

Contaminant Transport Component of the
Catchment Modelling System SHETRAN
(Published report not requiring QA sheet)

John Ewen

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AUTHOR(S) J. EWEN

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	NAME	SIGNATURE	DATE
AUTHOR(S)	John Ewen	<i>John Ewen</i>	9/12/96
CHECKED	John Ewen	<i>John Ewen</i>	9/12/96
APPROVED	John Ewen (Senior Officer)	<i>John Ewen</i>	9/12/96
APPROVED FOR EXTERNAL DISTRIBUTION	John Ewen (Principal Investigator)	<i>John Ewen</i>	9/12/96

Water Resource Systems Research Unit
Department of Civil Engineering
University of Newcastle upon Tyne
Newcastle upon Tyne
NE1 7RU

Tel: Tyneside (0191) 222 6259
Fax: Tyneside (0191) 222 6669

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Contaminant Transport Component of the Catchment Modelling System SHETRAN

JOHN EWEN

Water Resource Systems Research Unit, Department of Civil Engineering, University of Newcastle upon Tyne, UK

16.1 INTRODUCTION

The SHETRAN modelling system for water flow and sediment and contaminant transport in river catchments has been developed by the Water Resource Systems Research Unit at the University of Newcastle upon Tyne. The contaminant transport component of the system is described here.

Currently there is world-wide interest in environmental quality issues, including surface and groundwater pollution and the effects on water resources of changes in climate (e.g. global warming) and land use (e.g. deforestation). The aim in developing SHETRAN was to create a flexible tool which could be used in research and planning decision support to simulate the basic processes and pathways for flow and transport in river catchments. It is designed to have the capability to predict the consequences of given changes in climate and land use and to have a modular basis that will allow it to be upgraded in the future as our understanding of the processes improves.

SHETRAN has three main components: one each for water flow, sediment transport and contaminant transport. The water flow component is an updated version of the Système Hydrologique Européen (SHE) (Abbott *et al.*, 1986a, 1986b); the sediment component is an updated version of SHESED (Wicks, 1988), and the scientific basis for the contaminant transport component is given in Ewen (1990) and Purnama and Bathurst (1991).

The philosophy behind the SHE is that there are good physically based hydraulic models available for the main processes of water movement in catchments, and these can be integrated into a flexible spatially distributed (rather than lumped) catchment modelling system which can be successfully applied to a diverse range of catchment types and sizes (Abbott *et al.*, 1986a). Since the process models are physically based rather than conceptual or black box types, the parameters for the system can be based directly on field measurements, or literature values, for physical properties (e.g., the saturated hydraulic conductivity of soil). It is argued, then, that the effects of changes in climate and land use on the water flow in a catchment can be predicted

TABLE 16.1 Parameters for the contaminant transport component of SHETRAN

Variables	Description
D	Dispersion coefficient for porous media (varies with contaminant and media type and flow velocity)
D_s	Dispersion coefficient for river channels (varies with river type, size, and flow rate; nb dispersion with surface and horizontal subsurface flows is not accurately represented in SHETRAN)
f	Fraction of the adsorption sites in porous media associated with mobile water (varies with contaminant and media type)
K'_d	Reference adsorption distribution coefficient for porous media (varies with contaminant and media type)
K_d^*	Reference adsorption distribution coefficient for sediments (varies with contaminant type and sediment type and size)
n	Exponent for Freundlich adsorption equation for porous media and sediments (varies with contaminant type, porous media type and sediment type and size)
α	Coefficient for contaminant exchange between mobile and immobile water in porous media (varies with contaminant and media type)
α_{bd} and α_{bs}	Coefficients for contaminant exchange between the bed surface layer and the bed deep layer, and between the river water and the bed surface layer (varies with contaminant and river type)
λ	Radioactive decay constant (varies with contaminant type)
ϕ	Fraction of pore water which is mobile in porous media (varies with contaminant and media type)
ξ	Efficiency for plant uptake of mobile water (varies with plant type)

provided the changes in the physical properties are known or can be estimated. SHESED and SHETRAN were developed according to the same philosophy.

SHETRAN is basically a three-dimensional transient finite difference model written in a very general modular form which allows the user, via input data files, to use it as a flexible modelling system to build a model of any catchment to the appropriate level of detail. The input data files give values for the physical properties. Many of these properties will vary with location in the catchment and the depth below the surface, and this is allowed for using simple map and array data structures. (The full parameter list for the contaminant transport component of SHETRAN is given in Table 16.1.)

A catchment is modelled as an ensemble of columns and stretches of channels. As shown in Figure 16.1, each column comprises a rectangular area of the ground surface and vegetation canopy, and the parts of the unsaturated and saturated zones lying directly below that area. The main drainage channels are represented as networks of stretches of channels (called river links), with each river link running along the edge of a column.

The soil and rock in each column is divided, by horizontal slicing, into several (sometimes up to one hundred) parallelepipedal finite difference cells; each river link has three finite difference cells: one for river water and two for the river bed. Thin columns, typically only 10 metres wide, are positioned on either side of each link to ensure that some of the complexity of

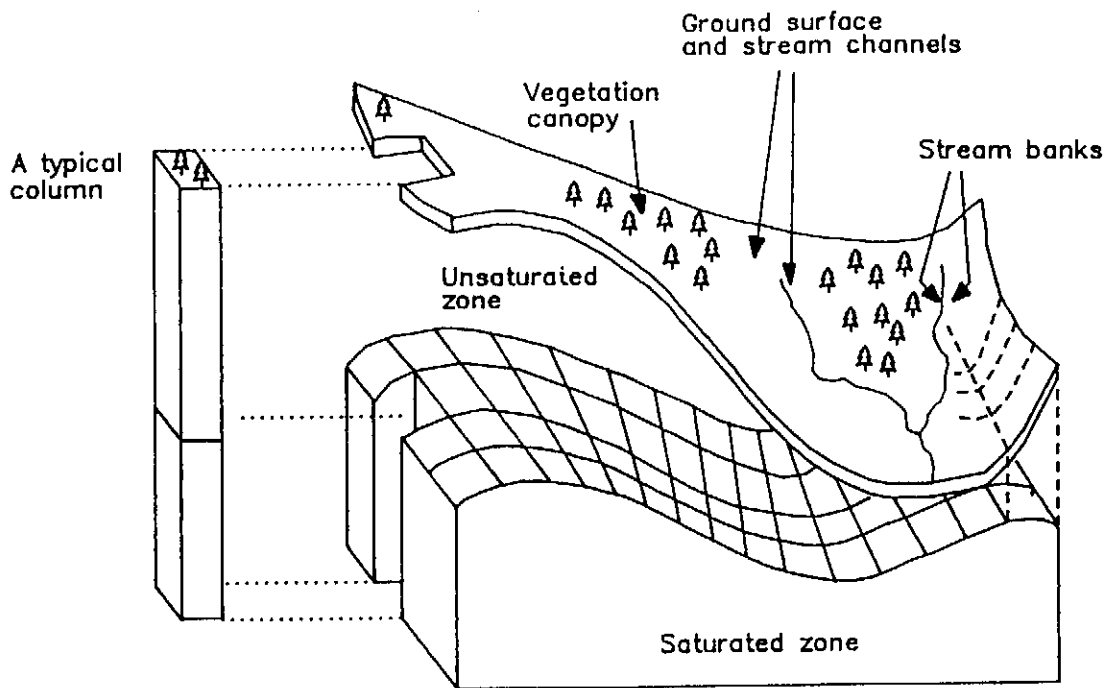


FIGURE 16.1 A typical SHETRAN column

the flow and transport paths close to channels is represented. (Ideally, some form of full grid refinement would be used near channels; however, at present, this is not practical.) When SHETRAN is running, a fully coupled three-dimensional description of the distribution and movement of water, sediment and contaminants is predicted in the usual finite difference fashion (i.e. the simulation steps through time, taking one time-step after another, giving a full three-dimensional picture of the catchment at the end of each time-step).

The water flow processes that are represented include: canopy interception of rainfall; evaporation and transpiration; infiltration; surface runoff (overland, overbank and in channels); snowpack development and snowmelt; soil moisture storage and flow in the unsaturated zone; and groundwater storage and flow in the saturated zone. Surface water flow, both overland and in channels, is modelled using the diffusion form of the Saint Venant equation; flow in the unsaturated zone is modelled using Richards' equation; and flow in the saturated zone is modelled using the two-dimensional Boussinesq equation for phreatic aquifers.

