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DESIGN AND APPLICATION OF A SEDIMENT AND CONTAMINANT TRANSPORT MODELLING SYSTEM

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ABSTRACT A physically-based modelling system for water, sediment and contaminant transport at the river basin scale, called SHETRAN-UK, is presented which has particular relevance to environmental change impact studies. Based on the SHE hydrological modelling system, components have been developed for soil erosion and sediment yield, and for dissolved and particulate contaminant transport. Particular emphasis is placed on sediment and contaminant interactions and sediment transport by size fraction (including cohesive sediments) to account for the preferential sorption of contaminants by the finer sediment sizes. Three typical application areas are described: simulation of radionuclide dispersal in the biosphere as part of the establishment of the safety case for deep underground disposal of radioactive waste; modelling the impacts of likely changes in climate and land use on basin hydrology and soil erosion in a study of desertification in Mediterranean Europe; and development of forestry practice guidelines for minimizing soil erosion.

INTRODUCTION

In recent years, considerable attention has been focussed worldwide on the impacts of environmental change induced by human activity. Current issues in the hydrological domain include the effects of large scale deforestation and climate change on soil erosion and flow regime, and the dispersal of contaminants from agricultural and industrial activities. From Amazonia to Eastern Europe there have been insistent demands for reducing the environmental degradation caused by human activity; within the European Community strict regulations have been introduced for water quality in river basins; and worldwide there is debate on the environmental consequences of climate change. At the same time, however, industrial and agricultural activity is essential for maintaining our physical, material and economic well-being. A trade-off is therefore required between the level of development (providing an economic return) and the maintenance of an acceptable environment. Establishing such a trade-off is a decision-making process involving many elements, one of which is an appreciation of how environmental systems respond to imposed change. Of particular concern is the movement of sediments and contaminants through the land phase of the hydrological cycle.

Supported by constantly increasing computer power and sophisticated numerical solution techniques, mathematical modelling plays a vital role in developing the necessary appreciation of response mechanisms. This paper describes the structure and typical application area for SHETRAN-UK, an advanced physically based, spatially distributed modelling system for water, sediment and contaminant transport at the river basin scale. Within the system, specific allowance is made for the interaction of sediments and contaminants, represented by the transport of contaminants in particulate form through sorption by sediment particles.

PHYSICALLY-BASED MODELLING SYSTEMS

Simulation of the hydrological consequences of environmental change requires models which can represent a river basin in its future altered state in advance of the change taking place. The task is beyond the traditional black box and conceptual hydrological models, which are essentially regression relationships relying on the availability of past rainfall and hydrological records for their calibration. Their parameters lack physical meaning, so cannot be specified in advance. Similarly, records derived for the past state of a basin cannot support model calibration for a future altered state. Such models do not, therefore, have any basis for representing the impacts of, for example, future land use or climate change. Further, they are spatially lumped, so cannot readily account for spatial variations in basin characteristics, rainfall input and hydrological response.

By contrast, physically based spatially distributed modelling systems have particular advantages for the study of basin change impacts and applications to basins with limited records. Their parameters have a physical meaning and can be measured in the field. Model set-up therefore is less dependent on the existence of past data record, while the ability to specify representative parameter values means that models can be set up for a future altered state of the basin. Basin response is represented on both a spatially and temporally distributed basis and in terms of multiple variable outputs: i.e. rather than providing just one output variable, such as sediment discharge, the models provide distributed predictions of all relevant hydrological, sediment and contaminant variables.

Disadvantages of physically based models include heavy computer requirements, the need to evaluate many parameters, and a complexity which implies a lengthy training period for new users.

SHETRAN-UK

The basis for SHETRAN-UK is the Système Hydrologique Européen (SHE) (Abbott *et al.*, 1986a, b). This is a physically based, spatially distributed, hydrological modelling system, incorporating the major components of the land phase of the hydrological cycle to give an integrated surface and subsurface representation of water movement through a river basin. Following the initial joint development of the SHE by the Danish Hydraulic Institute, the Institute of Hydrology (UK) and SOGREAH (France), subsequent UK activity has been concentrated at the Natural Environment Research Council's (NERC) Water Resource Systems Research Unit (WRSRU) at the University of Newcastle upon Tyne.

