

Numerical analysis of coupled hydrosystems based on an object-oriented compartment approach

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ABSTRACT

In this paper we present an object-oriented concept for numerical simulation of multi-field problems for coupled hydrosystem analysis. Individual (flow) processes modelled by a particular partial differential equation, i.e. overland flow by the shallow water equation, variably saturated flow by the Richards equation and saturated flow by the groundwater flow equation, are identified with their corresponding hydrologic compartments such as land surface, vadose zone and aquifers, respectively. The object-oriented framework of the compartment approach allows an uncomplicated coupling of these existing flow models. After a brief outline of the underlying mathematical models we focus on the numerical modelling and coupling of overland flow, variably saturated and groundwater flows via exchange flux terms. As each process object is associated with its own spatial discretisation mesh, temporal time-stepping scheme and appropriate numerical solution procedure. Flow processes in hydrosystems are coupled via their compartment (or process domain) boundaries without giving up the computational necessities and optimisations for the numerical solution of each individual process. However, the coupling requires a bridging of different temporal and spatial scales, which is solved here by the integration of fluxes (spatially and temporally). In closing we present three application examples: a benchmark test for overland flow on an infiltrating surface and two case studies – at the Borden site in Canada and the Beerze–Reusel drainage basin in the Netherlands.

Key words | Borden aquifer, control-volume finite element method, coupled hydrosystem modelling, Meuse river basin, nonlinear diffusion equation, object-oriented programming

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INTRODUCTION

Hydrological systems belong to the most complex, dynamic and fragile environmental systems affected by both natural and human pressures. Hydrological systems encompass not only hydro- and geosphere partitions, but are affected by the bio- and atmosphere as well. An integrated process understanding is required in order to evaluate the impact of anthropogenic influences and the evolution of hydrosystems (Chen *et al.* 2006).

The hydrosphere can be subdivided roughly into surface water, vadose zone and aquifer compartments (Figure 1). The unsaturated zone is denoted as soil compartment

hereafter. The corresponding hydrological processes on the surface are related to lakes as well as rivers and overland flow. In the subsurface, unsaturated flow in soils and groundwater flow in porous as well as fractured aquifers occurs. The hydrosphere directly interacts with the biosphere and the atmosphere. Water exchange with the atmosphere occurs via evaporation and precipitation whereas root water uptake and transpiration represent links to the biosphere. The transport of contaminants in the hydrosystems strongly depends on the water movement through the compartments. The same physical principles

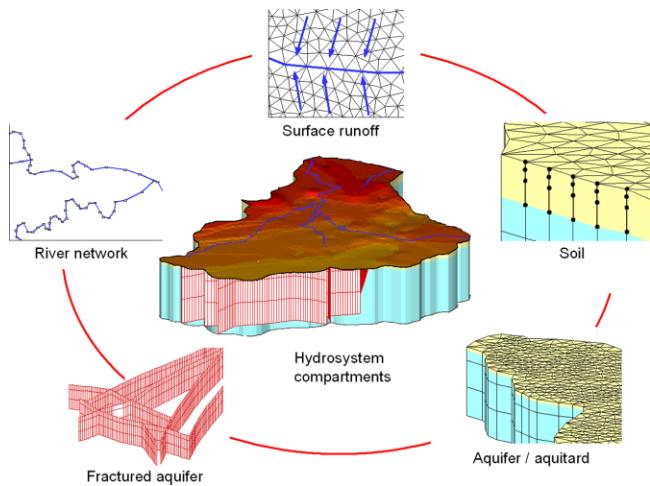


Figure 1 | Compartments of environmental hydrosystems. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

apply to water movement and contaminant transport in surface and subsurface hydrosystems. Thus, physically and chemically based mass, momentum and energy conservation laws expressed by partial differential equations are used to describe the processes and their interactions (Lees 2000; Abbott *et al.* 2001).

Hydrological analysis requires a complete model representation of the hydrological systems. Abbott *et al.* (2001) identified scaling, parameter uncertainty, process coupling, processing and visualisation of large datasets, software design and efficiency of computational methods as key challenges in hydrological analysis. A more and more realistic representation of hydrological processes has been achieved during the last thirty years as the accuracy of numerical algorithms and the feasible spatial and temporal discretisation has continuously improved. Computational modelling is a tool rapidly developed in hydrological analysis. In particular, advances in numerical mathematics and computer science have tremendously enlarged the variety and the nature of problems addressed by environmental scientists and engineers. It is certainly true that for each hydro-compartment (Figure 1) there exist many excellent simulation codes, but traditionally the development has been isolated within the specific disciplines. As a result, surface water models commonly lack rigorous representations of flow and transport in complex geological formations. On the other hand, groundwater models

typically ignore the dynamics of overland flow and surface water quality issues. There is a clear need to establish an integrative framework for the robust and sound analysis of terrestrial hydrological systems. Comprehensive overviews of physically based surface water and watershed hydrologic modelling can be found in (Anderson & Burt 1985; Abbott *et al.* 1986a; Singh & Frevert 2005). In subsurface hydrology well-established models exist for both saturated and variably saturated flow in porous media (Huyakorn & Pinder 1983; Simunek *et al.* 1999) and in dual-continua porous media (Vogel *et al.* 2001).

Coupled surface–subsurface flow models have been developed since they were first outlined in (Freeze & Harlan 1969). Examples of existing conceptual models and numerical codes include MODFLOW2000 (MODular three finite-difference ground-water FLOW model (Harbaugh *et al.* 2000)), TOPMODEL (physically based runoff production model (Bertoldi *et al.* 2004)), Feflow (Wasy Software (2004)), MIKE-SHE (Système Hydrologique Européen (Abbott *et al.* 1986b)), Hydrosphere (Sudicky *et al.* 2000) (see also <http://sciborg.uwaterloo.ca/~mclaren/public/> or <http://www.modhms.com/software/hydrosphere.html>), SWAT (Arnold *et al.* 1998), HSPF (Gunduz & Aral 2005; Donigian & Imhoff 2006) and ParFlow (Kollett & Maxwell 2006), to name just a few. These finite difference, element and volume implementations include a variety of monolithic and partitioned coupling schemes which rely on combinations of continuity assumptions and exchange flux calculations.

Object-oriented programming (OOP) has proven to be a key concept in developing complex software not only in engineering computation (e.g. Forde *et al.* 1990) but also in hydrogeology (Desitter *et al.* 2000; Wang & Kolditz 2007). Its advantages become particularly visible in the context of large developer teams and for the reuse, maintenance and extension of codes. In the field of water resources and hydrology, recent object-oriented software developments include models for flood analysis (Alfredsen & Saether 2000), topographically based watershed analysis (Wang *et al.* 2005), surface water quality (Elshorbagy & Ormsbee 2006) and pollutant transport in mine spoil heaps (Gandy & Younger 2007). The approval of integrated approaches also spawned object-oriented modelling software aimed at integration on a higher level. Within the hydrology community the CUAHSI (2007) Hydrologic Information System

(<http://river.sdsc.edu/HDAS/>) is dedicated to the linkage, visualisation and dissemination of numerous sources of hydrologic data. OpenMI ([Gregersen et al. 2006](#)) defines a generic modelling framework that allows communication and data exchange between different hydrological simulation models that are compatible with the according framework interface. JUPITER ([Banta et al. 2006](#)) describes an API (application programming interface) for hydrologic model analysis in terms of parameter identification and reliability. Finally, DANUBIA ([Barth et al. 2004](#)) provides an internet-based platform integrating the distributed simulation models of socio-economic and natural science disciplines taking part in the GLOWA-Danube project. The common idea to all of these initiatives is a flexible combination of existing models and software tools. An important backbone of hydroinformatics remains the existence and further development of open source software ([Harvey & Han 2002](#); [Abbott 2003](#); [Khatibi et al. 2004](#)).

