulse is switched off. The green line shows the break through in the final (45th) box and shows the retardation of the pulse (compared with the earlier example – with no sorption) and the "smearing out" and attenuation of the sharp step pulse caused by dispersion and sorption.

Click on the check box labeled "Log Conc" in the "Break-thru" section and click on the plot button in the same section. This will now display the above graph but with a logarithmic scale for the concentration. Now, click on the check box labeled "Log Hours", and press the plot button again. This will re-plot the graph with the x-axis in Logarithmic hours. The user can now select the graph of their choice and with the use of the "Save Graph" button can save the output as a Windows Metafile. This can then be directly imported to Microsoft Word (or other program) and scaled without loss of resolution.

That is the example of a run with sorption/dispersion completed, next we will add the process of diffusion.

8.3 Worked example 3, advection/dispersion, sorption and diffusion

Return to the input screen and, retaining the values already used, click on the check box labeled "Diffusion in Rock Matrix" in the "Main Options" section in the top left of the screen. This will now enable the section labeled "Rock Matrix".

Leave the default value of 10 boxes for the "Limit of Diffusion (boxes)" and enter the following values:

Effective Diffusivity [$m^2 s^{-1}$]:	1E-12
Matrix Porosity:	0.05

Click on the "Save" button and save as "testex3.sin". This will save the updated data to a file on your hard drive. Remember to update your comments in the comments box (this data is already contained in the file "wrkex3.sin").

Now click on "Use Values" to return to the main screen. In the section labeled "Setup of run" the text "-> Main Channel Sorption" and "-> Diffusion in Rock Matrix" should be visible. Click on the "Start" button.

The displays indicating the concentration in the first and last box will rise similarly to the previous example but will fall much slower. This is indicating the storage effect of the rock matrix retaining the tracer. Click on the "Grapher" button to go to the graphing screen.

Click on the "Plot" button in the distribution section. This shows the retardation effect of the rock matrix on the tracer pulse. It is noticeably retarded compared to the previous example, and at a higher concentration (ranging from 3E-9 to 2E-11 kg m^{-3}).

Click on the "Log Conc" and "Log Hours" check boxes in the "Break-thru" section and then the "Plot" button. This illustrates the effect of diffusion into the rock matrix with the retention of the tail, caused by the effect of the tracer coming back out of the rock matrix.

For a better illustration of this, change the "Duration of run (hours):" to 110 hours in the input screen and run again. This will show the development of the tail over a longer time period – remember to change this value back to 20 hours before continuing.

With diffusion now enabled it is possible to access the "Plot" button in the "Diffusion" section. Click on this button to access the diffusion screen. This section enables the user to see the concentration level in each of the rock matrix boxes (adjacent to the main channel box chosen in the main screen section "Extra:", left at the default first box, No. 1). The main feature of this section is being able to scroll through the time periods recorded by using the scroll bar, in real time. Click on the right end of the scroll bar and hold the button down. You will now see consecutive time periods illustrated, forming an animation of the development of the tracer pulse into the system. From cycle 22 (0.782 hours) onwards the input pulse has been switched off and the graph will now illustrate the tracer coming back out of the rock matrix (this is analogous with Chap. 7.2.3). Again the option exists to view the graph using Log concentration.

That is the example of a run with sorption/dispersion, diffusion and matrix diffusion completed, next we will add the process of sorption in the rock matrix.

8.4 Worked example 4, advection/dispersion, sorption and diffusion with sorption

Return to the input screen and click on the check box labeled "Sorption in Rock Matrix" (This option will only be possible if the previous "Diffusion in Rock Matrix option has been selected). Enter the following values:

Alpha for sorption:	0.0001
Leave Beta for sorption at:	1.

Click on the "Save" button and save as "testex4.sin". This will save the updated data to a file on your hard drive. Remember to update your comments in the comments box (this data is already contained in the file "wrkex4.sin").

Click on the "Use Values" button to return to the main screen. The section labeled "Setup of run" will now display the text "-> Main Channel Sorption", "-> Diffusion in Rock matrix" and "-> Rock matrix sorption" should be visible. Click on the "Start" button.

This run will take a little longer than the previous runs as SANTA is now calculating sorption in all of the rock matrix boxes in addition to the main channel boxes. Once the run is completed click on the "Grapher" button to access the graphing screen. The "Distribution" and "Breakthru" graphs will be similar to the previous example, the greatest changes having occurred in the rock matrix.

Click on the "Plot" button in the "Diffusion" section to access the diffusion screen. Scroll through the graph to view the development of the diffusion profile. This highlights the retardation caused by the sorption in the rock matrix. In the previous example the diffusion pulse reaches further into the rock matrix in a shorter time (load in the previous data, perform a run and compare the results).