Within the SHE, each of the processes (snowmelt, canopy interception, evapotranspiration, overland and channel flow, unsaturated and saturated subsurface flow and stream/aquifer interaction) is modelled either by finite difference representations of the theoretical partial differential equations of mass and energy conservation or by empirical equations derived from independent experimental research. The spatial distribution of basin characteristics, precipitation input and hydrological response is achieved in the horizontal through representation of the basin with an orthogonal grid network and in the vertical by a column of horizontal layers at each grid square. Further details are given in Abbott *et al.* (1986b).

Water movement is a basic driving mechanism for contaminant and sediment transport and the SHE therefore provides the framework for a growing family of overlay components. These make use of the hydrological information such as overland and channel flows, soil moisture conditions and groundwater flows supplied by the SHE, to determine, as appropriate, concentrations and rates of transport and deposition of sediments and contaminants on a spatially and temporally distributed basis. A major project underway at the WRSRU is the development of SHETRAN-UK as a powerful sediment and contaminant transport modelling system, with particular application to the surface and subsurface dispersal of radionuclides within river basins. The following gives a brief description of the sediment and radionuclide transport components for the surface region.

Sediment transport component

The basis for the sediment transport component is the SHESED-UK soil erosion and sediment yield component for the SHE developed at the University of Newcastle upon Tyne. This accounts for erosion by raindrop impact, leaf drip impact, and overland flow, and sediment transport by both overland and channel flow (Wicks & Bathurst, in press). However, to account for the transport of sorbed radionuclides, the component has undergone considerable upgrading within SHETRAN-UK. In particular, an improved representation of cohesive sediments and the size distribution of transported materials has been introduced, because radionuclides are sorbed preferentially to the finer, cohesive sediments. The processes incorporated in the component have also been expanded to include bank erosion and infiltration of fine sediments into the channel bed.

Space does not permit a full mathematical description of the component and only the central routing equations are presented here. For overland flow transport, sediment is routed as total load according to the two-dimensional mass conservation equation

$$\frac{\partial (ch)}{\partial t} + (1-\lambda)\frac{\partial z}{\partial t} + \frac{\partial g_x}{\partial x} + \frac{\partial g_y}{\partial y} = -e \qquad (1)$$

where h = water depth; c = sediment concentration; λ = soil porosity; z = the depth of loose soil; g_x, g_y = volumetric sediment transport rates per unit width in the x and y directions respectively; and t = time. In this equation the term involving $\partial z/\partial t$ represents the change in the depth of loose soil as material is either removed by the flow or added from incoming material from upstream. The term e represents the rate of generation of new loose soil by raindrop impact and overland flow and includes also a term for deposition of cohesive sediment as a function of flow shear stress. The transport rate is then limited either by the amount of loose soil available or by the capacity transport rate of the flow, determined by a sediment discharge equation. The above equation is applied to each size fraction in turn, with the cohesive material treated as a single size fraction.

For channel flow transport, mobile sediment is divided between the cohesive and the non-cohesive. For the non-cohesive fraction, separate allowance for the bed and suspended load components is not considered necessary for the purposes of modelling particulate radionuclide transport. The main reason for simulating the two components separately would be to account for dispersion of the suspended load: however, dispersion of non-cohesive sediment is considered relatively insignificant. Non-cohesive sediment transport therefore is simulated with the total load equation

$$\frac{\partial (Ac)}{\partial t} + (1-\lambda)\, W\frac{\partial z}{\partial t} + \frac{\partial Q_s}{\partial x} = q_s \tag{2}$$

where A = flow cross-sectional area; c = sediment concentration; λ = bed porosity; W = active bed width; z = channel bed elevation; and Q_s = volumetric sediment discharge. The term q_s represents the input of sediment from bed erosion, bank erosion and overland flow supply, and losses through infiltration of the finer sizes into the bed. This latter process is determined as a function of the difference between the concentration of sediment in the flow and concentration in the top layer of the bed material, and depends also on the ratio of the size of the infiltrating particles and the pore size of the bed material. As for overland flow transport, sediment discharge is determined as a function of the amount of sediment available and the capacity transport rate of the flow. Calculations are carried out for each size fraction in turn and allowance for sediment size distribution also enables armour layer development to be simulated at the bed surface.