Compartment approach

Two of the most difficult and challenging topics in hydro-system analysis are scale bridging and process coupling. To overcome these difficulties, we propose a compartment approach. The hydrologic compartments individually host the different flow and transport processes, which are coupled at their common compartment interfaces by exchange flux terms. This concept allows the consideration of each process appropriately at its specific time and space scale. To keep flexibility in the spatial resolution, each process is solved with a mesh optimized for its geological and hydrological structures, and numerical constraints. Together with the object-oriented method, this allows a use of multiple meshes tailor-made for each process ([Figure 5](#)), and leads to flexibility of the compartment approach. The central idea behind the multi-mesh concept is that the partial differential equation of each compartment can be solved numerically with the most suitable spatial discretisation. In addition, flexibility can also be achieved with sub-time steps for each individual process for the time discretisation. Thus, the time steps can be chosen according to the stability requirements of the process-specific numerical scheme (see Time-stepping synchronisation). Moreover, the compartment approach allows the combination of different numerical schemes,

such as a Galerkin finite element method (G-FEM) and a control-volume finite element method (CV-FEM) (see Numerical Methods). This separation of methods via the compartment is particularly powerful when the nonlinearity of each process does prefer certain numerical methods. Solution techniques for the coupled problem can be handled in the following two ways: partitioned coupling schemes and monolithic schemes to account for strongly coupled processes. In this paper, partitioned coupling is of interest. To harbor the flexibility over each process separable in the numerical scheme of the compartment approach, object-oriented programming was our choice for code implementation. In particular, the implementation of the multi-process concept ([Kolditz & Bauer 2004](#)) benefits from object orientation as the main steps of the numerical solution procedure for the partial differential equations are independent of the specific problem, i.e. calculation of element contributions, assembly of algebraic equation systems (including treatment of boundary conditions and source terms), solution of the algebraic equation systems and calculation of secondary variables.

This paper is structured as follows. After a brief overview of the governing equations for overland, soil water and groundwater flow used for the compartment approach we expand on the applied numerical solution methods. A comprehensive description of the coupling concept finishes the theoretical part of this paper. Subsequently we present three example applications of the compartment approach: a benchmark test based on the classic experiment by ([Smith & Woolhiser 1971](#)) and two case studies, the Borden site in Canada ([Abdul 1985](#)) and the Beerze–Reusel drainage basin in the Netherlands.

GOVERNING EQUATIONS

In this section we briefly summarise the governing equations of the compartment approach for three-dimensional groundwater flow (first subsection), one-dimensional flow in the unsaturated zone (second subsection) as well as a two-dimensional overland flow (third subsection). Each equation is based on mass conservation and a flux-primary variable relationship resulting in a parabolic

equation that is linear for groundwater and nonlinear for soil and overland flow.

Groundwater flow: Darcy equation

The groundwater flow is described by a three-dimensional fluid mass balance equation with fluxes given by Darcy's law which is restricted to laminar flow (Bear 1988).

Therefore the flow equation is

$$n^{gf} S_0^{gf} \frac{\partial h^{gf}}{\partial t} + \nabla \cdot \mathbf{q}^{gf} = q_s^{gf} \quad (1)$$

where h^{gf} , the hydraulic head, is the primary variable of the groundwater flow equation, n^{gf} is the aquifer porosity, S_0^{gf} is the aquifer storativity which accounts for the porous medium matrix and the fluid compression, ∇ is the three-dimensional nabla operator and q_s^{gf} is a source/-sink term. The groundwater flux \mathbf{q}^{gf} is given according to Darcy's law by

$$\mathbf{q}^{gf} = -\mathbf{K}^{gf} \nabla h^{gf} \quad (2)$$

where \mathbf{K}^{gf} is the aquifer hydraulic conductivity tensor.

Flow in the unsaturated zone: Richards' equation

A series of one-dimensional vertical Richards models are used in order to describe water flow in the unsaturated zone. The Richards model assumes that the air phase pressure is constant and makes use of a generalised form of Darcy's equation used in the groundwater model presented above. It is based on empirical capillary pressure–saturation and relative permeability–saturation functions given by (van Genuchten 1980). Furthermore we assume that the fluid is incompressible and the porous matrix is non-deformable. Therefore the pressure-based Richards equation is

$$n^{sf} \frac{\partial S^{sf}}{\partial t} + \frac{\partial q^{sf}}{\partial z} = q_s^{sf} \quad (3)$$

where n^{sf} is soil porosity, S^{sf} is soil water saturation and q_s^{sf} is a source/sink term. The flux q^{sf} is given by Darcy's law:

$$q^{sf} = -k_{rel}^{sf} \frac{\rho g}{\mu} k^{sf} \left(\frac{\partial h^{sf}}{\partial z} - 1 \right) \quad (4)$$

where h^{sf} , the soil water pressure head, is the primary variable of unsaturated flow, k_{rel}^{sf} denotes relative permeability, k^{sf} the saturated soil permeability, μ the water viscosity, ρ the water density and g the gravitational acceleration. Two material-dependent constitutive relationships for saturation and permeability are required to close the fluid mass balance equation. The van Genuchten functional relationships $h^{sf}(S^{sf})$ and $k_{rel}^{sf}(S^{sf})$ are used neglecting hysteresis. With the effective saturation

$$S_{eff} = \max \left(0, \frac{S^{sf} - S_{res}}{1 - S_{res}} \right) \quad (5)$$

where S_{res} is the residual saturation, the empirical functions for capillary pressure and relative permeability are

$$h_{cap} = -h^{sf} = \frac{1}{\alpha} \left(S_{eff}^{1/m} - 1 \right)^{1-m} \quad (6)$$

$$k_{rel}^{sf}(S^{sf}) = S_{eff}^{1/2} \left[1 - \left(1 - S_{eff}^{1/m} \right)^m \right]^2 \quad (7)$$

where α and m are soil material parameters.

Overland flow: diffusive wave shallow water equation

For the simulation of overland flow a two-dimensional diffusive wave approximation of the Saint-Venant equations is used. The Saint-Venant equations are derived by depth integration of the Reynolds averaged Navier–Stokes equations with the main assumptions of a hydrostatic pressure distribution, small morphology variations and empirical flow resistance distributions (Vreugdenhil 1994; Gerbeau & Perthame 2001). These equations are hyperbolic and capable of handling extreme conditions such as dam breaks (LeVeque 2002). The diffusive wave approximation of the Saint-Venant equations is parabolic and is derived by neglecting the inertial terms such that they are restricted to subcritical flow conditions (Beinhorn 2005). For runoff simulations they have proven their reliability (VanderKwaak 1999). Criteria for the applicability of this equation as well as the kinematic wave equation are given in Ponce *et al.* (1977) and Singh (1994).

The diffusive wave shallow water equation is given by

$$\frac{\partial h^{of}}{\partial t} + \nabla \cdot \mathbf{q}^{of} = q_s^{of} \quad (8)$$

where $h^{\text{of}} = H + z$, the hydraulic head, is the primary variable of surface water flow, H is surface water depth, z is the elevation, ∇ is the two-dimensional nabla operator and q_s^{of} is a source/sink term for surface water. The use of Manning's resistance to flow distribution, as well as neglecting the inertia terms in the Saint-Venant equations, gives the flux \mathbf{q}^{of} :

$$\mathbf{q}^{\text{of}} = -k_{\text{rel}}^{\text{of}} K^{\text{of}} \nabla h^{\text{of}}. \quad (9)$$

The conductivity terms $k_{\text{rel}}^{\text{of}}$ and K^{of} are given by

$$k_{\text{rel}}^{\text{of}} = H^{5/3} \quad (10)$$

$$K^{\text{of}} = \frac{1}{n^{\text{of}} S_s^{1/2}} \quad (11)$$

where n^{of} is the Manning coefficient and S_s is the friction slope coefficient given by

$$S_s = \left[\left(\frac{\partial h^{\text{of}}}{\partial x} \right)^2 + \left(\frac{\partial h^{\text{of}}}{\partial v} \right)^2 \right]^{1/2}. \quad (12)$$

Nonlinear diffusion equation

The previously introduced governing equations for groundwater, soil and overland flow belong to the general class of (nonlinear) diffusion type partial differential equations which can be written as

$$A(u) \frac{\partial u}{\partial t} - \nabla \cdot B(u) \nabla u = Q(u) \quad (13)$$

where U is the unknown field function (primary variable), A is a capacitance matrix (representing time dependences), B is a conductivity matrix (representing space dependences) and Q is a source/sink term. In general A , B and Q are dependent on the unknown field function U which results in nonlinearities. The object-oriented numerical solution of different types of partial differential equations is described in (Wang & Kolditz 2007).