You have now created 4 example files with increasing complexity. Explore SANTA further by changing parameters and settings in the saved files and plot the results. Consult the user manual for further details on the running of the code.

9 Concluding remarks on accuracy and limitations

The limitations of SANTA are determined by restrictions on the geometry, the limited choice of processes, conceptual shortcomings, and by limits to the numerical accuracy. These limitations render SANTA useful for the development of concepts, scoping and exploratory calculations, sensitivity studies, and for teaching purposes. SANTA was not developed as a tool for rigorous performance assessment.

The restrictions on geometry limit SANTA to calculations along a single flow path in a single fracture. The model is essentially one-dimensional, with a pseudo-dimension to represent interaction with a rock matrix adjacent to the flow-path. The major limitation on processes is the lack of generalised rock-water interaction to account for the transient chemical evolution. Sorption and desorption of a single solute is the only mechanism of retardation. Sorption is of the Freundlich type, either linear or non-linear, and can be defined individually for the fracture medium and the rock matrix. The Freundlich model does not permit the definition of an upper limit for sorption capacity, but the non-linear option does allow for effects such as self-sharpening fronts.

The combined equation implemented for advection, dispersion and retardation requires that the length of the flow path, the travel time and the number of boxes be no longer independent variables. SANTA calculates the number of boxes required given the length of the flow path, travel time, dispersivity, and sorption parameters (for retardation). The user should therefore avoid combinations of input parameters that result in either too few boxes or too many boxes, and for example, adjust the length of the flow path.

The conceptual shortcomings include the crude approximation of gradients for relatively large steps in space and time. Also, the processes of dispersion, sorption and diffusion are computed sequentially rather than simultaneously. Diffusion in the rock matrix is treated in one-dimension without accounting for mass transfer between rows of boxes (e.g. parallel to the fracture). The implementation of combined dispersion and sorption is numerically exact only for the case of linear Freundlich-type sorption. Flow within the fracture is assumed to be represented by one-dimensional flow through an equivalent homogeneous porous medium.

The numerical errors associated with the conceptual shortcomings have been assessed by calculations in comparison to exact analytical solutions or numerically more accurate models. Errors associated with gradients are largest when gradients are largest, as demonstrated in the case of diffusion form the fracture into the first box of the rock matrix during the first time step. Subsequent time steps are modeled with sufficient accuracy such that incremental mass transfers are accurate for all but the initial time step of diffusion. The sequential computation of the processes does not appear to induce significant error as demonstrated with a computation involving linear sorption in the rock matrix, dispersion and radioactive decay. Errors associated with non-linear sorption have not been quantified, but it is expected that results are reasonably accurate as long as the non-linearity is not extreme, e.g. within the bounds of most experimental observations on rock material. The implementation of dispersion by an equivalent amount of numerical dispersion is numerically accurate.

The distinct advantages of the simple box model are the non-iterative and rapid computations, the simplicity of the required input parameters, and the transparent and modular implementation. The comparative calculations presented in the previous section impressively demonstrate the capability of a rather simplistic approach.

The application of SANTA calculations to field problems is mostly limited by restrictions to the geometry and the simplified treatment of chemical processes. Well defined portions of a natural system may, however, be explored and interpreted by SANTA simulations. Also, worst-case scenarios for natural systems tend to minimize complexity and rely on simple concepts, and hence, might be explored with rather simple numerical models.

10 Coding of SANTA

SANTA was coded using a combination of FORTRAN and Visual Basic. All the main numerical modules were coded in FORTRAN and checked first in a DOS environment. This chapter outlines the method SANTA employs to combine FORTRAN code with a Windows front-end or Graphical User Interface (GUI).

The front-end that controls SANTA and allows the saving of graphs was created in Visual Basic. The main reason for this approach was to retain the proven mathematical functions in FORTRAN that are familiar to most coders while adding the user-friendly and familiar front-end environment offered by Windows.

The basic component approach is outlined below along with the method employed in coding SANTA:

