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Coupling spatially distributed river and groundwater transport models to investigate contaminant dynamics at river corridor scales

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ABSTRACT

Rivers and aquifers are mutually dependent components of the hydrological cycle, typically characterised by temporal dynamics that are a few orders of magnitude apart. This characteristic is often advocated to justify the use of independent single-system models to maximise the outcome for the available computational resources. However, the rapid increase in computational power presently provides means to explore new and more complex modelling schemes, which better reflect the complex physical reality. We present a new modelling framework, FLUXOS, developed from the full coupling of modified versions of state-of-the-art standalone river and groundwater flow and transport models. The model is validated against analytical solutions and applied to real world scenarios in the complex urban corridor of the Ciliwung River in Jakarta to show its flexibility for practical applications and its capabilities as an exploratory tool for realistic investigation of contamination sources and pathways determining non-linear behaviours of river-aquifer interactions.

Software availability

Program name: FLUXOS
Developer: Diogo Costa
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Year first available: 2016
Program language: Fortan 90 and Fortran 77
Software requirements: MS Windows, libifcoremdd.dll, libiomp5md.dll, libmmd.dll and msvcr100d.dll
Software development: MS Visual Studio 2010, Intel(R) Visual Fortran Composer XE 2011, or above, and Intel(R) Fortran Compiler XE 12.0
Software availability: contact the authors
Web page: http://www.fcl.ethz.ch

1. Introduction

Half of the world's population lives in cities and the number is still rising. Particularly in developing countries, many urban areas are rapidly sprawling into sizable megacities (Zipperer and Pickett, 2012) without developing adequate sanitary infrastructures. By 2050 the number of people residing inside urban perimeters is expected to reach 70% (Heilig, 2012), turning the conservation of water resources and the protection of human and ecological health from increasingly polluted rivers into a foremost challenge.

Solid waste and widespread water pollution are currently major sources of contamination of many urban rivers (Un-Habitat, 2008). Urban runoffs, which often carry high levels of heavy metals originating from road traffic, are now becoming also increasingly rich in pathogens and organic substances (Zoppou, 2001) because of the imbalance between growth of spontaneous settlements and construction of infrastructures.

Urban pollution is visibly affecting the quality of water in many rivers around the world. Moreover, numerous studies have shown over the years that contamination is reaching the underlying groundwater resources despite the highly impermeable surfaces of urban areas. Cases of contamination of urban groundwater by sewage leakage from damaged sewers and infiltration of polluted

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river waters are commonly found in the literature (e.g., Lerner, 2002).

In many cases, the problem is further aggravated by increased interaction between shallow and deeper aquifers due to excessive pumping, which favours the propagation and/or migration of contamination across different layers in the groundwater system.

Finally, evidences of an increase in the frequency of flooding has been observed in many regions around the globe (Hallegatte et al., 2013) and attributed to different phenomena, thereby including climate change, reduced permeability and increased encroachment of river margins. In some cases, such changes affect the hydraulic regime of rivers, which in turn, significantly reverberates in the river-aquifer dynamics and has been linked to pollution problems (e.g., Wong et al., 2010).

The number of urban areas, where pollution, flooding, excessive pumping and dependency on groundwater emerge as phenomena that induce more complex interaction across water bodies, is continuously rising, thus requiring a more integrated approach to rivers-aquifers systems management.

Accordingly, determining the circumstances which can generate flow and transport dynamics across river and aquifer systems leading to critical pollution states (e.g. Rassam et al., 2008) is extremely important. Unfortunately such processes are yet poorly understood and there is a lack of appropriate modelling tools to address river-aquifer interaction, particularly in urban environments and for cases involving unsteady contaminant exchange. This is best addressed by the joint simulation of flow and transport processes across the river-aquifer boundary (Rassam, 2011), as done by the modelling framework presented in this article.

2. State-of-the-art

It is well known that rivers and groundwater exchange flow and mass at rates that vary over space and time (e.g. Tian et al., 2015; Kalbus et al., 2006). These fluxes depend on the hydraulic and water quality characteristics at the interface (Winter, 1999). These are dynamic and can determine conditions, which lead to exchange patterns that are non-linear (Sophocleous, 2002).