NUMERICAL METHODS

A variety of finite difference, finite element and finite volume methods are available to solve the partial

differential equations appearing in hydrosystems (Weiyan 1992; Vreugdenhil 1994; LeVeque 2002; Starke 2005). In general, either of these methods leads to a (nonlinear) algebraic system of equations. In order to resolve nonlinearities in the governing equations, Picard and Newton–Raphson iteration schemes are used. For a comparison of both see, for instance, Paniconi *et al.* (1991). For the demonstration examples (see Examples) we use finite element methods, more specifically the Galerkin and the control volume finite element method with Picard and Newton–Raphson iteration, respectively, to solve the governing equations of the form (13) as these are well suited for problems with complex geometries. For time discretisation a weighting parameter enables the choice between fully explicit and implicit Euler stepping schemes. Usually time stepping for parabolic equations is chosen in accordance with the Neumann criterion (36).

Finite element method

The finite element method is based on the weak formulation of a partial differential equation, which allows the search for generalised solutions in Sobolev spaces. These contain discontinuous solutions and allow the assignment of discontinuous functions for material properties. The model domain is subdivided into small subdomains, the finite elements. The division can be performed according to geological structures, hydrological structures or other requirements. Calculations for these finite elements are performed after a transformation to a basis element. On each element the solution is locally approximated with piecewise polynomial functions forming the basis of an approximated solution space. The equation system for the solution of the unknown field function u is assembled from all element contributions.

Galerkin finite element method

The standard Galerkin finite element method is used for the subsurface compartments (soil and groundwater) because of the slow water movement. In order to obtain the weak formulation of the general diffusion equation, the expression (13) is multiplied by test functions v and

integrated over the domain Ω , giving

$$\int_{\Omega} v \left(A \frac{\partial u}{\partial t} - \nabla \cdot B \nabla u \right) d\Omega = \int_{\Omega} v Q d\Omega. \quad (14)$$

Applying Green's formula gives

$$\begin{aligned} & \int_{\Omega} v A \frac{\partial u}{\partial t} d\Omega + \int_{\Omega} \nabla v \cdot B \nabla u d\Omega \\ &= \int_{\Gamma} v (B \nabla u) \cdot \mathbf{n} d\Gamma + \int_{\Omega} v Q d\Omega \end{aligned} \quad (15)$$

where $\Gamma = \partial\Omega$ is the domain boundary. These equations are valid for all test functions v in the Sobolev space $H^1(\Omega)$. In the Galerkin and the control volume finite element method (see the next subsection) the unknown field functions U as well as test functions v belong to the same Sobolev space. For the numerical solution u is replaced by a finite-dimensional subspace spanned by polynomial basis functions. This is

$$u(t, x, y, z) \approx \hat{u}(t, x, y, z) = \sum_{j=1}^{ng} \phi_j(x, y, z) u_j(t) = \sum_{j=1}^{ng} \phi_j u_j \quad (16)$$

$$v(t, x, y, z) \approx \hat{v}(t, x, y, z) = \sum_{i=1}^{ng} \phi_i(x, y, z) v_i(t) = \sum_{i=1}^{ng} \phi_i v_i \quad (17)$$

where \hat{u} and \hat{v} are the approximate solutions, ϕ_i are the basis functions and ng the dimension of the subspace which is equal to the number of grid nodes in the finite element discretisation.

Therefore, Equation (15) is transformed into an algebraic equation system

$$\begin{aligned} & \sum_{j=1}^{ng} \left(\left[\int_{\Omega} \phi_i A \phi_j d\Omega \right] \frac{du_j}{dt} + \left[\int_{\Omega} \nabla \phi_i \cdot B \nabla \phi_j d\Omega \right] u_j \right) \\ &= \int_{\partial\Omega} \phi_i (B \nabla u) \cdot \mathbf{n} d\Gamma + \int_{\Omega} \phi_i Q d\Omega \quad i = 1, \dots, ng. \end{aligned} \quad (18)$$

The basis functions are subdivided into local basis functions for each element e with the domain Ω^e giving

$$\begin{aligned} & \sum_{s=1}^{ne} \left(\left[\int_{\Omega^e} \phi_r A \phi_s d\Omega \right] \frac{du_s}{dt} + \left[\int_{\Omega^e} \nabla \phi_r \cdot B \nabla \phi_s d\Omega \right] u_s \right) \\ &= \int_{\partial\Omega^e} \phi_r (B \nabla u) \cdot \mathbf{n} d\Gamma + \int_{\Omega^e} \phi_r Q d\Omega \quad r = 1, \dots, ne \end{aligned} \quad (19)$$

where ne is the number of element nodes. Equation (19) can be written as

$$\sum_{s=1}^{ne} \left(A_{rs}^e \frac{du_s}{dt} + B_{rs}^e u_s \right) = g_r^e + s_r^e + r_r^e \quad r = 1, \dots, ne \quad (20)$$

where A_{rs}^e is the capacitance matrix, B_{rs}^e is the conductance matrix, g_r^e accounts for the gravity term, s_r^e for the source terms and r_r^e for the boundary fluxes. The integrals are calculated with the Gaussian integration scheme, yielding for the capacitance matrix entries

$$\begin{aligned} A_{rs}^e &= \int_{\Omega^e} \phi_r A \phi_s d\Omega = \int_{\hat{\Omega}^e} \hat{\phi}_r \hat{A} \hat{\phi}_s \det \mathbf{J} d\hat{\Omega} \\ &= \sum_{k=1}^{gp} W_k(\hat{x}_k) \hat{\phi}_r(\hat{x}_k) \hat{A}(\hat{x}_k) \hat{\phi}_s(\hat{x}_k) \det \mathbf{J}(\hat{x}_k) \end{aligned} \quad (21)$$

with the Jacobian matrix \mathbf{J} of the coordinate transformation from the basis element domain $\hat{\Omega}$ to the element domain $\hat{\Omega}^e$ and the Gauss weights W_k . Entries of the capacitance matrix as well as of gravity, source and boundary flux vector are calculated accordingly. Applying an Euler finite difference scheme to Equation (20) for the approximation of the time derivative yields

$$\begin{aligned} & \sum_{s=1}^{ne} \left(\frac{A_{rs}^e}{\Delta t} + \theta B_{rs}^e \right) u_s^{n+1} = g_r^e + s_r^e + r_r^e \\ &+ \sum_{s=1}^{ne} \left(\frac{A_{rs}^e}{\Delta t} - (1 - \theta) B_{rs}^e \right) u_s^n \quad r = 1, \dots, ne \end{aligned} \quad (22)$$

where θ is an implicit-explicit weighting parameter. Frequently mass lumping schemes are employed in order to stabilise the numerical method. Defining

$$M_r^e = \int_{\Omega^e} A \phi_r d\Omega \quad (23)$$

the mass matrix lumped form of Equation (20) is

$$M_r^e \frac{du_r}{dt} + \sum_{s=1}^{ne} B_{rs}^e u_s = g_r^e + s_r^e + r_r^e \quad r = 1, \dots, ne \quad (24)$$

After the derivation of a general finite element scheme for the nonlinear diffusion Equation (13), the resulting finite element matrices are specified for the corresponding flow processes.

Control volume finite element method for overland flow

The traditional finite element methods such as the Galerkin and Petrov–Galerkin schemes tend to show non-physical oscillations for overland flow simulations (Giamarco *et al.* 1996; Beinhorn 2005). On the other hand, finite volume methods have shown how to handle these difficulties (LeVeque 2002). Giamarco *et al.* (1996) suggested the control volume finite element method which effectively combines the finite element with the finite volume method. It avoids oscillations by mass matrix lumping as well as conductivity term upwinding (Forsyth & Kropinski 1997) and guarantees local mass conservation. Using Lagrange polynomial basis functions ϕ_r where $\sum \phi_r = 1$, for the numerical approximation of the solution u and for the test function v , we have

$$\nabla \sum_{s=1}^{ne} u_s \phi_s = \nabla \sum_{s \neq r} \phi_s (u_s - u_r). \quad (25)$$