For each time-step, Richards' equation is applied at each column in turn and is solved to give the moisture content within each unsaturated cell, and the vertical flow rates into and out of each unsaturated cell. (Lateral flow is not allowed for in the Richards solution, so flow and transport in the unsaturated zone of the catchment are restricted to the vertical direction only.) The Boussinesq equation is applied to the entire saturated zone, and the Richards and Boussinesq solutions are coupled in a way that ensures water mass is conserved within each column. To allow the simulation of three-dimensional contaminant transport, the results from the Boussinesq solution are used to generate a three-dimensional velocity field for the saturated zone (following the approach of Connorton, 1985). (A fully three-dimensional saturated/unsaturated flow model is being developed for SHETRAN at present. This new model will allow three-dimensional water flow and contaminant transport to be simulated for the entire

subsurface, including combined systems of unsaturated regions, and phreatic, perched and confined aquifers.)

The simultaneous transport of several classes of sediment (usually based on particle size) can be simulated. The sediment transport processes that are represented include: erosion by raindrop and leaf drip impact and overland flow; deposition and storage of loose sediments on the ground surface; total-load convection with overland flow; overbank transport; erosion of river beds and banks; deposition on the river bed; down-channel convection; and infiltration of fine sediments into the river bed.

16.1.1 Contaminant transport component

Since the SHE philosophy is to be followed, the contaminant transport component must be physically based and spatially distributed; the transport equations for the contaminant transport component must therefore be partial differential equations with parameters that are physical properties. The convection–dispersion equation has been adopted, as it is the only transport equation that is well established and satisfies these requirements (see, for example, the review for contaminant transport in soil of Addiscott and Wagenet, 1985). The transport equations are developed and discussed in Sections 16.2 to 16.5 below. The preferred form of the equation for soil and rock is the version developed by Kasten *et al.* (1952) and extended by Coats and Smith (1964) and van Genuchten and Wierenga (1976); for transport in river channels the preferred approach follows Shih and Gloyna (1969) and Onishi (1981).

SHETRAN can be used to simulate the simultaneous transport of several contaminants. At present, however, radioactive decay and generation (as required for a parent–daughter radioactive decay chain) are the only contaminant transformations allowed for; models for more complex transformations, including those for the main species of nitrogen involved in the soil phase of the nitrogen cycle, are being developed for incorporation in SHETRAN in the future.

In the current version of SHETRAN (Version 3.4), it is assumed that water flow and sediment transport are not influenced by the presence of the contaminants; so, when SHETRAN is running, no information on contaminant distribution or transport need be passed back from the contaminant transport component to the water flow or sediment transport components. A cold-region heat-transport component, based on the contaminant transport component, is being developed for a future version of SHETRAN. Since temperature has a strong effect on water flow (especially during frozen periods), the three-dimensional temperature distribution calculated in the heat-transport component will be fed back, in the future version, to the water flow component at the end of every time-step, where it will be used in determining the current status and hydraulic properties of the surface and subsurface waters.

16.1.2 General

The computer memory and processing times required by SHETRAN are quite large. For example, to simulate five years of combined water flow and sediment and contaminant transport for a catchment modelled using 200 columns (each with 50 cells) and 60 links requires an overnight run on a standard computer workstation (64 Mb memory; 20 Mflops processing).

The computer code for the contaminant-transport component of SHETRAN was written in FORTRAN 77. It was developed and tested within a quality assurance system for software development, based on BS 5750, and has been in place since 1991.

16.2 PHYSICS OF TRANSPORT PROCESSES

The transport of a contaminant in a catchment is effected by three main processes — convection, molecular diffusion and mechanical dispersion — and is affected by two other main processes — adsorption and absorption. Two other contaminant processes are modelled by the current version of SHETRAN: radioactive decay and plant uptake.

16.2.1 Convection

The convection equation below describes the distribution of contaminant in a one-dimensional steady flow of water down a hillslope, channel or column of porous media, provided there is no dispersion. It is simply an expression of the law of conservation of mass:

$$\frac{\partial c}{\partial t} = - \frac{\partial(uc)}{\partial x} \quad (1)$$

where c [ML^{-3}] is the concentration in solution, t [T] time, u [LT^{-1}] the magnitude of the average water flow velocity and x [L] distance. (A list of symbols used is given in the Appendix.)

16.2.2 Molecular diffusion and mechanical dispersion

Molecular diffusion is a microscopic process involving molecule/molecule collisions, and therefore takes place even if there is no flow. Mechanical dispersion arises through mechanical mixing, and takes place only if there is flow. For soil and rock, continuous mechanical mixing occurs within the pores in the medium, as previously adjacent packets of solution move relative to one another under the velocity gradients near the solid walls of the pores; and separation and mixing of packets occurs as a variety of tortuous flowpaths are taken by the water as it moves from pore to pore. In surface water flows there is mechanical mixing associated with turbulence and the velocity gradients within planes perpendicular to the flow direction. In general it is not possible to distinguish between the contributions of molecular diffusion and mechanical dispersion, so both are usually considered together under the general term dispersion.

Taylor (1953) found that the dispersion of a contaminant injected into a solvent flowing through a tube can be accurately modelled using a diffusion equation. Strictly, dispersion does not act like diffusion and a diffusion equation should only be applied to dispersion after the transport paths are well developed, i.e. when all the molecules have had a good chance of sampling the full range of velocities seen in the flow.

Adding a term for dispersion to the convection equation gives the convection–dispersion equation for one-dimensional steady flow:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - \frac{\partial(uc)}{\partial x} \quad (2)$$

where D [L^2T^{-1}] is the effective longitudinal dispersion coefficient.

Dispersion is a complex process which is not limited to the pore and turbulent eddy scale as discussed above. For example, there is dispersion when a contaminant migrates with water flow through an interconnected network of fractures in rock; for such a case the dispersion process

should be viewed on a large physical scale, covering a volume of rock at least sufficient to contain a fully representative sample of the network. (Dispersion in rock is discussed in Jefferies *et al.*, 1993.)

In the equations developed below for contaminant transport in SHETRAN columns and river links, a diffusion term, as in eqn (2) above, is used to model dispersion. The magnitude of the dispersion coefficients used with SHETRAN should therefore be consistent with the physical scale of the columns and river links.

16.2.3 Adsorption

Contaminants in solution can be adsorbed to the microscopic surfaces of soil, rock and sediments. Adsorption can be positive or negative, as the contaminant can accumulate preferentially either at surfaces or in the bulk solution. In general the rate at which adsorption takes place will depend on the concentration in solution and the amount adsorbed (Kasten *et al.*, 1952). However, under nearly all circumstances, an appropriate description for the kinetics is not known. A practical approach is to assume that the adsorbed contaminant is in thermodynamic equilibrium with that in solution. At the low concentrations expected when contaminants migrate through the near-surface and surface zones, the Freundlich equation is probably the most appropriate (Bohn *et al.*, 1985):

$$s = K_d c \quad (3)$$

where s [ML^{-3}] is the mass adsorbed per unit volume of the medium and K_d [1] the (dimensionless) distribution coefficient, which varies with the concentration in solution:

$$K_d = K'_d (c/c')^{n-1} \quad (4)$$

where K'_d is the distribution coefficient at some arbitrarily chosen reference solution concentration c' and n [1] is an empirical constant.

If the empirical constant n in the Freundlich equation is set to one, the Freundlich equation is reduced to a linear equilibrium adsorption equation. For most simulations, the linear equation will be the better choice: full data on non-linear adsorption is often not available for all the materials in a catchment, or is available only with limited accuracy, and the results of simulations can often be shown to be insensitive to the exact form of the adsorption equation used.

A convenient and compact form of the convection–dispersion equation for porous media including the effects of adsorption can be written by following the approach of Hashimoto *et al.* (1964). When there is adsorption, if the volumetric moisture content is θ [1] the total effective concentration at a point is $c + \theta s$, yet the concentration for convection and dispersion with water flow is simply c . Therefore, for mass balance, in one-dimensional steady flow:

$$\frac{\partial(c + \theta s)}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - \frac{\partial(uc)}{\partial x} \quad (5)$$

giving

$$\frac{\partial(Rc)}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - \frac{\partial(uc)}{\partial x} \quad (6)$$

where

$$R = 1 + K_d \theta \quad (7)$$

For transport in porous media, adsorption tends to retard the rate of transport of contaminant relative to the rate of water flow. The factor R [1] is therefore called the retardation factor when applied to contaminant transport in soil and rock. An equation with the same form as eqn (6) also applies to contaminant transport in surface water if there is adsorption to stationary surface soils and sediments.