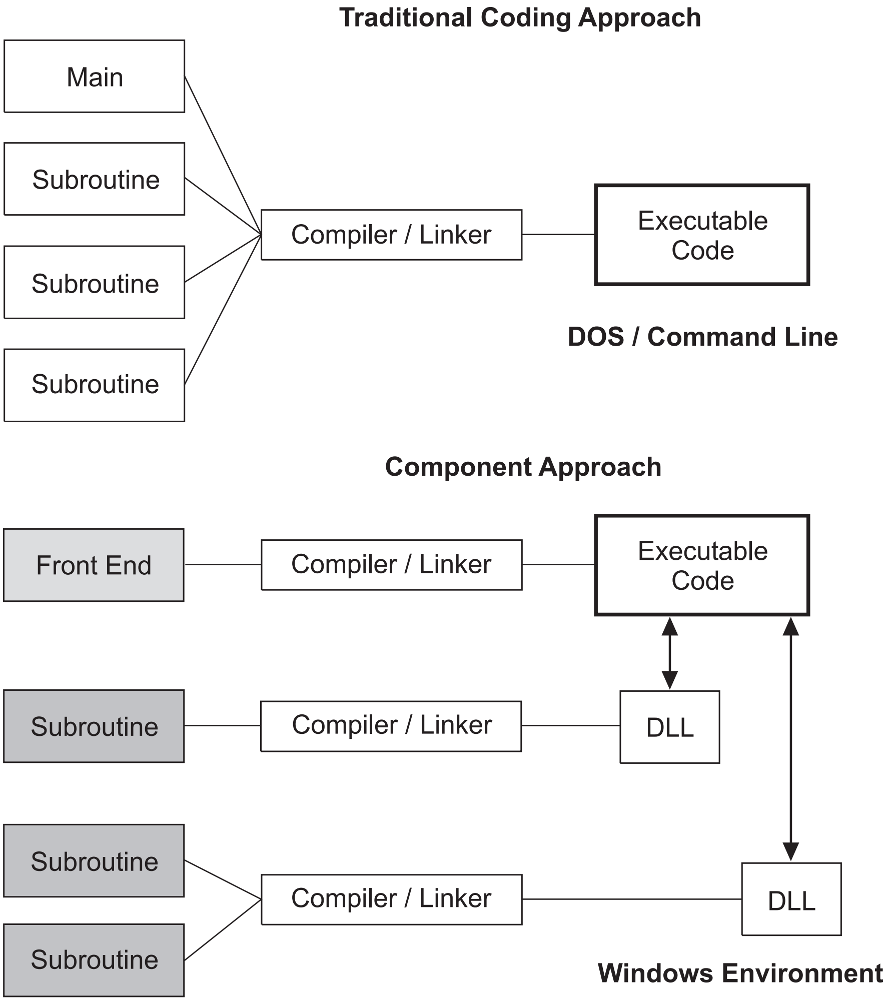

Fig. 10.1: Comparison of coding methods

Traditionally all subroutines were compiled into a single executable file (*.exe). An alternative approach is to use Dynamic Link Libraries (DLLs). DLLs are program modules that contain code, data, or resources that can be shared among Windows applications. A DLL is basically the same as a Windows EXE file but one major difference is that a DLL is not an independently executable file, although it may contain executable code. A program can be constructed modularly using DLLs containing maths routines or other commonly called code. The program, while running, loads in the relevant DLLs when required. This is all done automatically and the end user need not be aware of the process.

The main advantage that SANTA gains by using DLLs is the way that existing, and rigorously checked and proven FORTRAN code, can be implemented within a Windows programmed front-end. These front-ends are usually far more user-friendly than a DOS prompt. Another advantage is the ability to escape the 640 K memory limitation that programming in standard DOS dictates, and the ability to use complex graphing routines and output directly to the printer.

The modular approach while using DLLs simplifies updating a program, because one need replace only DLLs instead of replacing the entire program. Thus when an updated or new method needs to be added, the DLL containing the code need only be changed, leaving the rest of the project unaffected.

DLLs can be accessed from any code capable of supporting DLLs, thus any code present in a DLL can be utilised by other codes or Windows applications. Packaging often used codes or routines into DLLs means that a selection of DLLs will be available for future programming projects.

11 Acknowledgments

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APPENDIX A: Quick start – run something now

Follow these instructions, after installing SANTA, to perform a run.

1. Start SANTA by double clicking on the SANTA icon. As SANTA holds a large amount of information in large arrays it is better to close any Programs you presently have running that also require a lot of memory (i. e. Word, Excel etc.) to prevent too much Hard drive activity as your machine uses virtual memory.

2. From the main screen, click on the "Create/Load/Update" button. This will take you to the Input screen.

3. From the input screen click on the "Load" button. This will show a standard windows file requester.

4. Select "quick.sin" from the list shown (this file should be included).

5. Click on the "Use Values" button on the input screen. This should return you to the main screen.

6. Click on the "Start" button. The program will start to run. A progress meter will show the state of calculations, and the other meters show the log concentration in the first and last boxes in the main channel.

7. When the code has finished the message "Run Completed" will be shown in the text box next to the "Start" button.

8. Click on the "Grapher" button. This will display the Graphing screen. Select any of the options you want and click on a "Plot" button. Try looking at the diffusion profile.

Go back to the Input Screen and try running the same file but this time turn off the diffusion by clicking on the check box that says: "Diffusion in Rock Matrix", and see the effect diffusion has on the system.

That is a very quick start to using SANTA. If you have a query at any point while running SANTA click on the "Help" button. This will jump to the relevant section in the Help file.