To capture these phenomena, hydrological models coupling surface water (SW) and groundwater (GW) components have emerged with the purpose of investigating the hydrology of river basins thereby including SW-GW systems at catchment scales. Some popular models belonging to this category are MODHMS (Loague et al., 2006), InHM and HydroGeoSphere (Brunner and Simmons, 2012), MIKE-SHE (Refsgaard et al., 1995; Ma et al., 2016) and tRIBS (Ivanov et al., 2004). However, while the target scale of these models (watersheds) allows for the diffusion wave assumption or other simplified overland flow routing methods, for river reach and corridor scale studies such simplifications are unsuitable, especially to simulate phenomena such as flooding and turbulence, and the associated transport processes, which require a greater level of detail.

Models coupling surface unsteady hydrodynamic and groundwater flow solvers started emerging little more than 10 years ago when computers became increasingly faster and more efficient (e.g. Shaad, 2015). Examples of these models are SWIFT2D-SEAWAT (Langevin et al., 2005), MODFLOW-LGR-VSF-newCFL (Borsi et al., 2013), MODFLOW-OWHM (Hanson et al., 2014) and 2dMb-MODFLOW (Ruf, 2007; Shaad, 2015).

However, the full coupling of 2-dimensional surface and 3-dimensional groundwater flow models is still incipient (Furman, 2008), e.g. not many of the models allow for moving boundary problems for flooding and wetland studies, and the further integration of transport and water quality subroutines is largely unexplored (e.g. Zerihun et al., 2005).

A wide range of popular surface and groundwater models, which can generally simulate either river or aquifer dynamics only, are currently available. However they are not suitable for detailed river-aquifer flow and mass flux estimations in complex cases involving transient conditions and/or in irregularly-shaped streambeds due to a number of reasons, namely:

1. Most are single-system models developed to address typical river (e.g., QUAL2E, Brown and Barnwell, 1987) or aquifer (e.g., PHT3D, Prommer et al., 2003) problems. While processes affecting the targeted systems are explicitly modelled, those arising from interactions with the other, non-modelled systems are, if included at all, forced through a set of boundary conditions, the definition of which is in many cases simplified or difficult to link with reality (see Fig. 1).
2. The interaction between river and aquifer in both the channel and the floodplain is a complex and dynamic process. It may occur in both directions, depending on the relative position of the water table and the river water level. Flow and mass exchange between river and aquifer are however often ignored or simplified to uniform or linearly-varying predefined rates (e.g., MT3DMS and MODFLOW; Zheng and Wang, 1999; Harbaugh et al., 2000).
3. Thus, reversing the direction of the fluxes across the interface may occur, in turn causing each system to act alternatively as source or sink (see Fig. 2).

Therefore, a realistic simulation of the exchange of mass through the river-aquifer interface, which depends on the continuously changing pressure gradients and distribution of concentrations across the system acting as a source, which may change over time, requires solving river and groundwater flow and transport equations in parallel, alongside with explicit tracking of interactions and continuous update of the surface and groundwater systems. In the case of externally coupled river and groundwater models, such flux oscillations caused by river-aquifer interdependent dynamics are not simulated and are typically forced through boundary conditions.

4. Externally coupled flow and transport models have additionally the disadvantage that flow information needs to be stored by the flow model for subsequent use by the transport subroutine/model. This may lead to a disproportionate growth of storage needs during long term simulations, thus making external coupling unattractive or sometimes impossible.

An example of a fully coupled model attempting to solve the limitations enumerated above is provided by the coupling of MIKE FLOOD – a 1D/2D surface hydrodynamic model – to FEFLOW – a 2D/3D groundwater flow, transport and water quality finite element model. The coupling makes use of MIKE11 – the 1D hydrodynamic solver of the river network in MIKE FLOOD – through the *ifmMIKE11* plug-in, which allows both models to exchange flow and mass information at all time steps, thus allowing the coupled model to mimic a possible exchange of flow and transport direction during transient conditions. However, the interaction between river and aquifer is limited to the pre-defined river network, due to the 1D character of the surface hydrodynamic model, thus making impossible the simulation of inundation events, which extend over the broader river corridor.

Another model worth to mention is the control-volume finite element hydrological model HydrogeoSphere (HGS), which aims at simulating the terrestrial portion of the hydrological cycle. It is a fully-integrated subsurface and surface flow and solute transport that solves the 2D diffusion wave equation. This is appropriate for