The factor R can also be used in the convection–dispersion equation for contaminant transport in flowing water that is carrying adsorbing sediments. The name retardation factor is best avoided in such a case, however, as the contaminant adsorbed on the sediments will move with the sediments, and, provided the sediments move with the flow velocity, the rate of contaminant transport will not be retarded relative to the rate of flow. For transport in one-dimensional steady flow, with adsorption to suspended sediments that are moving with the flow velocity:

$$\frac{\partial(Rc)}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - \frac{\partial(Ruc)}{\partial x} \quad (8)$$

where the coefficient D accounts for the combined dispersion of the dissolved and adsorbed phases.

16.2.4 Absorption in porous media

Soil and rock have a strong tendency to become wetted, and a dry sample placed in a reservoir of solution will absorb the solution into its pores by capillary action. Also, if there is a change in the concentration in the solution flowing past a point in saturated or unsaturated soil or rock, that change will not be transmitted instantaneously to all the solution: there are dead spaces in which there is little or no flow, and into which (at least under steady flow conditions) a contaminant can be transported only by diffusion (Nielsen and Biggar, 1961). In general terms, the transfer of contaminant into dead-space is a form of absorption.

One of the most successful approaches to modelling the absorption of contaminant into dead-space involves assuming that the pore water can be divided into two parts: mobile water and immobile water. The mobile water is in the “dynamic region” of the medium and the immobile water is in “dead-space”; convection through the medium and mechanical dispersion take place only in the dynamic region. This division into the dynamic region and dead-space is in some ways a modelling simplification. However, the value for the fraction of pore water which is mobile has been measured in field soils (e.g. Gvirtzman and Magaritz, 1986), and the division is clearly physical if there is significant preferential flow through macropores in soil (Beven and Germann, 1982) or fractures in rock (Jefferies *et al.*, 1993).

Following the approach of Deans (1963) and Coats and Smith (1964), the convection–dispersion equations for one-dimensional steady flow in saturated porous media, without adsorption, extended to include the effect of absorption into dead-space, are

$$\frac{\partial(\phi c)}{\partial t} + \frac{\partial[(1-\phi)c^*]}{\partial t} = \frac{\partial}{\partial x} \left(\phi D \frac{\partial c}{\partial x} \right) - \frac{\partial(\phi u c)}{\partial x} \quad (9)$$

and

$$\frac{\partial[(1-\phi)c^*]}{\partial t} = \alpha(c-c^*) \quad (10)$$

where ϕ [1] is the fraction of the pore water which is in the dynamic region (i.e. the fraction that is mobile), c^* [ML^{-3}] is the concentration of contaminant in solution in dead-space and α [T^{-1}] the coefficient for mass transfer between the dynamic region and dead-space.

16.2.5 Sources

Any direct gain or loss of contaminant can be modelled using a source term added to the right-hand side of the convection–dispersion equation. The convection–dispersion equation without adsorption or absorption into dead-space but with a spatially distributed time-varying source of strength B [$ML^{-3}T^{-1}$] is

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - \frac{\partial(uc)}{\partial x} + B(x,t) \quad (11)$$

The important sources are for radioactive decay, plant uptake and lateral convection. For radioactive decay, the source term for the parent contaminant is

$$B = -\lambda c \quad (12)$$

where the decay constant λ [T^{-1}] is related to the half-life of the contaminant. The decay of a contaminant results in the generation of its daughter products; for conservation of mass, the combined strength of generation of daughter products at any point must equal the strength of decay of the parent contaminant at that point.

The second important source is plant uptake. If plants take up contaminant from the rooting zone and return some contaminant with recycled dead plant material, the net strength of source involved can be calculated using a plant uptake and recycling model, and this can be coupled to the convection–dispersion equation via a spatially distributed time-varying source term.

The final important source is lateral convection. If contaminant transport in a river or a column is modelled using a one-dimensional convection–dispersion equation, transport into or out of the river or column with lateral flow can be modelled using a spatially distributed time-varying source term. The strength of this source will be proportional to the product of the rate of lateral flow and the concentration in solution in the lateral flow.

16.3 EQUATIONS FOR CONTAMINANT TRANSPORT IN SHETRAN COLUMNS

The convection–dispersion equation for one-dimensional flow with adsorption and dead-space was adapted for non-steady flow conditions in unsaturated porous media by van Genuchten and Wierenga (1976):

$$\frac{\partial(\phi\theta c)}{\partial t} + \frac{\partial[(1-\phi)\theta c^*]}{\partial t} + \frac{\partial(fs)}{\partial t} + \frac{\partial[(1-f)s^*]}{\partial t}$$

$$= \frac{\partial}{\partial x} \left(\phi \theta D \frac{\partial c}{\partial x} \right) - \frac{\partial(\phi \theta u c)}{\partial x} \quad (13)$$

In this equation the superscript * indicates dead-space, and the adsorption sites are assumed to be divided between the dynamic region and dead-space, with fraction f [1] of the total being associated with the dynamic region.

The general equation for absorption into dead-space which complements eqn (13) was not developed by van Genuchten and Wierenga (1976). To account for both diffusional and convective exchanges between the dynamic region and dead-space, this equation must be of the form:

$$\begin{aligned} \frac{\partial[(1-\phi)\theta c^*]}{\partial t} + \frac{\partial[(1-f)s^*]}{\partial t} = \alpha(c-c^*) + 0.5 \frac{\partial[(1-\phi)\theta]}{\partial t} (c+c^*) \\ + 0.5 \left| \frac{\partial[(1-\phi)\theta]}{\partial t} \right| (c-c^*) \end{aligned} \quad (14)$$

where the vertical lines in the final term indicate that the absolute value is taken. The final two terms in this equation account for the transfer of contaminant with water moving between the dynamic region and dead-space. It is assumed that the concentration in water entering dead-space will be c whereas the concentration in water leaving dead-space will be c^* ; the rate of transfer of water simply depends on the rate of change of the moisture content in dead-space.

To create the equations for transport within the soil and rock part of a SHETRAN column, the van Genuchten and Wierenga equations were rewritten to include the retardation coefficients R and R^* , and were extended by the addition of terms for radioactive decay, plant uptake and convection with lateral water flow to and from the four neighbouring columns. The full equations for the transport of a single contaminant in the soil and rock in a SHETRAN column are

$$\begin{aligned} \frac{\partial}{\partial t} \{ \theta[\phi R c + (1-\phi)R^*c^*] \} = \frac{\partial}{\partial z} \left(\phi \theta D \frac{\partial c}{\partial z} \right) - \frac{\partial(\phi \theta u c)}{\partial z} \\ - \lambda \theta[\phi R c + (1-\phi)R^*c^*] \\ + e_d + e_{ds} + \sum_{j=1}^4 (v \bar{c})_j / A \end{aligned} \quad (15)$$

and

$$\begin{aligned} \frac{\partial}{\partial t} [(1-\phi)\theta R^*c^*] = \alpha(c-c^*) - \lambda(1-\phi)\theta R^*c^* + e_{ds} \\ + (\gamma + |\gamma|)c/2 + (\gamma - |\gamma|)c^*/2 \end{aligned} \quad (16)$$

where

$$R = 1 + fK_d/(\phi\theta) \quad (17)$$

$$K_d = K'_d(c/c')^{n-1} \quad (18)$$

$$R^* = 1 + (1-f)K'_d/[(1-\phi)\theta] \quad (19)$$

$$K_d^* = K'_d (c^*/c')^{n-1} \quad (20)$$

and

$$\gamma = \frac{\partial[(1-\phi)\theta]}{\partial t} + (1-\zeta\phi)\eta \quad (21)$$

The boundary conditions, based on Danckwerts (1953), are

$$c = c_b(t) \quad \text{or} \quad Q_b(t) = \phi\theta \left(uc - D \frac{\partial c}{\partial z} \right) \text{ at } z = 0 \quad (22)$$

and

$$c = c_{gs}(t) \quad \text{at } z = z_{gs} \text{ if } (d_{sw} + d_{ls}) > 0 \quad (23)$$

$$Q_{gs}(t) = \phi\theta \left(uc - D \frac{\partial c}{\partial z} \right) \text{ at } z = z_{gs} \text{ if } (d_{sw} + d_{ls}) = 0$$

The new subscripts introduced in these equations are: b for bottom boundary, d for the dynamic region (in which mobile water can flow), ds for dead-space, gs for the ground surface, ls for loose sediments lying on the surface of the column and sw for free water lying on the surface of the column. A bar over a symbol for a variable indicates that the variable is evaluated at one of the vertical faces of the column. The new variables are: A [L^2], the plan area of the column; d [L], depth; j [1], the index for the four vertical faces of the column; e [$ML^{-3}T^{-1}$], the combined rate of input from plant uptake and recycling, and generation by decay of parent contaminants; Q [$ML^{-2}T^{-1}$], the rate of transfer (positive upwards) of contaminant at the ground surface or the bottom of the column, with rainfall, irrigation, direct application, dry deposition or regional flow of groundwater; v [L^2T^{-1}], the volumetric lateral flow rate into a face of the column, per unit depth; z [L], elevation within the column; ζ [1], the efficiency of water uptake, by plants, from the dynamic region (a fraction between 0 and 1); and η [T^{-1}], the volumetric rate, per unit volume of soil, of uptake of water by plants.