This allows us to express the diffusion term in Equation (19) as a function of the primary variable difference between node r and its neighbours. Using this scheme, the lumped mass matrix Equation (24) becomes

$$V_r^e \frac{du_r}{dt} + \sum_{s \neq r} B_{rs}^e (u_s - u_r) = s_r^e + r_r^e \quad r = 1, \dots, ne \quad (26)$$

where

$$V_r^e = \int_{\Omega^e} \phi_r d\Omega. \quad (27)$$

The conductance term can be written as $B = k_{\text{rel}} \mathbf{K}$, where $k_{\text{rel}}(u)$, \mathbf{K} represent primary variable dependent and independent parts, respectively. They are given for overland flow by Equations (10) and (11), respectively. Therefore, Equation (26) becomes

$$V_r^e \frac{du_r}{dt} = \sum_{s \neq r} \lambda_{rs+1/2} \gamma_{rs}^e (u_s - u_r) + s_r^e + r_r^e \quad r = 1, \dots, ne \quad (28)$$

where

$$\begin{aligned} \gamma_{rs}^e &= \int_{\Omega^e} \nabla \phi_r \mathbf{K} \nabla \phi_s d\Omega = \int_{\Omega^e} \hat{\nabla} \hat{\phi}_r \hat{\mathbf{K}} \hat{\phi}_s \det \mathbf{J} d\hat{\Omega} \\ &= \sum_{k=1}^{\text{gp}} W_k(\hat{x}_k) \hat{\nabla} \hat{\phi}_r(\hat{x}_k) \hat{\mathbf{K}}(\hat{x}_k) \hat{\nabla} \hat{\phi}_s(\hat{x}_k) \det \mathbf{J}(\hat{x}_k) \end{aligned} \quad (29)$$

and upwinding is implemented by

$$\lambda_{rs+1/2} = \begin{cases} k_{\text{rel}s}; & \text{if } \gamma_{rs}(u_s - u_r) > 0 \\ k_{\text{rel}r}; & \text{if } \gamma_{rs}(u_s - u_r) < 0 \end{cases} \quad (30)$$

such that k_{rel} represents a weighted conductivity. The right-hand-side terms s_r^e, r_r^e are coupling terms to the soil compartment. The Euler time stepping scheme gives

$$\begin{aligned} \frac{V_r^e}{\Delta t} u_r^{n+1} + \theta \sum_{s \neq r} \lambda_{rs+1/2}^{n+1/2} \gamma_{rs}^e (u_s^{n+1} - u_r^{n+1}) \\ = s_r^e + r_r^e - \frac{V_r^e}{\Delta t} u_s^n - (1 - \theta) \sum_{s \neq r} \lambda_{rs+1/2}^n \gamma_{rs}^e (u_s^n - u_r^n) \end{aligned} \quad (31)$$

$$r = 1, \dots, ne$$

with the implicit-explicit weighting parameter θ . For linearisation a Newton–Raphson scheme is applied. The Jacobian matrix in this iteration is approximated by a numerical derivative, which provides an effective matrix assembly method (Forsyth *et al.* 1995).

Object orientation

Object-oriented programming regards a software programme as a collection of objects and their defined interactions. Hereby, objects are instances of (abstractly) defined classes that contain both data (also called properties) and functions (also called methods) to manipulate this data. Thus the so-called encapsulation is achieved, as an object's (protected) properties can only be accessed by its own methods. Defined interaction between objects (also of objects belonging to different classes) is achieved by one object calling the other object's methods and vice versa. Another fundamental concept is inheritance, where new classes may be defined by inheriting properties and methods from already existing classes. If properly designed, these concepts achieve two of the big advantages of object

orientation: easy extendability of the software's functionality and code reuse.

In the scientific software environment GeoSys/RockFlow a central unit is the top-level process class (PCS). All numerical processes described above are instances of this base class. Each PCS object contains its relevant PDE solution procedure objects: FEM (for finite element method), TIM (for time discretisation), EQS (equation system including solver) as well as process-related material properties (MAT), boundary condition (BC), initial condition (IC) and source term objects (ST) (Kolditz & Bauer 2004) as well as a computational mesh object (MSH). The development and implementation of the MSH class for instantiation of meshes for the different hydrological compartments is the novel part of the GS/RF code development in this work.

Geometries are defined process-independent by geometrical objects such as points, polygons, surfaces and volumes (GEO). These can be used for a computationally efficient visualisation of overall geometries as well as for initialisation of MSH objects, e.g. for the initial definition of the individual compartments. However, depending on the flow process and/or the coupling of processes the MSH object itself is allowed to adapt in accordance with the temporal and/or spatial evolution of the process(es). Thereby, (adjacent) MSH objects of coupled processes are required to be topologically consistent at their mutual interface. The latter means that each coupling boundary element of a MSH object always has a defined neighbouring element belonging to a coupled MSH object. Based on these topological mesh relations the assignment of correct coupling fluxes is facilitated.

COUPLING CONCEPT

In general, two concepts exist for equation coupling: monolithic schemes for strongly coupled systems (e.g. Wang & Kolditz 2007) and partitioned (or staggered) techniques for weakly connected systems. If we focus on hydrological systems, distinct and separate compartments such as surface, soil (vadose zone) and aquifers can be recognised. In fact, compartment interactions take place only at their combined interfaces, such as the ground

surface, capillary fringe and water table. Moreover, the time and space scales of hydraulic processes in different compartments typically differ substantially. Time scales of flow processes can easily range from seconds (e.g. overland flow) to years (e.g. flow in low-permeability aquitards). Therefore, we have adopted a partitioned coupling scheme for hydrosystems modelling. For the surface/soil/groundwater hydrosystem the equation system becomes

$$\begin{aligned} [P^{\text{of}}][u^{\text{of}}] &= [r^{\text{of}} + r^{\text{of/sf}}] \\ [P^{\text{sf}}][u^{\text{sf}}] &= [r^{\text{sf}} + r^{\text{sf/of}} + r^{\text{sf/gf}}] \\ [P^{\text{gf}}][u^{\text{gf}}] &= [r^{\text{gf}} + r^{\text{gf/sf}}] \end{aligned} \quad (32)$$

where P^* , u^* , r^* are system matrix, solution vector and RHS vector for overland, soil and groundwater flow, respectively, the exponents of, sf, gf indicate overland flow, soil and groundwater flow, respectively, and $r^{\text{of/sf}}$, $r^{\text{sf/of}}$, $r^{\text{sf/gf}}$ denote compartment exchange terms. In the partitioned scheme the computation of the individual processes can be conducted at completely different temporal and spatial discretisations using different numerical methods. The computational advantage is that the numerical schemes for each process can be optimised despite the differences in their corresponding physical scales.

Flux coupling

The coupling concept is based on first-order flux exchange relationships at the compartment interfaces (Figure 2). Depending on hydrological/hydrogeological considerations, each compartment may be subdivided into sub-domains ($A_i^{\text{of}}, A_j^{\text{sf}}, A_k^{\text{gf}}$). An important requirement for flux

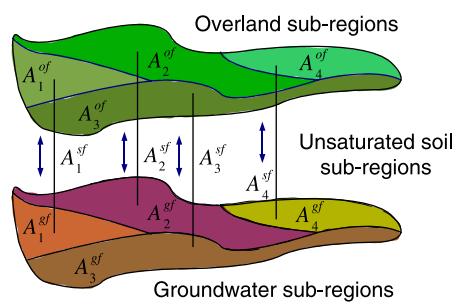


Figure 2 | Flux-oriented coupling approach. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

coupling is topological consistency, specifically, the interface area between coupled compartments has to be the same for both.

If we consider the coupling between overland flow and unsaturated flow in soils, the vertical fluxes of the former are collected and passed to the latter process within hydraulically relevant time periods. This means integrating fluxes on certain compartment elements over proper time intervals, yielding source terms. The overland and soil process coupling is

$$Q_i^{\text{of}} \Delta t = -Q_i^{\text{sf}} \Delta t = \int_{\Delta t^{\text{sf}}} \int_{A_i^{\text{sf}}} q^{\text{of/sf}} \times (\Lambda^{\text{of/sf}}(x, y, t), u^{\text{of}}(x, y, t), u^{\text{sf}}(x, y, t)) d\Omega dt \quad (33)$$

where the exchange flux $q^{\text{of/sf}}$ depends on both an exchange coefficient $\Lambda^{\text{of/sf}}$ and the hydraulic heads of both processes. For first-order coupling it is

$$q^{\text{of/sf}} = \Lambda^{\text{of/sf}}(u^{\text{sf}} - u^{\text{of}}). \quad (34)$$

As an example we provide the coupling equation for the surface and soil compartments which is based on an interface layer concept (Delfs et al. 2007, 2008). The interface layer allows the definition of a discrete exchange flux to couple the flow processes in both compartments mutually. The description of the interface flux is motivated by a Darcy approach (VanderKwaak 1999):

$$q^{\text{of/sf}} = -k_r^c K^c \frac{h^{\text{of}} - h^{\text{sf}}}{a} \quad (35)$$

where $k_r^c \in [0, 1]$ is a infiltration capacity, K^c is the interface layer conductivity and a is the interface layer thickness. The infiltration capacity is given by $k_r^c = \min((\theta^{\text{sf}})^{2(1-S)}, 1)$, where $\theta = h^{\text{of}}/a$.

