Modelling *Escherichia coli* dynamics in the river Zenne (Belgium) using an OpenMI based integrated model

Narayan Kumar Shrestha, Olkeba Tolessa Leta, Bruno De Fraine, Tamara Garcia-Armisen, Nouho Koffi Ouattara, Pierre Servais, Ann van Griensven and Willy Bauwens

ABSTRACT

In 2000, the European Union (EU) launched the Water Framework Directive (WFD), calling for a good ecological status for water bodies by 2015 through integrated river basin management. Despite huge investments, the river Zenne (Belgium) still acquires high loads of pollutants. A multidisciplinary research project was therefore launched to evaluate the effects of river basin wastewater management plans on the river's ecological functioning. Different water quantity and quality processes were considered, and different models were used for each process. For the integration of these models – in view of a holistic analysis – we opted for the Open Modelling Interface (OpenMI). This paper discusses early results of integrated faecal bacteria modelling considering five models. The integrated model is shown to reproduce concentrations of *Escherichia coli* (used as indicator faecal bacteria) with 'Very Good', and 'Satisfactory' accuracy for dry weather, and long-term simulations respectively. For both cases, it is found that the *E. coli* concentrations in the river are well above EU level for bathing water, with occasional combined sewer overflows (CSOs) from the Brussels' sewer systems making the ecological status even worse. We also found OpenMI-based integration to be very useful. However, the calculation time overhead for such OpenMI integrated models remains significant.

Key words | *E. coli*, integrated modelling, OpenMI, river Zenne, WFD

Narayan Kumar Shrestha (corresponding author)
Olkeba Tolessa Leta
Ann van Griensven
Willy Bauwens
Department of Hydrology and Hydraulic Engineering,
Vrije Universiteit Brussel, Brussels,
Belgium
E-mail: *nashrest@vub.ac.be*

Bruno De Fraine
Department of Computer Science,
Vrije Universiteit Brussel, Brussels,
Belgium

Tamara Garcia-Armisen
Nouho Koffi Ouattara
Pierre Servais
Ecologie des Systèmes Aquatiques,
Université Libre de Bruxelles, Brussels,
Belgium

Ann van Griensven
UNESCO-IHE Institute for Water Education,
Core of Hydrology and Water Resources,
The Netherlands

INTRODUCTION

The use of modelling and modelling tools to represent reality in a simplified form has been practised for a long time (Maria 1997; Parker *et al.* 2002; Knapen *et al.* 2013). These modelling tools exist and are implemented in various forms (Argent *et al.* 2006) even though generally meant for a single purpose (Parker *et al.* 2002). However, the real problem is much more complex and interrelated (Argent *et al.* 2006), hence the growing consensus that an integrated approach is required in any attempt to seek insights into these complex problems (Parker *et al.* 2002; Candela *et al.* 2012; Bulatewicz *et al.* 2013). Regulatory frameworks such as the European Union Water Framework Directive (EU-WFD) (EU 2000) also require practitioners to adopt an integrated approach towards exploring if not mitigating environment-related problems. While the need for integrated modelling is generally recognised, there is, however, little consensus on how to proceed towards achieving a feasible integration of models on different concepts, and different spatial and temporal scales (Parker *et al.* 2002). Parker *et al.* (2002) stressed that a new, open and transparent tool is needed to achieve easy and feasible integration. Laniak *et al.* (2013) envisioned a similar approach and roadmap for the future of integrated environmental modelling. They suggested that for the integrated modelling to succeed: (a) it requires a system framework and approach; (b) it should ensure the involvement of stakeholders; (c) it

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should encourage global practitioners to facilitate learning, sharing and communication with one another; (d) practitioners should be open towards cooperation, collaboration, and even sharing the results of research and development. More importantly, they stressed that the community concerned should use and accept globally recognised standards and interface when designing and implementing software-based products. Similar conclusions were also found by the Open Modelling Interface (OpenMI)-Life project (OpenMI 2009). The project recommended practitioners to follow an 'open source route' and create a functional collaborative community. This is an important statement as there is a growing number of modelling tools and platforms for model integration, one different from the other, and importantly, the tools and platforms are designed for similar purposes, and there is little or no communication and sharing of information among developers. Over the years, a number of coupling approaches have been tried and tested. Brandmeyer & Karimi (2000) presented a hierarchical view of the coupling practices in environmental modelling, considering one-way, loose, shared, joined and tool coupling. The one-way coupling is traditionally the most common practice and at the bottom line of the coupling hierarchy. The most sophisticated coupling methodology, the tool coupling, is inspired by the so called 'component based software engineering' philosophy (Argent 2004). It is certainly advantageous to practitioners if the coupling framework allows for sufficient flexibility, such that the user can delete, replace or add any specific component with a certain ease. Such component based modelling systems have gained increased attention in recent time (Castronova & Goodall 2010) because they allow to interchange specific components of the integrated modelling system, in order to better represent the specific process or to test the impact of a specific component in the integrated system (Castronova et al. 2012). A major advantage of model coupling is that it allows practitioners to use the 'most suitable' existing models, thereby preserving the previous investments made in those models.

The OpenMI (Moore & Tindall 2005; Gregersen et al. 2007) is an example of a tool coupling methodology. It is an interface that allows models (that are compliant to its standard) to exchange data as they run. It therefore eliminates the cumbersome and error-prone tasks of transforming the output of one model into an input to another model (Reußner et al. 2009) and allows for bi-directional interactions between model components. Obviously, the usefulness of OpenMI depends on the availability of OpenMI compliant models (Gregersen et al. 2007). For this, existing models can be migrated to the OpenMI platform, while new models can be developed in such a way that they directly become OpenMI compliant (Moore & Tindall 2005). While the OpenMI can be applied in different scientific domains, its applications are currently limited to water and environmental disciplines (Knapen et al. 2013). Several studies have been conducted where the platform is used to integrate different models in view of simulating different catchment processes, including water quality processes (Reußner et al. 2009; Bulatewicz et al. 2010; Betrie et al. 2011; Leta et al. 2011, 2012; Shrestha et al. 2012b, 2013).