16.3.1 Overland transport

At the ground surface, there are exchanges of contaminant between the subsurface and surface waters. Equations (15) to (23) must therefore be coupled (at $z = z_{gs}$) to the overland transport equations.

The basic equation for overland transport of contaminant is a two-dimensional version of the convection–dispersion equation. It is assumed that the surface water, sediments and associated contaminants are in direct contact with the underlying soil and rock. It is convenient here, therefore, to write the overland convection–dispersion transport equation, for a single contaminant, in the form in which it applies to the top of a soil and rock column. In effect, this is the equation for the ground surface concentration, c_{gs} in eqn (23):

$$\begin{aligned}
\frac{d}{dt} [(d_{sw} R_{sw} + d_{ls} \theta_{ls} R_{ls}) c_{gs}] = & \left[\phi \theta \left(uc - D \frac{\partial c}{\partial z} \right) \right]_{z=z_{gs}} - \lambda (d_{sw} R_{sw} + d_{ls} \theta_{ls} R_{ls}) c_{gs} \\
& + v [\theta (\phi R c + (1 - \phi) R^* c^*)]_{z=z_{gs}} \\
& - Q_{gs} + e_{ss} + \sum_{j=1}^4 (\bar{q}_{sw} \bar{R}_{sw} \bar{c}_{gs} + \bar{b})_j / A
\end{aligned} \quad (24)$$

where

$$R_{sw} = 1 + \sum_{l=1}^{ns} (\delta K_d^*)_l \quad (25)$$

$$R_{ls} = 1 + \sum_{l=1}^{ns} (\beta K_d^*)_l / \theta_{ls} \quad (26)$$

and

$$K_{d_l}^* = K_{d_l}^{*'} (c_{gs}/c')^{n-1} \quad (27)$$

In order, the terms in eqn (24) are for: change in amount of contaminant stored; exchange of contaminant with the underlying soil and rock; radioactive decay; erosion of surface soils; loss of contaminant to the atmosphere; net input of contaminant as the result of plant uptake and generation by the decay of parent contaminants; and net input with lateral convection and dispersion with surface water flow and sediment transport to and from the four neighbouring columns and river links.

One new subscript has been introduced here: *ss* is for ground surface water and suspended sediments combined. The new variables introduced are: *b* [MT^{-1}], the rate of dispersion into the column with surface water flow; *ns* [1], the total number of sediment classes (e.g. *ns* will be 3 if the clay, silt and sand fractions are treated separately); *l* [1], the index for the sediment classes; *q* [L^3T^{-1}], the volumetric rate of flow; β_l [1], the fractions of the local loose (i.e. lying on the surface) sediments that are in class *l*; δ_l [1], the relative density of suspended sediments in class *l*; and *v* [LT^{-1}], the rate of vertical erosion of the ground surface. Only two extra parameters have been introduced in these equations: the reference distribution coefficients for adsorption to the sediments in the different classes, $K_{d_l}^{*}$ [1], and the Freundlich equation exponent, *n*, for the sediments. (In the current version of SHETRAN, the amount of the soil and rock and in a column does not change when soil is eroded or loose sediments consolidate; eqn (15) therefore does not have a term corresponding to the erosion term in eqn (24).)

16.3.2 Plant model

A plant model for contaminant uptake, storage and recycling has been incorporated in SHETRAN. Uptake is modelled using a linearised version of the Michaelis–Menten equation

(Barber, 1984), and each plant type on each column is modelled using two computational storage compartments, one of which grows and decays in size with the canopy leaf area index prescribed for the plant type. The plant model is not described here.

16.3.3 Simultaneous transport of several contaminants

In simulations where several contaminants are transported simultaneously, the full set of column and river link transport equations are solved for each contaminant.

16.4 EQUATIONS FOR CONTAMINANT TRANSPORT IN RIVER CHANNELS

A three-layer description of contaminant transport in river channels has been developed for SHETRAN. At every point along a channel it is assumed that there are three distinct layers: a river water layer (subscript *s* is used to denote this layer) which includes the suspended and bed-load sediments; the bed surface layer (subscript *bs*, this layer is assumed to have a small fixed thickness) which contains the materials of the bed which are in direct contact with the river water; and the bed deep layer (subscript *bd*) which contains the bulk of the river bed and includes deposited materials and, if appropriate, some parent bed materials. This three-layer approach makes it possible to represent both quick and slow transfers of contaminant between the river water and the bed, and both long- and short-term storage of contaminant in the bed. (For a single river link, the two bed layers are, in effect, dynamic finite difference cells for a one-dimensional convection–dispersion equation for contaminant transport down through the river bed.)

The equations below are for the transport of a single contaminant down a river, and include a term for inputs from tributaries and losses to distributaries. The simultaneous transport of several contaminants in an entire river network can be modelled using simultaneous sets of these equations.

At any point along a channel, there are three concentrations, one for each layer. Three equations are therefore required. The first equation (eqn (28)) is for overall mass balance within the three layers; the second (eqn (29)) is for mass balance within the bed surface layer on its own; and the third (eqn (30)) for mass balance within the bed deep layer on its own.

$$\begin{aligned} \frac{\partial}{\partial t} (a_s R_s c_s + a_{bs} \theta_{bs} R_{bs} c_{bs} + a_{bd} \theta_{bd} R_{bd} c_{bd}) &= \frac{\partial}{\partial x} \left(a_s D_s \frac{\partial c_s}{\partial x} \right) \\ &- \frac{\partial}{\partial x} [(q_s + q_D) R_s - q_D] c_s \\ &- \lambda (a_s R_s c_s + a_{bs} \theta_{bs} R_{bs} c_{bs} + a_{bd} \theta_{bd} R_{bd} c_{bd}) \\ &+ \sum_{nk=1}^2 \left[\int_0^{z_{gs}} \nu_{bk} (Fc + Gc^*)_{bk} dz \right]_{nk} \\ &+ \hat{Q}_s + \hat{e}_s + \hat{e}_{bs} + \hat{e}_{bd} + \psi_s \end{aligned}$$

$$\begin{aligned}
& + 0.5 \sum_{nk=1}^2 \left\{ \int_0^{z_w} [(\hat{q}_{bk} + |\hat{q}_{bk}|)c + (\hat{q}_{bk} - |\hat{q}_{bk}|)c_s] dz \right. \\
& + (\hat{q}_{sw} + |\hat{q}_{sw}|)R_{sw}c_{gs} + (\hat{q}_{sw} - |\hat{q}_{sw}|)R_s c_s \\
& \left. + (\hat{q}_{sb} + |\hat{q}_{sb}|)c + (\hat{q}_{sb} - |\hat{q}_{sb}|)c_{bd} \right\}_{nk} \quad (28)
\end{aligned}$$

In order, the terms in eqn (28) are for: change in amount of contaminant stored; dispersion; down-channel convection with water and sediments; radioactive decay; erosion of the river banks; inputs with rainfall, irrigation and dry deposition; net input of contaminant with plant uptake and generation by decay of parent contaminants (the three e terms); net contaminant input with tributary and distributary water flow and sediment transport; and net input with convection with water flow through the river bank, over the river bank and through the bed.