Cohesive sediment is assumed to move essentially as suspended load and is simulated by the equation

$$\frac{\partial (Ac)}{\partial t} + \frac{\partial (UAc)}{\partial x} = \frac{\partial}{\partial x}\left[D_x A\frac{\partial c}{\partial x}\right] + q_s \tag{3}$$

where U = longitudinal velocity of the suspended load particles; D_x = longitudinal dispersion coefficient; and q_s represents sediment input from bed erosion, bank erosion and overland flow supply and losses through infiltration into the bed and deposition (determined as a function of flow shear stress). A dispersion term is included since the fine particles are prone to dispersion and it is the fine particles to which the radionuclides are preferentially sorbed.

Surface radionuclide transport component

The component simulates the spatial and temporal distributions of radionuclide concentration arising from transport in both dissolved form and particulate form (through sorption to sediment particles). The concepts behind the component are such that simulation can also be extended more generally to other contaminants.

A particular difficulty is dividing the radionuclide load into the sorbed and the dissolved components. Sorption is a highly complex effect which can occur by several different processes and which depends on the chemical, mineralogical and size distribution characteristics of the sediment load, as well as the concentration and types of dissolved radionuclides. Lack of information does not justify a complex approach to the problem and a practical approach is used, based on the Freundlich equilibrium sorption isotherm (Bencala *et al.*, 1983). This has the advantages of simplicity and an accumulated body of experience in its application. Radionuclide sorption is quantified in terms of a (partition) distribution coefficient K_d where

$$K_d = \frac{\text{Amount of radionuclide sorbed to sediment}}{\text{Amount of radionuclide left in solution}} \tag{4}$$

The concept was developed for ideal solutions under the constraints that the system is at equilibrium and the temperature is constant. Under real conditions these constraints may not be satisfied and the method may therefore provide only a first approximation to the sorption process.

Within SHETRAN-UK, radionuclide routing is carried out using the convection-dispersion equation. By building in an allowance for sorption, though, just one form of the equation needs to be solved to account for both dissolved and sorbed transport, i.e. the calculations can be carried out in terms of the dissolved radionuclide concentration only. To achieve this, the terminology applied to solute transport in porous media has been used, to introduce a retardation factor, R, (Onishi *et al.*, 1981) where

$$R = 1 + cK_d \tag{5}$$

and c = concentration of sediment particles in the flow. The retardation factor represents the enhancement of the storage capacity at a point, resulting from some of the radionuclides being sorbed to sediment particles. Then, within the routing equation, with sorption loss given by the retardation factor, the proportion of radionuclide load travelling in particulate (sorbed) form can be determined knowing sediment concentration and K_d.

For overland flow, radionuclide transport is simulated by the equation

$$\frac{\partial\left[(hr + \theta z r_s)\, c_D\right]}{\partial t} + \frac{\partial (hruc_D)}{\partial x} + \frac{\partial (hrvc_D)}{\partial y} = e_r \tag{6}$$

where r = retardation factor for the surface water layer; r_s = retardation factor for the water in the loose sediment layer; θ = soil moisture content; z = thickness of loose sediment; c_D = concentration of solute radionuclide; u, v = water velocity in the x and y directions respectively; and e_r represents the net addition of radionuclides resulting from inputs from above and from the subsurface, generation of daughter products and loss through decay and plant uptake.

For channel flow a three-compartment representation of the channel is used. The top compartment represents the flow zone (carrying dissolved and particulate radionuclides) and incorporating longitudinal convection and dispersion. The middle compartment is the bed surface layer, introduced to account for rapid bed/flow interactions. The bottom compartment is the deep bed layer, introduced to account for longer term subsurface storage.