Technically, during the source/sink term calculations, node and element contributions from corresponding areas (e.g. A_1^{of} for A_1^{sf}) are exchanged. The same technique is used for the soil/groundwater interface.

Time stepping synchronisation

Besides spatial discretisation, time stepping schemes need to meet process-specific requirements. This is critical for

numerical stability as each individual flow process may require completely different time steps. This is underlined by the Neumann criteria for maximum time steps in diffusion type partial differential Equations (13):

$$\Delta t = \frac{1}{2} \frac{\Delta l^2}{D} \quad (36)$$

where Δl is a characteristic length scale of the spatial discretisation and D is a process-related diffusivity coefficient.

The time stepping for all processes was synchronised in order to calculate exchange terms according to Equation (33). Table 1 illustrates the implementation of the synchronisation scheme between the different processes. In the Borden site demonstration example (see Rainfall-runoff experiment) we use fully implicit time stepping with the following intervals: $\Delta t = 10^2$ s for overland flow, $\Delta t \sim 10^3$ s (adaptive) for soil flow and $\Delta t = 10^4$ s for groundwater flow.

Ultimately, the above illustrates the central feature of the compartment approach: each individual flow and transport process can have its own discretisation in space and in time (Figure 1).

EXAMPLES

In this section three examples are provided in order to verify the compartment approach and to demonstrate the applicability of this concept to field data.

The verification of the present numerical code for the individual processes is given, for example, in Kolditz et al. (1998) and Beinhorn (2005). Despite abundant test cases for flow in saturated and unsaturated porous media (e.g. Segol

Table 1 | Coupling scheme for time discretisation

Δt	Overland (OF)	Soil (SF)	Groundwater (GF)	Coupling
1	Δt_1^{of}			
⋮	⋮			
<i>i</i>	Δt_i^{of}	Δt_1^{sf}		OF/SF
⋮	⋮	⋮		
<i>j</i>	Δt_j^{of}	Δt_k^{sf}	Δt_1^{gf}	OF/SF/GF
⋮	⋮	⋮	⋮	

1993) or overland flow (e.g. van Rijn 1986) only a few examples are available for testing numerical models for coupled surface–subsurface systems. In order to prove the correct coupling between overland and soil water flow, the Smith & Woolhiser (1971) problem is considered (see the next subsection). In this laboratory experiment the soil conditions were found to dominate the coupled hydrosystem behaviour. In addition, an example in the Borden aquifer with the focus on coupling of the overland, soil and groundwater processes across temporal and spatial scales is demonstrated (see Rainfall–runoff experiment). Finally, through a field application to the Beerze–Reusel catchment in the Meuse river basin (see Beerze–Reusel drainage basin), a high resolution of the infiltration dynamics could be achieved with the compartment approach.

Smith & Woolhiser laboratory experiment

A well-known problem in process coupling is that, even if numerical models for the individual processes are implemented correctly, their combination can fail if the coupling scheme is not appropriate. Therefore, the compartment approach was tested against experimental data. Delfs *et al.* (2007) provided a detailed analysis of the classic experiment by Smith & Woolhiser (1971) on infiltration excess (Hortonian) overland flow. The Smith & Woolhiser problem is one of the few experimental datasets available for the analysis of coupled surface/subsurface flow systems and was used for a code intercomparison study (Figure 3).

The study by Delfs *et al.* (2007) was focused on (i) a comparison of different conceptual models and (ii) a parameter sensitivity study. Therein, different conceptual approaches were compared for overland flow (i.e. Saint-Venant vs kinematic and diffusive wave approximations), soil water movement (Richards vs Green–Ampt models) and, in particular, their coupling. It could be shown that a flux-based coupling concept using an interface layer reproduces the experimental results appropriately. Moreover, further reduction in model complexity was achieved as the Green–Ampt model could successfully reproduce water flow in the unsaturated zone. As an example Figure 3 shows a comparison of computed hydrographs for the overland flow of the GS/RF code and those obtained from several studies on the Smith & Woolhiser experiment.

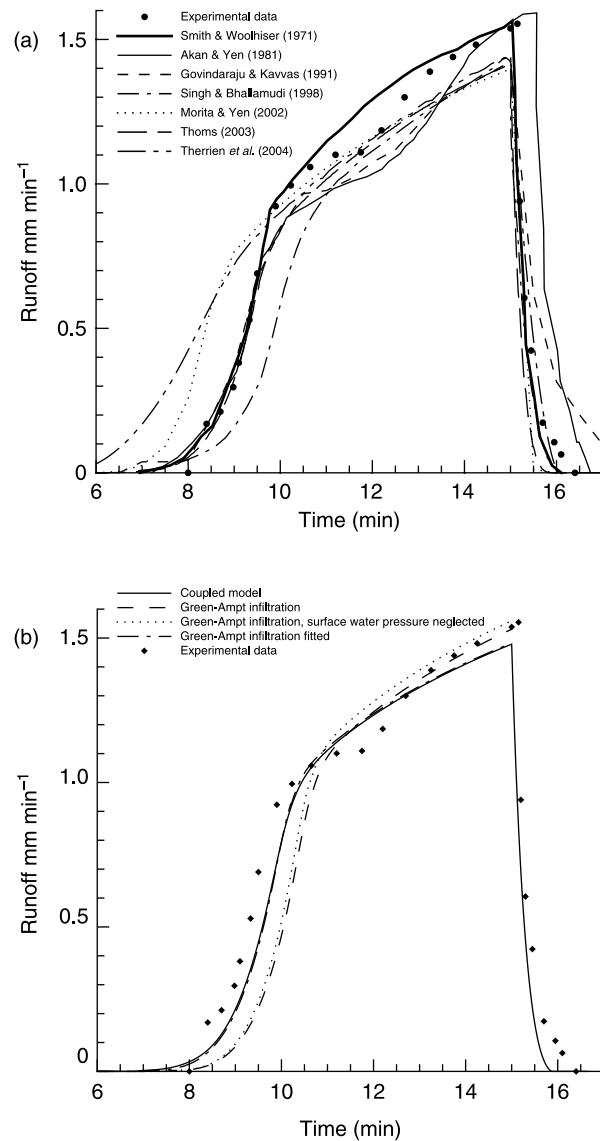


Figure 3 | Hydrograph results for the Smith & Woolhiser problem. Left: existing studies, right: GS/RF present results (interface layer/compartment approach).

Rainfall–runoff experiment at the Borden aquifer

The second example is based on a field-scale rainfall–runoff experiment at the Canadian Forces Base, Borden, Ontario. The experimental set-up and evaluation are described in Abdul (1985) and Abdul & Gilham (1989). A comprehensive documentation of site details, flow characteristics and results can be found in VanderKwaak (1999) and Hydro-sphere (2004). In order to apply the presented compartment approach for the coupling of overland, soil water and

groundwater flow, we modified the description of the subsurface zone. We introduced two separate compartments, one for an unsaturated and one for a groundwater domain of two and ten meters thickness, respectively.

Figure 4 shows the elevation of the land surface with the stream bed in the middle. It consists of a man-made channel surrounded by grass-covered land and has a depth of approximately 1.2 m. Prior to the beginning of the experiment the channel is dry. Then uniform artificial recharge is applied at a rate of 0.02 m h^{-1} over the entire area for 50 min. The rainfall intensity is the same over the entire area. The total experiment lasts 24 h. The following hydrologic processes were recognised to govern the field experiment (Abdul 1985; Abdul & Gilham 1989): water infiltration in upland region, discharge into lower areas and surface runoff.