$$\begin{aligned}
\frac{d}{dt} [a_{bs} \theta_{bs} R_{bs} c_{bs}] &= \alpha_{bs} g U (c_s - c_{bs}) - \alpha_{bd} g (c_{bs} - c_{bd}) - \lambda (a_{bs} \theta_{bs} R_{bs} c_{bs}) \\
& + 0.5 [(a_{bd})_t + |(a_{bd})_t|] (\theta_{sd} R_{sd} c_s - \theta_{bs} R_{bs} c_{bs}) \\
& + 0.5 [(a_{bd})_t - |(a_{bd})_t|] (\theta_{bs} R_{bs} c_{bs} - \theta_{bd} R_{bd} c_{bd}) \\
& + (1-U)\hat{Q}_s + i_{bs} - i_{bd} + \hat{e}_{bs} \\
& + 0.5 \sum_{nk=1}^2 [(\hat{q}_{sb} + |\hat{q}_{sb}|) (c_{bd} - c_{bs}) + (\hat{q}_{sb} - |\hat{q}_{sb}|) (c_{bs} - c_s)]_{nk} \quad (29)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dt} [a_{bd} \theta_{bd} R_{bd} c_{bd}] &= \alpha_{bd} g (c_{bs} - c_{bd}) - \lambda (a_{bd} \theta_{bd} R_{bd} c_{bd}) \\
& + 0.5 [(a_{bd})_t + |(a_{bd})_t|] \theta_{bs} R_{bs} c_{bs} \\
& + 0.5 [(a_{bd})_t - |(a_{bd})_t|] \theta_{bd} R_{bd} c_{bd} + i_{bd} + \hat{e}_{bd} \\
& + 0.5 \sum_{nk=1}^2 [(\hat{q}_{sb} + |\hat{q}_{sb}|) (c - c_{bd}) + (\hat{q}_{sb} - |\hat{q}_{sb}|) (c_{bd} - c_{bs})]_{nk} \quad (30)
\end{aligned}$$

In order, the terms in eqns (29) and (30) are for: change in amount of contaminant stored; inter-layer transfers by diffusion (the α terms); radioactive decay; two terms for transfers with bulk movement of bed materials (associated with deposition and erosion of the bed, and consistent with the fact that the thickness of the bed surface layer is fixed); input from the

atmosphere (in eqn (29) only); infiltration of fine sediments into the bed (the i terms); net input of contaminant with plant uptake and generation by decay of parent contaminants; and convection with water flow through the bed.

The R factors in eqns (28) to (30) are evaluated in the same way as R_{sw} and R_{is} . The new subscripts introduced above are: bk for river bank; D for sediment dispersion; s for river water; sb for river bed; sd for newly deposited sediments; and t for time derivative. The new variables are: a [L^2], the cross-sectional area of a layer (measured on a plane perpendicular to the river direction); \hat{e} [$ML^{-1}T^{-1}$], combined rate (per unit length of channel) of plant uptake and generation by decay of parent contaminants; F and G [1], factors accounting for contaminant adsorbed to eroded bank materials; g [L], the effective width of the bed surface layer (measured following its contour across the width of the channel); i [$ML^{-1}T^{-1}$], rate (per unit length of channel) of contaminant infiltration with sediments infiltrating from the river water; nk [1], river bank number (1 or 2); \hat{q} [L^2T^{-1}], lateral volumetric flow rate per unit length of channel; \hat{Q} [$ML^{-1}T^{-1}$], rate (per unit length of channel) of surface input of contaminant with rainfall, irrigation or dry deposition; U [1], unitary function (zero when there is no river water, one when there is); ψ [$ML^{-1}T^{-1}$], rate (per unit length of river) of contaminant input with tributary and distributary flow.

16.5 SOLUTION METHODS

Within SHETRAN there are two main computational algorithms (solvers) for contaminant transport: COLM, for the equations for the transport of a single contaminant in a column (including the water and sediments lying at the ground surface), and LINK, for the equations for the transport of a single contaminant in one river link. COLM and LINK are both single subroutines written in FORTRAN 77. To create these solvers, the differential equations describing contaminant transport were scaled, reduced to finite difference equations and an algorithm chosen which solves the finite difference equations. (The fact that the transport equations were scaled — i.e. reduced to non-dimensioned form — is invisible to users of SHETRAN, but was of benefit in developing and testing the solvers.)

Fully implicit finite difference approximations were used to reduce the scaled process equations to finite difference equations. Such approximations give great numerical stability to the solvers, even under extreme storm conditions, but can lead to (overly damped) unphysical solutions if very large time-steps are taken. In practice, however, time-steps much larger than two hours cannot be taken, as they result in inaccuracy in the water flow component of SHETRAN.

16.5.1 COLM

It is assumed that every column is areally homogeneous, and at every depth in every column the contaminant is uniformly distributed over the plan area. As described in Section 16.1, each column is divided, by horizontal slicing, into parallelepipedal finite difference cells; this allows the vertical distribution of contaminant to be simulated.

For compatibility with the water flow solvers used in the SHE, a mesh-centred approach is used (i.e. cell boundaries lie halfway between nodes). A 'staggered mesh' approach is not required, so the cells for contaminant transport are the same as those for water flow. The mesh need not be uniform; this allows the possibility of using a finer mesh (giving higher resolution)

within the plant rooting zone and thin high-permeability or strongly adsorbing layers of the soil and rock.

To ensure strong coupling (which reflects strong physical coupling) between the equations for contaminant transport in the soil and rock and in surface waters and sediments, the top cell of the column holds the top few centimetres of the soil and rock and all the surface waters and sediments. The finite difference equations for the top cell satisfy both the column porous media transport equations, (15 to 23), and the overland transport equations, (24 to 27). With this approach, if there is surface water on a column, the concentration of contaminant in solution in the top few centimetres of soil and rock is always equal to that in solution in the surface water.

A fully implicit hybrid finite difference approximation (upwind/central, with harmonic mean values for the dispersion coefficients) has been used for the terms describing vertical convection and dispersion within a column. This ensures numerical stability and, provided the cell Peclet number is less than two for all cells, gives very accurate results for vertical convection and dispersion in both the saturated and unsaturated zones.

To ensure numerical stability, fully implicit upwind finite difference approximations have been used for the terms describing horizontal convection (including downstream convection in river channels). Since the upwind approximations introduce numerical dispersion which is usually stronger than the expected physical dispersion, finite difference representations of the physical dispersion terms for horizontal transport should not be, and are not, included in the contaminant transport component.

If there is linear adsorption, the finite difference equations for the contaminant contained in the dynamic region in each column form a tridiagonal set of simultaneous linear algebraic equations. This set is solved at each time level using the Thomas algorithm (see, for example, Ames, 1977). The finite difference equations for dead-space are a set of independent linear algebraic equations. These equations are solved after those for the dynamic region, using direct calculation. If there is non-linear adsorption, all the algebraic equations are non-linear, and the full set is solved using a simple iteration procedure which involves the repeated use of the Thomas algorithm and direct calculation.

16.5.2 LINK

There are three finite difference cells for each river link: one each for the river water, the bed surface layer and the bed deep layer. The thickness of the cell for the bed surface layer does not vary with time; to ensure that the concentration in the cell can respond quickly to changes in the concentration in river water, this thickness should be a few centimetres at most. The thickness of the river water cell will vary with time as the level of water in the river rises and falls. Similarly, the thickness of the cell for the bed deep layer will vary when there is erosion or deposition.

The finite difference equations for each river link form a set of three simultaneous non-linear algebraic equations, which is solved, at each time level, using an iteration method based on Demidovich and Maron (1987).

16.5.3 Coupling at catchment scale

When SHETRAN is running, the overall water, sediment and contaminant simulation progresses step by step from time level to time level. At each time level, the contaminant

calculations are carried out only after the water and sediment calculations have been completed and their results are available for use. In finite difference terminology, water and sediment data at time level $m + 1$ are passed to the contaminant component, and are then used in the calculation of the contaminant concentrations at time level $m + 1$.

It is important to have very robust, mass-conserving methods of coupling the solutions for the transport in any column or link to the transport in neighbouring columns and links, and for coupling the transport of one contaminant to the transport of other contaminants. Within the contaminant component, when a solver is called it returns the final values for the concentrations at time level $m + 1$. There is, therefore, no iteration involving repeated calls to the solvers COLM and LINK. At each time level, the whole catchment is swept once. Columns and river links are processed one by one; for each column or river link, one call is made to COLM or LINK, as appropriate, for each contaminant. The order of processing is an important feature of the overall approach to obtaining a stable solution for the entire catchment. The basic rules for ordering are:

1. Columns and river links are processed in decreasing order of the elevation of the free surface of the surface waters associated with them (there is a secondary ordering system for the columns on which there is no surface water).
2. For each solver, calls for the first contaminant are always made before calls for the second, etc.

As a result of the first rule, when a column or link is being processed, the upstream concentration of contaminants is known at time level $m + 1$ for all the surface water flowing into the column or river link from neighbouring columns and river links. This makes it possible to use a fully implicit upwind approach for modelling contaminant convection with surface water flows and sediment transport. This method of coupling columns and river links ensures the stability of the solutions, even during extreme storms. It does, however, as noted earlier, introduce numerical dispersion.

The second rule in the list above makes it possible to use a mass-conserving approach to coupling the transport of daughter contaminants to the transport of parent contaminants.