Particulate radionuclides can pass from the top to the middle compartment as sediment is exchanged between the bed and the flow. Deeper infiltration of sediment into the channel bed allows the passage of particulate radionuclides to the bottom compartment. The mass balance equation for channel flow is:

$$\frac{\partial(ARc_D)}{\partial t}+\frac{\partial(Q_rRc_D)}{\partial x}=\frac{\partial}{\partial x}\left[AD\frac{\partial c_D}{\partial x}\right]+q_r \qquad (7)$$

where R = retardation factor; Q_r = radionuclide discharge, incorporating dissolved and particulate load and dispersion of particulate radionuclides; D = longitudinal dispersion coefficient for dissolved radionuclides; and q_r represents the net addition of radionuclides resulting from inputs from overland flow, from the bank, from above and from the bed, generation of daughter products, loss due to decay and plant uptake, erosion and deposition, and exchanges between the flow-zone, the bed surface layer and the deep bed layer.

Comments on the design of SHETRAN-UK

Development of a practically oriented modelling system has required certain compromises in the detail of process representation (to keep computational requirements within reason) and in complexity (since several of the processes are not yet satisfactorily quantified). For example, little research has been done on bank erosion and bed infiltration equations and relatively simple approaches therefore are used in SHETRAN-UK. Radionuclide sorption similarly is not well quantified and there is a general lack of information on cohesive sediment dynamics in rivers and overland flow: most available information is based on studies in estuarine environments. However, a radionuclide transport model would be incomplete without allowance for the various processes: at the same time, the modelling approach will enable the sensitivity of the simulations to the inherent uncertainty to be investigated.

APPLICATIONS OF SHETRAN-UK

Three projects in which SHETRAN-UK is either being used or is proposed for use demonstrate the need for this type of model in examining the impacts of changing environments on sediment and stream water quality.

Radionuclide dispersal

Development of SHETRAN-UK for radionuclide transport modelling forms one project within a large research program, funded by UK NIREX Ltd. and concerned with establishing the safety case for deep underground disposal of low and intermediate level radioactive waste in the UK. Assessment of the consequences of disposal activity must apply not only while the repository is operating but also after closure and for a very long time into the future.

The natural pathway for the radioactivity contained within the repository to travel back to man is via the groundwater that penetrates the deep rock strata. Assessment of the pathways to be followed and the concentrations likely to occur at the surface in the long term involves a variety of mathematical models: amongst these are a geosphere model to simulate radionuclide migration from the repository towards the ground surface and a biosphere model to simulate radionuclide dispersal in the ground surface and near surface regions. Information on radionuclide concentrations obtained from the biosphere model will then be used in predictions of the risk to man. The simulations will need to be carried out for the periods of thousands to hundreds of thousands of years over which trace quantities of radionuclides could be released to the environment. Of necessity, though, simulations over such time scales will require assumptions and approximations in the models about processes, pathways and spatial and temporal dependencies. The biosphere model therefore will not be fully physically based and its relatively simple level of representation will consequently need to be justified through comparison with more sophisticated representations, to be provided in this case by SHETRAN-UK. Because it is currently limited to simulation periods of a few years to decades, SHETRAN-UK cannot itself be used for the long-term biosphere simulations.

Typical processes which may be simulated by SHETRAN-UK include the reconcentration in the biosphere of radionuclides previously dispersed in the geosphere, so increasing their radiological input, for example the build-up of particulate radionuclides in channel beds or the build-up of dissolved radionuclides in areas undergoing salinisation. Conversely the model can simulate the possible dilution within the biosphere of relatively high radionuclide concentrations delivered to the top of the geosphere. In both cases it will be important to consider spatial and temporal variations in concentration, since time and space averaged values may ignore short term or local fluctuations of significance.

Conditions must also be simulated for the possible climates which may evolve at the repository site over the next million years or so: these include a possible warmer climate brought on by global warming and, in the longer term, the next ice ages. The advantage of using SHETRAN-UK is that its parameters and input data, which are physically-based, can be specified for any desired state of climate and at any catchment. As a first step, the flow components of the system are being validated using present day basins from various climatic regions as analogues for future conditions.