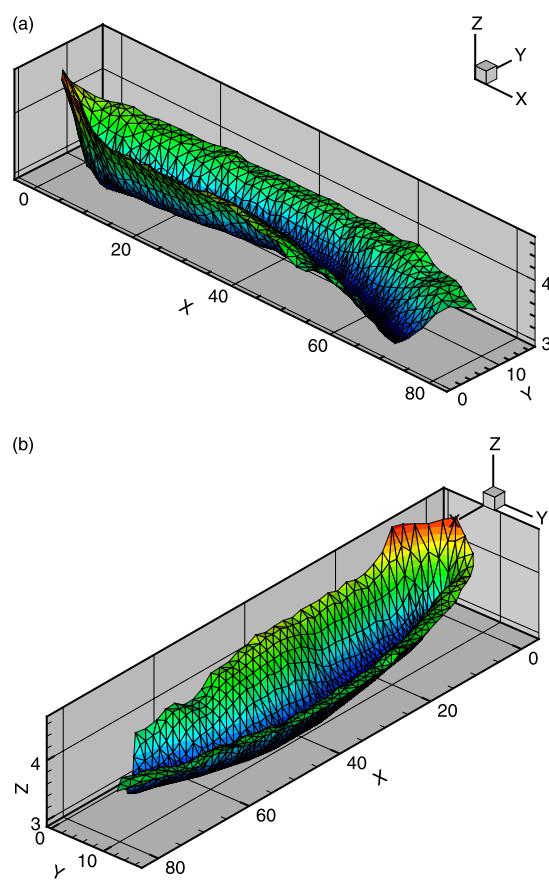


Figure 4 | Channel geometry of the field-scale rainfall–runoff experiment. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

The parameter values for overland, Richards, and Darcy flows in this model set-up are provided in Table 2.

Figure 5 depicts the discretisation of the multi-mesh system for the Borden study. Three topologically coupled meshes are used for the surface, soil and groundwater compartments. The multi-mesh system consists of the following numbers and types of elements: 2,651 triangles for the surface, 106,040 line elements for the soil and 26,510 prisms for the aquifer. Each soil column has 40 line elements and the groundwater compartment is split into 10 element layers. The governing equations are solved fully implicitly with fixed time steps of $\Delta t = 10^2 \text{ s}$ and $\Delta t = 10^4 \text{ s}$ for overland flow and groundwater flow, respectively. For soil water flow a self-adaptive time stepping is applied, resulting in time steps of the order of $\Delta t = 10^3 \text{ s}$.

The results of the coupled flow modelling are depicted in Figures 6–8. The surface water level within the stream channel is shown in Figure 6 for the first hour. The water level rise is a result of the uniform recharge applied during the first 50 min. The water flows rapidly into the topographically lowest part of the channel in the middle of the domain and follows its course to the outlet at $x = 80 \text{ m}$ (lower domain boundary). After precipitation has stopped, the water level in the channel commences to decline.

Figure 7 illustrates the infiltration process resulting from overland flow. The water saturation is shown for different times at a soil depth of 1 m. With increasing simulation time the water saturation keeps increasing – even after the artificial recharge was stopped. An overland/soil coupling flux is used which depends solely on the hydrostatic surface water

Table 2 | Properties of the coupled hydrosystem

Parameter	Symbol	Value	Unit
Manning coefficient	n^{of}	0.15	$\text{s m}^{-1/3}$
Soil porosity	n^{sf}	0.37	–
Soil permeability	k^{sf}	$2.95 \times 10^{-13} \text{ m}^2$	
Residual saturation	S_{res}	0	–
van Genuchten parameter	α	1.43	m^{-1}
van Genuchten parameter	M	0.336	–
Aquifer porosity	n^{gf}	0.33	–
Aquifer storage coefficient	S_0^{gf}	$1.2 \times 10^{-7} \text{ m}^{-1}$	
Aquifer hydraulic conductivity	K^{gf}	10^{-5} m s^{-1}	

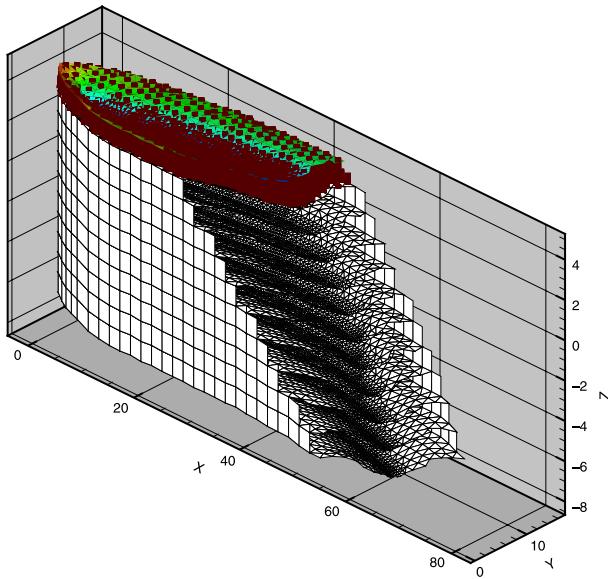


Figure 5 | MultiMSH discretisation of the test catchment consisting of triangle elements for overland flow, line elements for soil water movement, and prism elements for groundwater flow. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

pressure, leading to a large contrast in overland and soil velocities and spatially distinctive head profiles. As the surface water depth drives the infiltration rate, the largest increase in water saturation is found in the middle of the channel.

The hydraulic head distribution in the groundwater compartment is shown in Figure 8. Due to the buffering effect of the increasing soil moisture content, no significant hydraulic reaction of the aquifer is observed at the beginning of the rainfall event. After 12 h the infiltrated rainfall water reaches the aquifer top and causes a local increase in hydraulic head along the channel bottom. This leads to a small deformation of the flow pattern, resulting in some lateral flow towards the left and right domain boundaries. This effect slowly decreases as less water reaches the groundwater table at the end of the simulation time period. These results are in good qualitative agreement with the expected system response. This example demonstrates the ability of the compartment approach to couple surface and subsurface processes across distinct temporal and spatial scales.

Beerze–Reuzel drainage basin

In this subsection we present a real-world application of the compartment approach. The study region is located in

the Province of North Brabant in the southern half of the Netherlands. The size of the Beerze–Reuzel drainage basin is about 440 km² large (Figure 9 (left)). The subsoil mainly consists of sandy deposits formed in the Pleistocene. The generally flat region gently slopes in a north to northeast direction. There are several aeolian sand ridges up to a few metres in height that are oriented in a west to east direction. In the valleys alluvial soils have been formed consisting of redeposited sand, loam and peat. Because of the intensive agricultural drainage of the areas these peaty soils are strongly oxidized and have often become very shallow. Agriculture is the dominant land use in the region – grassland and maize being the most frequently used crops. Hence, the movement of soil moisture appears very important to assess the nitrate transport into the groundwater system.

The objective of the case study is, at first, to develop a hydrologic soil model for the Beerze–Reuzel drainage basin at a regional size in order to evaluate the nitrate cycle at the catchment scale later on.

A comprehensive soil database was made available from the Geological Survey of the Netherlands for this study. The database represents the result of a soil classification survey where more than 12,000 influence areas were identified that represent the lateral extent of distinct soil profiles (van der Grift *et al.* 2006). These influence areas are outlined by polygons as shown in Figure 9 (right). The more densely arranged polygons follow the river sediments indicate the flow network of the Beerze–Reuzel catchment. For each of these influence areas the vertical stratification of soil types, as well as the corresponding hydraulic (van Genuchten) parameter, is given. Based on this unique dataset the concept of a regional hydrological soil model (RHSM) for the entire drainage basin (440 km²) was developed. It allows us to keep a high vertical resolution (here 5 cm) of the soil compartment for the solution of the Richards' equation over a large lateral extent. The time step was made adaptive for numerical reasons. The high resolution of the soil compartment is indispensable in order to represent the unsaturated flow through the heterogeneous soil properly by a numerical Richards' model.