16.6 VERIFICATION

The solvers COLM and LINK have been tested independently of the rest of the SHETRAN computer code. They were embedded in specially written FORTRAN harnesses which produce synthetic water flow and sediment data, and were verified against analytic solutions and self-consistent physical descriptions of contaminant distribution and transport. A programme of testing requiring one man-year of time was designed and successfully carried out. This involved testing the description of each process for contaminant transport on its own and in association with the other processes. Many of the tests on COLM used the analytic solution given by van Genuchten and Wierenga (1976) for the convection—dispersion equation with adsorption and absorption into dead-space. The tests on LINK used specially derived solutions.

Both COLM and LINK were found to be numerically stable under all the conditions considered, and both were found to be accurate provided the time-step was kept to a reasonable level. The recommended time-step (for a typical catchment) is two hours during quiet periods, dropping to 15 minutes during storms. It is not possible to give an overall figure for accuracy, which will apply under all conditions. However, typical mass balance errors are extremely

small and are usually best measured in hundredths of a per cent; typical results are well within 1% of analytic solutions. A paper on the verification of SHETRAN is in preparation. This includes full details on the testing of COLM and LINK, and on the catchment simulations described briefly in the next section.

16.6.1 Catchment simulations

Analytic solutions are not available for the full set of coupled equations for three-dimensional integrated surface and subsurface contaminant transport. The only criteria for testing the full system are therefore self-consistency and physical reasonableness. As part of a verification programme, SHETRAN has been run for several simple hypothetical catchments. The main test catchment is a V-shaped catchment, 14 km N–S by 3 km E–W, drained by a single central channel running N–S. This catchment is shown, schematically, in Figure 16.2; each rectangle on the figure represents the top of a column. The figure is not drawn to scale: the main columns are 1 km N–S by 0.25 km E–W, so are not square in shape, and the 1 km N–S by 10 m E–W stream bank columns located on either side of the river are relatively much thinner than they appear in the figure. At all points on the ground surface there is a N–S slope and a slope towards the river. The subsurface has a simple layered structure, with 20 m of Quaternary deposits, including sandy and clayey layers, overlying sandstone. A variety of heterogeneous surface soil and vegetation covers have been considered. The main meteorological data used are from a several-year-long set for a catchment in Finland.

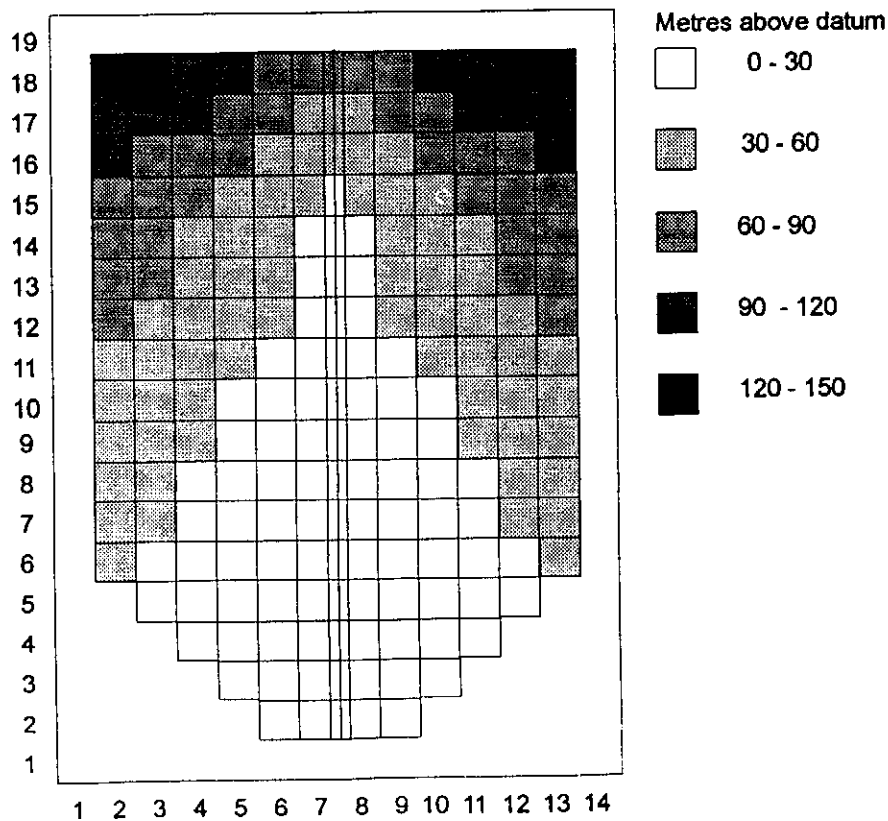


FIGURE 16.2 Typical ground surface elevations for the hypothetical V-shaped catchment

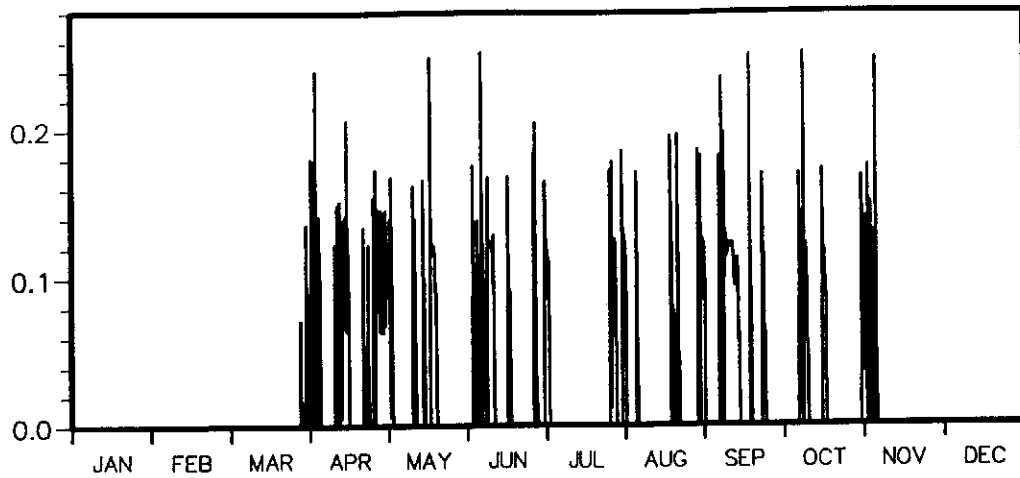


FIGURE 16.3 Typical relative concentration in river water as the result of erosion of highly adsorbing contaminated soils

To date, in the hypothetical catchment simulations, every process of contaminant transport that can be simulated using SHETRAN has been simulated (except for infiltration of fine sediments into the river bed) and the simulation of each process and each combination of processes has been self-consistent and physically reasonable. There is not space here for anything other than a few representative results which give a flavour of the types of results that can be obtained using SHETRAN. These are shown in Figures 16.3 to 16.6.

Figure 16.3 shows pulses of contaminant being discharged into the river during storms, with highly adsorbing sediments. The sediments were eroded from column 5,17 (see Figure 16.2) and washed down the hillslope into the channel. The only significant process for contaminant transport under these high adsorption conditions is convection with sediment. Between storms, therefore, when there is little or no input of sediment, the relative concentration in solution in the river is negligible. (Relative concentration is the ratio of the local concentration to the reference concentration c' ; for the simulation resulting in Figure 16.3, the concentration in solution in the soil water in the surface soils at column 5,17 was maintained at c' .)

Figure 16.4 shows results for a special type of simulation designed to test whether contaminant mass is conserved within a SHETRAN simulation. The initial concentrations at all points within the catchment and the concentration in all incoming water (including rain and snowmelt water) were set to the reference value c' . Under these circumstances, the only physical process that should cause the concentration at any point in the catchment to change from the reference value is evaporation, which should cause an increase. The figure shows the relative concentration of contaminant in solution at a point on the ground surface; for the meteorological data used there is no evaporation until late April, and, as it should, the relative concentration stays at one until this time. This test is run every time a dataset is assembled for a new catchment and, to date, every test has been successful, showing that SHETRAN conserves contaminant mass.