Mediterranean desertification

The water and sediment components of SHETRAN-UK are being used in an international multiorganization study of desertification and its impacts in Mediterranean Europe. The study, known as MEDALUS (Mediterranean Desertification And Land Use), is funded under the CEC EPOCH scheme (European Programme on Climatology and Natural Hazards) and headed by the University of Bristol, UK. It is aimed at supporting the formulation of future policy and strategies to take account of desertification trends (especially as they may be affected by climate change) and to prevent and mitigate the impacts of these trends. The project involves field and modelling studies of the interactions between climate, land use, soil degradation and water resources in the light of expected climate and land use changes.

The role of SHETRAN-UK is as follows:

(a) As an established modelling system, SHETRAN-UK and its data needs will provide a valuable input to the field program design by indicating what types of data are needed for modelling the hydrological and erosion processes associated with desertification. Efficient calibration of physically based models requires field studies to form an integrated part of the calibration procedure rather than appearing as an isolated activity.

(b) SHETRAN-UK will play an important role in extrapolating from the hillslope and plot scales, at which much of the field process study and modelling effort in MEDALUS is concentrated, to the basin and regional scales, at which the impacts of desertification have socio-economic importance. The link will be established by applying SHETRAN-UK to a focus basin and to hillslope and plot sites within the basin. This will provide information on the effect of model grid square size on simulation results and on the evaluation of effective model parameters representative at different grid scales. Extrapolation of results can then be carried out for other basins within the MEDALUS study.

(c) SHETRAN-UK will be used to simulate the impacts of likely changes in climate and land use on basin hydrology and soil erosion. Because of its physical basis, models can be constructed and calibrated using the results of short term field studies under present basin conditions and then applied to simulate the response to specified future changes in basin characteristics and inputs. Specific impacts to be studied will include: impacts of different spatial and temporal distributions of rainfall input on basin hydrology and erosion; impacts of different land covers; and impacts of different land management options. The impacts will be examined in terms of the responses of soil moisture, phreatic surface level, stream discharge, soil erosion and basin sediment yield. Results in terms of water availability and soil loss will form an input to the MEDALUS modelling projects dealing with soil degradation and plant productivity.

Land management

The possibility is currently being examined of applying SHETRAN-UK in Central Chile to establish guidelines for minimizing soil erosion as part of a land management study. In the past there has been considerable degradation of the vegetation cover along the Southern Andes and the Coastal Range as a result of deforestation, overgrazing and poor agricultural practices (Solbrig, 1984, pp. 163-173). As a consequence soil erosion has become a major problem, causing on-site loss of soil fertility and downstream siltation of river channels and degradation of drinking water quality. In addition, the decreased ability of the soil to absorb rain means that surface runoff has increased in volume and velocity (e.g. Glaser & Celecia, 1981). Reduced soil moisture storage, increased surface runoff and increased loss of moisture through transpiration are also the consequence of an extensive afforestation program involving replacement of native forests by plantations of imported tree species such as Radiata Pine (Monterrey Pine). As a result the seasonal fluctuations in river flow have become more extreme, ranging from damaging floods in winter to dry river beds (and reduced drinking water supplies) in summer.

Minimization of such impacts requires sound land management. In particular, careful management of forest reserves and careful implementation of forestry practices is needed in order to sustain continued commercial operations while minimizing adverse environmental impacts on downstream communities and infrastructure. A contribution to establishing such a trade-off can be provided by systems such as SHETRAN-UK which enable the impacts of different levels of project sophistication and of different approaches to basin management on soil erosion, sediment yield and flood discharge to be assessed, in advance of any change being implemented. In the case of forestry practices, SHETRAN-UK could be used to examine the impacts of different areal patterns of logging in a basin, different degrees of ground disturbance arising from different logging and planting practices, and the introduction of different tree species. Those practices which were simulated as minimizing soil erosion and sediment yield would then be considered for implementation.

CONCLUSION

SHETRAN-UK is introduced as a system for modelling water, sediment and contaminant transport at the basin scale. Because of its physical and spatially distributed basis it is especially suited to assessing the impacts of land use change, different land management strategies and waste disposal schemes in advance of any course of action being implemented. It is thus a powerful tool for examining the urgent hydrological, sediment and contaminant problems with which river basins are currently being afflicted.

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