Figure 10 (right) shows calculated moisture profiles for an example influence area. Figure 10 (left) illustrates the regional moisture pattern which is assembled from all influence areas. As within the modelled time span the

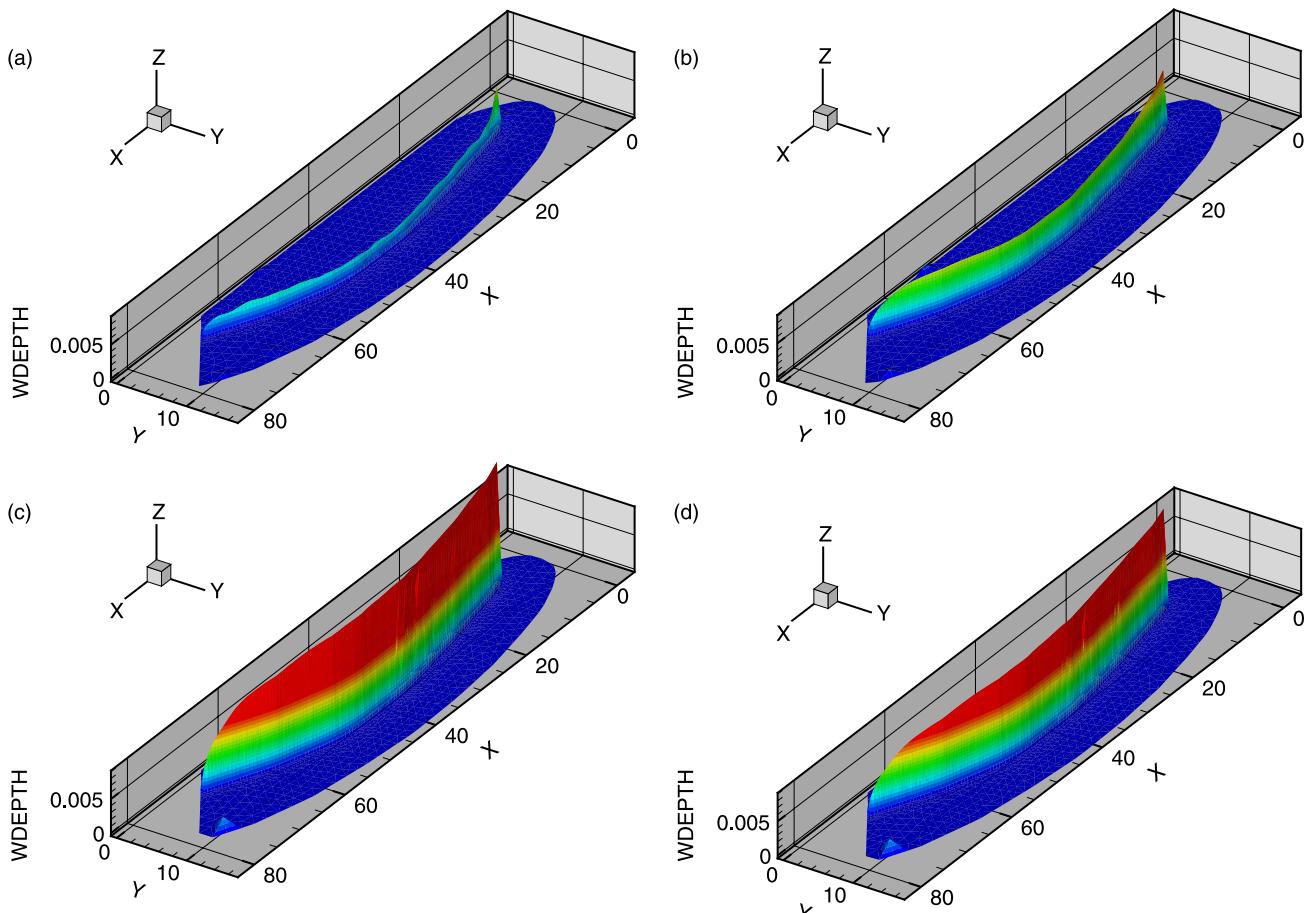


Figure 6 | Water depth in the channel after 10, 20, 50 min and 1 h ((a)–(d)), respectively. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

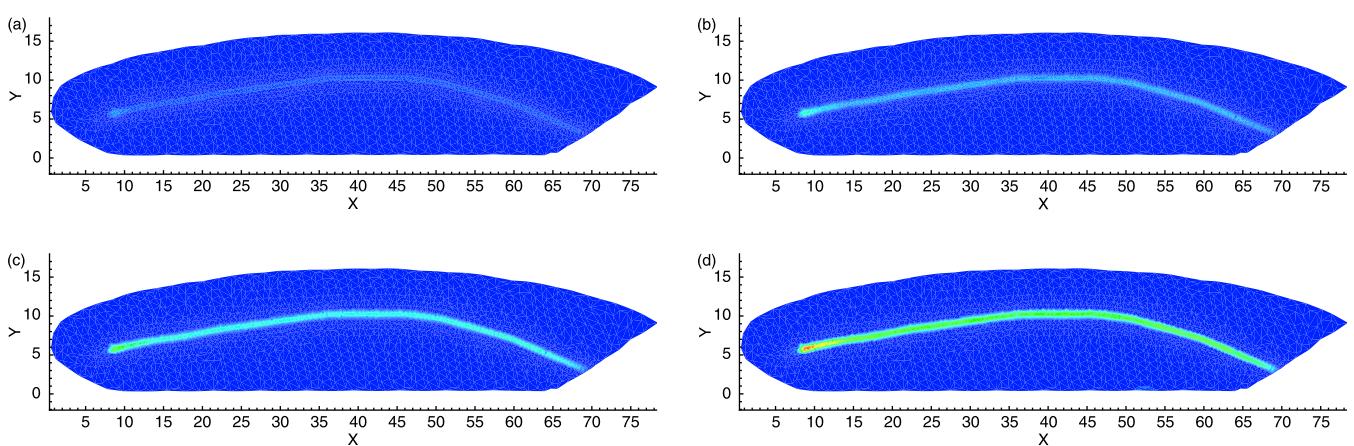


Figure 7 | Water saturation in the soil compartment at 1, 3, 6 and 12 h ((a)–(d)), respectively. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

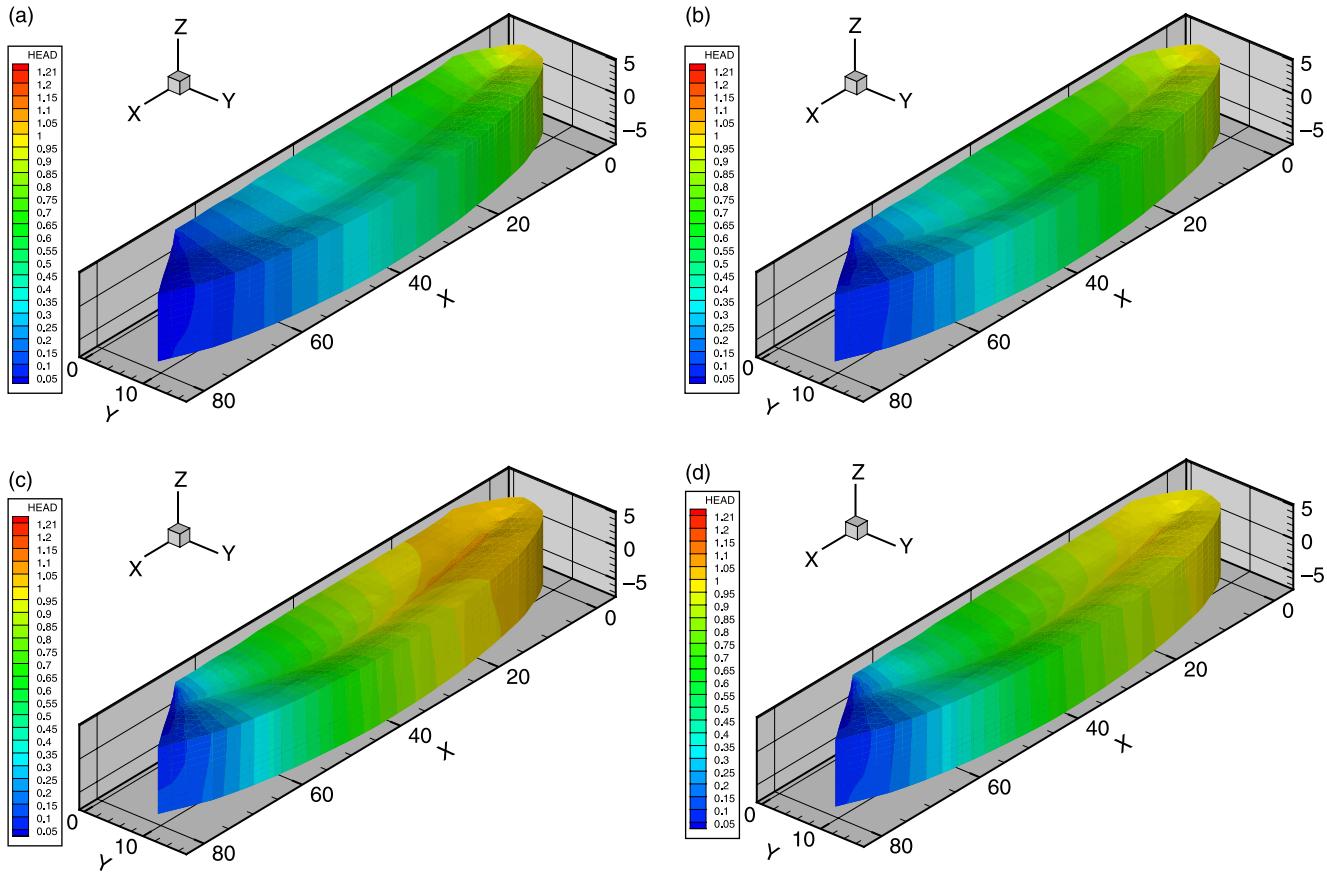


Figure 8 | Hydraulic head in the groundwater compartment at 1, 3, 12 and 24 h ((a)–(d)), respectively. The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

precipitation–evaporation conditions were rather homogeneous in the region, the pronounced differential moisture propagation is interpreted as being primarily due to the local variation of hydraulic soil properties. The regional groundwater recharge distribution is calculated from the soil water Darcy velocities multiplied by the corresponding influence area of each soil profile. More details including software development, data import and conversion tools are described in Kolditz *et al.* (2007).