Figure 16.5 shows typical relative concentrations on a river bank and in river water. The source of contaminant is groundwater (at the reference concentration c') flowing steadily upwards, through the base of the modelled aquifer, into the catchment at some distance from the river. From the gradual rise in concentration over the nine years, it is clear that it will take

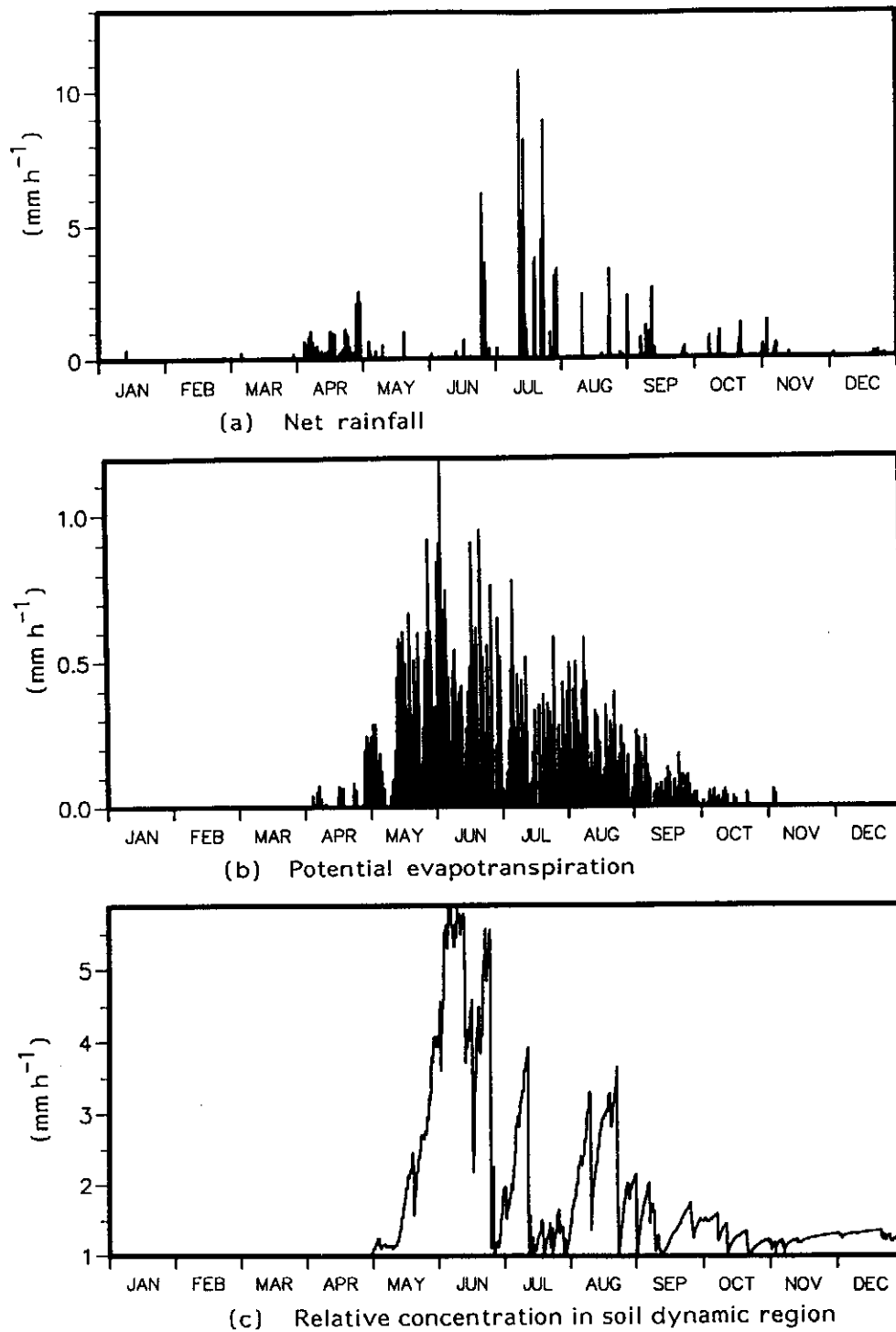


FIGURE 16.4 Typical mass balance verification result: (a) combined effective rainfall and snowmelt rate at the ground surface; (b) potential evapotranspiration rate; (c) relative concentration in solution at a point on the ground surface

many years, or decades, for near-steady transport conditions to develop. The figure shows that there are two distinct dilution regimes: the curves are smooth when there is a snowpack and little or no melt, and rough when there is dilution by rainfall and meltwater and re-concentration by evaporation.

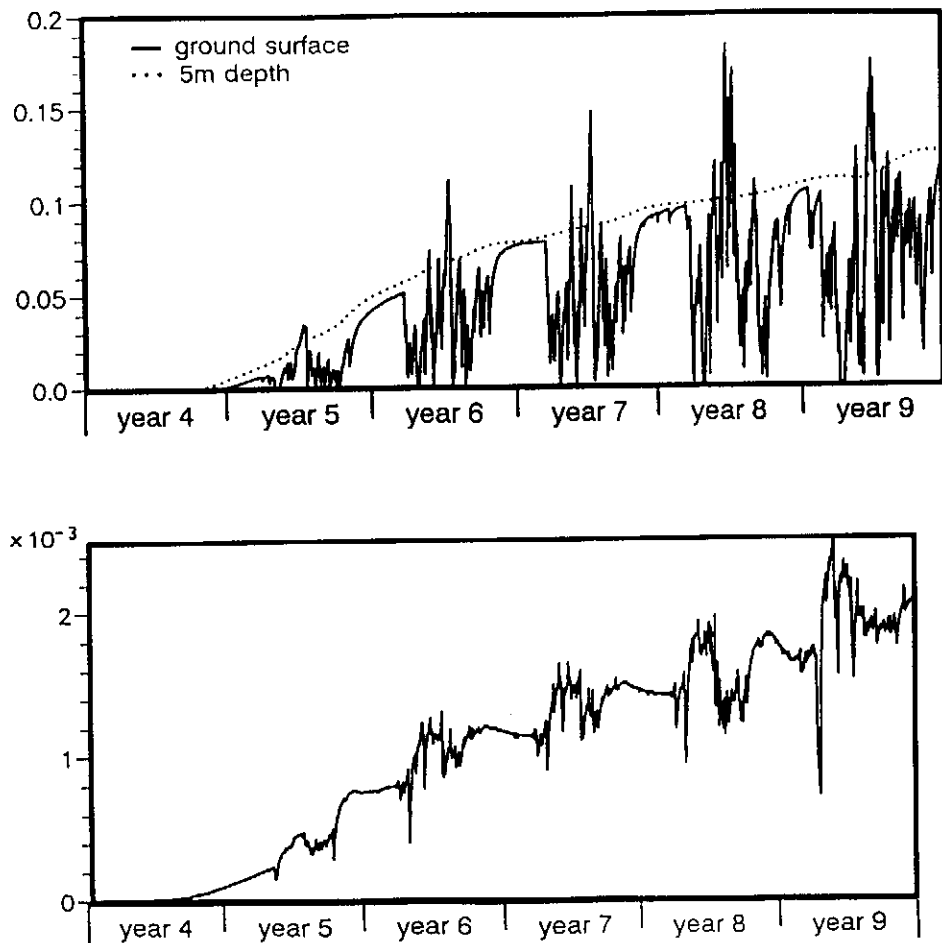


FIGURE 16.5 Typical relative concentration in solution for a non-adsorbing contaminant rising from the subsurface: (a) on the river bank; (b) in the river water

Figure 16.6 shows typical relative concentrations resulting in the subsurface when contaminated groundwater enters the catchment from below and flows to the river through a layer of permeable sand.

16.7 VALIDATION METHOD

The strength of SHETRAN and the SHE lies in their physically based spatially distributed nature; the cost of this strength, however, is complexity and many parameters. As it is for any complex model which has many parameters, the process of calibrating SHETRAN or the SHE is fraught with practical and philosophical difficulties. Yet calibration has been used in all the SHE application studies published to date (e.g. Bathurst, 1986; Refsgaard *et al.*, 1992; and Jain *et al.*, 1992), so these studies are clearly open to criticism. A new approach to the validation of catchment models against field data has therefore been developed (Ewen and Parkin, in press). The new method involves testing on research catchments. It is based on the idea that a model should be tested under conditions similar to those under which it will be used, and is designed to show whether a model is fit for purpose. When applying the new method, appropriate features like weekly runoff and the frequency with which a particular agricultural field will flood

are chosen, and bounding values for the magnitude of these features are set using the results from “blind” simulations. By “blind” it is meant that the measured data for the catchment (e.g. the data describing water storage and flow) are not available to the modeller in any form until all the predictions have been made (so calibration is not possible). The quality of the predictions must also be specified by the modeller. For example, the modeller may say that, for success, the measured data must lie within the predicted bounds 90% of the time.

Since the new method involves “blind” validation, it is especially appropriate for validating models which are to be used on ungauged catchments or for the prediction of the effects of future changes in climate and land use.