Due to the still enormous number of finite elements for the RHSMS of the Beerze–Reusel drainage basin, computation times are very expensive (about one month CPU time for a one-year simulation). Therefore, RHSMS parallelisation became necessary for computation of this type of real-world applications.

CONCLUSIONS AND FUTURE WORK

In this paper we presented a compartment approach for the numerical simulation of coupled processes in hydrosystems comprising of overland, unsaturated and groundwater flows. We demonstrated the applicability and limitations of this approach in three example studies spanning from laboratory to catchment scale:

- The classic laboratory experiment by Smith & Woolhiser (1971) on infiltration excess (Hortonian) overland flow (1–10 m scale),
- a (small) field-scale experiment at the Borden site by Abdul & Gilham (1989) (10–100 m scale), and
- a field-scale study on regional infiltration in the Beerze–Reuzel drainage basin (about 440 km² catchment size).

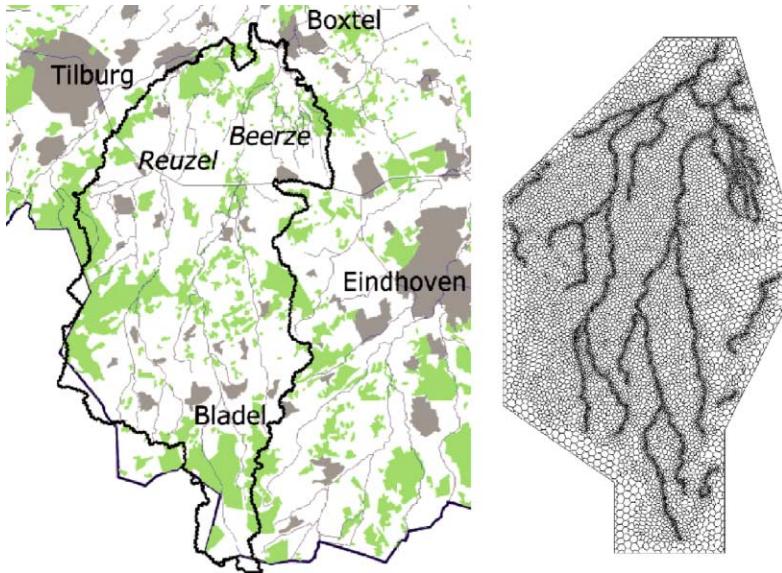


Figure 9 | Beerze–Reusel study area in the Meuse basin (left), identified influence areas for soil type characterization (right). The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

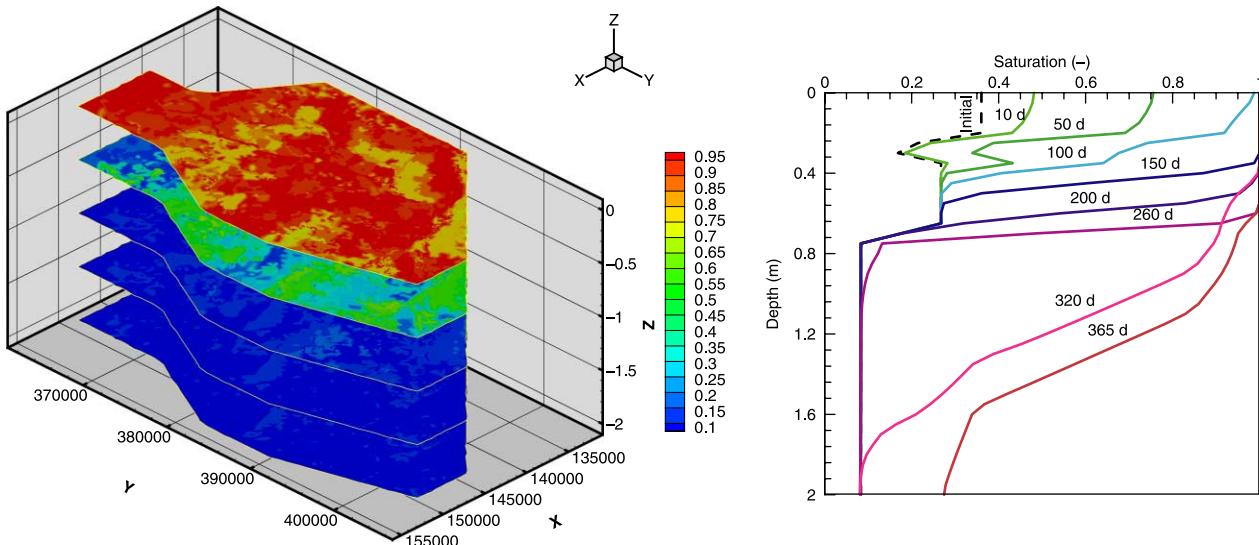


Figure 10 | Snapshot of the regionally heterogeneous moisture distribution (left), evolution of vertical moisture profiles in a selected influence area (right). The colour version of this figure is available in the online version of the paper (<http://www.iwaponline.com/jh/toc.htm>).

The case studies show that the underlying (nonlinear) diffusion-type Equations (13) can be solved efficiently utilising the compartment approach's inherent flexibility for combining different numerical methods (G-FEM and CV-FEM) with accordingly adapted spatial and temporal discretisations. The object-oriented software concept, which was originally developed for hydrogeological problems (Kolditz & Bauer 2004),

can be identified as a key component for this achievement. Based on the earlier work only two basic features had to be developed in a new mesh class to extend the GeoSys/RockFlow (GS/RF) scientific software environment for a hydrological compartment approach: (1) mesh instances are used for distinct compartment discretisations and (2) coupling terms are located based on topological mesh relations.

Using the regional hydrologic soil model (RHSM) concept (see Beerze–Reuzel drainage basin), comparatively thin soil layers can be incorporated into large catchment areas and coupled to overland and groundwater flow. A potential application of the RHSM could be hydrological upscaling analysis, e.g. for the calculation of groundwater recharge from precipitation without losing accuracy due to restrictions on the vertical soil resolution.

Although the presented work shows the flexibility and potential of the compartment approach for numerical analysis of hydrosystems at different scales, future work is needed, for example in the following directions:

- The development of qualified benchmarks for quantitative verification of fully coupled surface/soil/groundwater hydrosystems: a major focus hereby is the evaluation of numerical coupling errors. These are expected to be dominated by the consideration of the influence of the exchange terms on the stability in the numerical scheme, which limits the compartments individuality. The Neumann criterion given by Equation (36) ignores flux terms such that its application as a guideline is restricted in coupled hydrosystem models.
- The evaluation of lateral flow effects in the soil compartment: Using column elements for the RHSM we neglect lateral flows in the soil. This assumption holds for flat ground surface areas and a relatively homogeneous infiltration process. If significant lateral pressure or moisture gradients, even in flat areas, should exist, horizontal flow components in the soil layer have to be considered. This shortcoming can be solved by the use of prism instead of line elements for the soil layer discretisation.

ACKNOWLEDGEMENTS

This work was funded by the European Union FP6 Integrated Project “AquaTerra” (project no. 505428) under the thematic priority “Sustainable development, global change and ecosystems”. We thank the anonymous reviewers for their careful reviews based on which the manuscript was substantially improved. We are grateful to the Tübingen coordination team (J. Barth, E. Frank and P. Grathwohl) for saving us lots of time for research. We

would also like to thank C. Chen, Y. Du, M. Hess, C. McDermott, R. Walsh, W. Wang and M. Xie for commenting on the manuscript.

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First received 20 December 2007; accepted in revised form 14 April 2008