In practice it is impossible to validate a complex modelling system like SHETRAN for use at all catchments under all conditions. Also, the performance in a particular test will depend on the quality and experience of the modeller as well as the quality of the data and model. The new method therefore involves testing the model, whenever possible, throughout its life, and keeping a full record of its performance. Potential users can then look at this record and, bearing in mind the amount and quality of the catchment data they have available, judge for themselves whether or not the model and modeller can give them useful results for their particular catchments and problems.

The new validation method has been used to test the capability of SHETRAN to predict the flow discharge for Rimbaud, a subcatchment of the Real Collobrier research catchment in Mediterranean France. A paper giving the results of this test is in preparation.

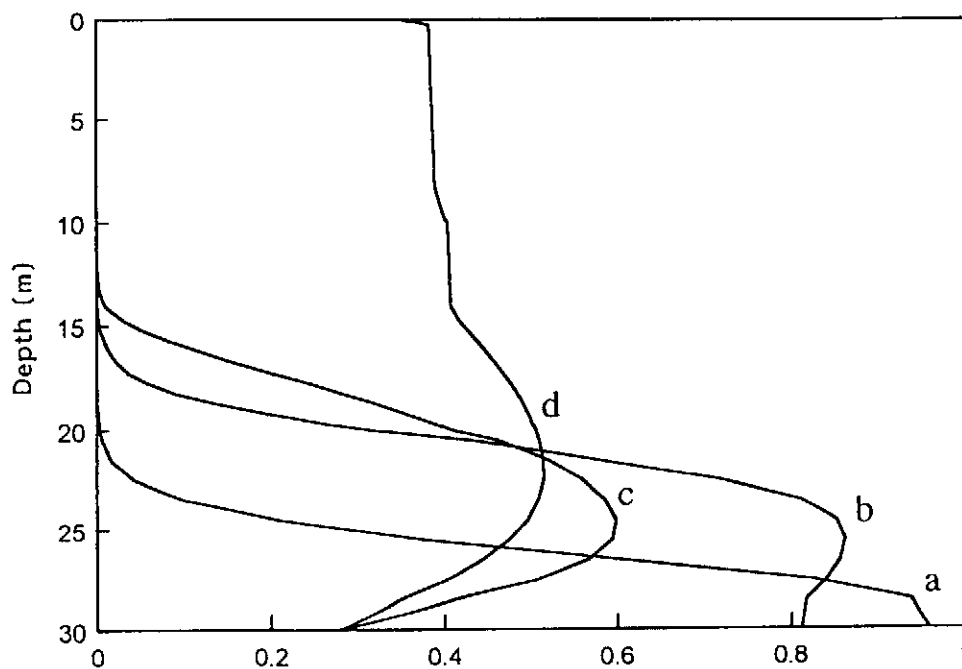


FIGURE 16.6 Typical relative concentrations in solution in subsurface waters, for a non-adsorbing contaminant, as a result of contaminated upflow through a region of the base of the modelled aquifer: a is for the column above the entry point; b and c are for the columns lying between a and the river bank at d. There is a very permeable sandy layer at 20–25 m depth

16.8 DISCUSSION

The main advantage of following a physically based spatially distributed approach in the development of SHETRAN is that the results from SHETRAN simulations are traceable to basic physical descriptions and physical property data that are independent of SHETRAN, and the prediction of the effects of changes in climate and land use on water resources is therefore possible. Since catchments are naturally complex, however, following the physically based spatially distributed approach has led to a contaminant transport component which is quite large and complex; it has twelve parameters, some of which vary spatially and with contaminant type. Despite this complexity, only one significant compromise has been made in the approximation of the governing partial differential equations by finite difference equations: a falsely dispersive upwind approximation has been used to represent the combined terms for horizontal convection and dispersion.

SHETRAN is a fully detailed fully integrated three-dimensional modelling system for combined water flow and sediment and contaminant transport in catchments. The contaminant transport component of the system has been fully verified and gives self-consistent and physically reasonable simulations of the simultaneous transport of several contaminants in, and between, the surface and subsurface zones. Catchments modelled using SHETRAN can be represented in quite fine physical detail, accounting for the heterogeneity of both surface and subsurface conditions; a typical ten-year simulation can show both storm responses and the slow development of contaminant transport pathways.

The new "blind" validation method is a practical scientific approach to the validation of catchment models against field data. We look forward to putting the method to use in validating the contaminant transport component of SHETRAN.

ACKNOWLEDGEMENTS

Work on the development of the contaminant transport component of SHETRAN was initiated in 1988 by Enda O'Connell, James Bathurst and Rae MacKay. A considerable amount of preparatory work (including the upgrading of the water flow component) was carried out before the contaminant transport component was installed. The major part of this preparatory work was undertaken by Geoff Parkin; a contribution was made by Anton Purnama. (Papers giving a general introduction to SHETRAN and describing the preparatory work are in preparation.) Significant contributions to the verification studies were made by Geoff Parkin, Stephen Anderton and Carl Ishemo. The work was funded by UK Nirex Ltd.

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APPENDIX: SYMBOL LIST

a L^2 cross-sectional area of a river channel layer, measured on a plane

		perpendicular to the flow direction
A	L^2	plan area of a column
b	MT^{-1}	rate of dispersion into a column
B	$ML^{-3}T^{-1}$	strength of source
c	ML^{-3}	concentration of contaminant in solution (for the column and link equations, c without a subscript is for the solution in a column)
d	L	depth
D	L^2T^{-1}	dispersion coefficient
e	$ML^{-3}T^{-1}$	combined rate of input from plant uptake and recycling, and from generation by decay of parent contaminants
\hat{e}	$ML^{-1}T^{-1}$	as e , but for channels
f	—	fraction of the adsorption sites in porous media which are associated with the mobile water
F	—	factor accounting for contaminant adsorbed to eroded river bank materials
g	L	effective width of the bed surface layer
G	—	factor accounting for contaminant adsorbed to eroded river bank materials
i	$ML^{-1}T^{-1}$	rate (per unit length) of contaminant infiltration, with fine sediments, into the river bed
j	—	index for the vertical faces of a column ($j = 1, 2, 3$ or 4)
K_d	—	adsorption distribution coefficient (ratio of the mass adsorbed per unit volume of the porous material or surface water to the concentration in solution)
l	—	index for sediment classes
n	—	exponent for Freundlich adsorption equation
nk	—	river bank number ($nk = 1$ or 2)
ns	—	total number of sediment classes
q	L^3T^{-1}	volumetric flow rate
\hat{q}	L^2T^{-1}	volumetric lateral flow rate per unit length of channel
Q	$ML^{-2}T^{-1}$	vertical (positive upwards) rate of transport of contaminant at the ground surface or the bottom of a column
\hat{Q}	$ML^{-1}T^{-1}$	rate of input of contaminant to the surface of a channel
R	—	factor accounting for the contaminant adsorbed to porous media or sediments (for porous media only, called the retardation factor)
s	ML^{-3}	concentration of contaminant adsorbed
t	T	time
u	LT^{-1}	velocity of flow (for the column equations, u is the pore water velocity)
U	—	unitary function (0 when there is no water in a channel, 1 when there is)
v	L^2T^{-1}	volumetric lateral flow rate, per unit depth, into a face of a column
x	L	distance
z	L	elevation within a column
α	T^{-1}	coefficient for exchange between the dynamic region and dead-space, and between the layers of a river channel
β	—	fraction of the loose sediments which are in a given class
γ	T^{-1}	volumetric rate, per unit volume of porous media, of water flow into

		dead-space
δ	—	relative density of the suspended sediments in a given class
ζ	—	efficiency of water uptake by plants from the dynamic region (a number between 0 and 1)
η	T^{-1}	volumetric rate of uptake of water by plants, per unit volume of porous media
θ	—	volumetric moisture content
λ	T^{-1}	radioactive decay constant
ϕ	—	fraction of the pore water which is in the dynamic region (i.e. the fraction which is mobile)
v	LT^{-1}	rate of erosion
ψ	$ML^{-1}T^{-1}$	rate (per unit length) of contaminant input to a stretch of a river with tributary and distributary flow

Special symbols and subscripts

*	dead-space
'	reference value
—	evaluated at the face of a column
$ h $	absolute value of variable h
b	bottom boundary of column
bd	bed deep layer
bk	river bank
bs	bed surface layer
d	dynamic region
D	sediment dispersion
ds	dead-space
gs	ground surface
l	index for the sediment classes
ls	loose sediments on the ground surface
s	river water
sb	river bed
sd	newly deposited sediments
ss	free surface water combined with loose sediments on the ground surface
sw	free water lying on the ground surface
t	time derivative