The Zenne river (Belgium) is a small river located in the Scheldt watershed that traverses the city of Brussels. Parallel to the river is a canal (Brussels-Charleroi) which interacts with the river, allowing the river to flow into it at three locations for the purpose of protecting Brussels from flooding. Downstream of Brussels, excess water is returned back from the canal to the river. During dry weather flow (DWF) periods, at least 50% of the river flow downstream from Brussels consists of treated sewer discharges, mainly originating from the two waste water treatment plants (WWTPs) of Brussels (Garnier et al. 2012). Hence, the WWTP effluents have serious impacts on the quality of the water in the downstream part of the river. In this part, the river is also subjected to the tidal influence of the river Scheldt. During storm conditions, the combined sewer overflows (CSOs) within Brussels have a major impact on the flow regime and on the quality of the river. Considering all these components and interactions, the system can be considered as quite complex. Since 2000, large investments were made for the management of the wastewaters, which resulted in an increase in the river water quality (Garnier et al. 2012). Despite these investments, the river still receives high loads of pollutants, especially considering the low discharge of the river, and the water quality downstream from Brussels does not comply with the requirements set by the EU-WFD. It is in this context that an interuniversity, multidisciplinary research project 'Good Ecological Status of the river Zenne (GESZ)' was launched to evaluate the effects of the wastewater management plans in the river basin on the ecological functioning of the river. Hereto, different water quantity and quality processes need to be considered: the hydrology in the river basin, the hydraulics in the river, in the canal and in the sewers, erosion and sediment transport, the carbon-nitrogen-phosphorus (C-N-P) cycle, the transport of trace metals and the transport and decay of faecal indicator bacteria (FIB). For the simulation of the hydrologic processes in the river basin, the Soil and Water Assessment Tool (SWAT) (Arnold *et al.* 1998) was used. SWAT was chosen as it considers the interactions between the water, the soil and the plants and thus allows for an assessment of the erosion and nutrients processes (Srinivasan *et al.* 1998; Santhi *et al.* 2001; White & Chaubey 2005; Jha *et al.* 2007; Lam *et al.* 2010). The representation of the river processes in SWAT is, however, too simplified for a complex system as the Zenne basin: backwater effects, tidal effects or complex interactions between system components cannot be considered. In addition, hydraulic structures such as weirs, locks, orifices, pumps and gates cannot be implemented (Betrie *et al.* 2011). Hence, to be generally applicable for integrated catchment modelling, SWAT needs an improvement of its routing modules, e.g. by replacing these modules by a dynamic wave routing approach, or it should be coupled to a hydraulic model that uses such an approach. As opposed to most hydrologic models, the hydraulic models generally consider the full dynamic wave equation for river routing and are thus able to account for backwater or tidal effects and to represent various hydraulic structures. One of the widely used hydraulic simulators is the Storm Water Management Model (SWMM) (Rossman 2009). The weak point of these models is that they generally represent the upland catchment processes in a simplified way (Betrie *et al.* 2011). Therefore, the hydraulic models also need to be complemented by more detailed hydrological models. An optimal solution to the problem consists of integrating various types of models, thereby making use of one's strength over the other's weakness. A general model to represent all the above stated processes hardly exists. Also, such a tight coupling lacks flexibility (Betrie *et al.* 2011). Another option would be to use the 'most suitable' model for each of the processes and to make them use each other's outputs. However, such an offline file based linking is a time consuming and error-prone procedure (Brandmeyer & Karimi 2000). Hence, we opted for the use of existing models in addition to the development of new models and for linking all these components through OpenMI.

The paper presents a new OpenMI based development for the integrated modelling which was applied to the *Escherichia coli (E. coli*) dynamics, as a tool to assess the microbiological level of pollution of a river. The integrated model involves five model components: a hydrological model (SWAT), a hydraulic model (SWMM), a new model for sediment transport, a new stream water temperature model and a new model for faecal bacteria. All these components are dynamically linked, using an OpenMI platform. The integrated model is applied to simulate the *E. coli* dynamics in the river Zenne (Belgium). The main objective of the paper is to demonstrate the use of OpenMI for coupling different models to form a feasible integrated model. Hereby, the use of OpenMI to couple different component models (e.g. the hydraulic model with the bacteria model) in parallel is – to our knowledge – a novelty.

THE STUDY AREA

The river Zenne is a part of the international Scheldt basin. It drains an area of 1,162 km² and runs through the three administrative regions of Belgium: the Walloon Region (574 km²), the Brussels Capital Region (162 km²) and the Flemish Region (426 km²). After a length of about 103 km, it finally meets the river Dijle, where it is subject to the tidal influence of the river Scheldt. Upstream of Brussels, the river follows a natural meandering course, while in the Brussels-Capital Region, the river has been vaulted over a distance of approximately 8 km. Downstream of Brussels, the bed level of the river has been re-profiled. The river basin is crossed by the canal Brussels-Charleroi and the Sea Canal Brussels-Scheldt. In the Walloon Region, the canal is fed by former tributaries of the river (Figure 1). In the reach between the borders of the Walloon and the Brussels Region, different tributaries discharge into the river. The canal also receives water from the river through several overflow structures, to prevent flooding in the Brussels

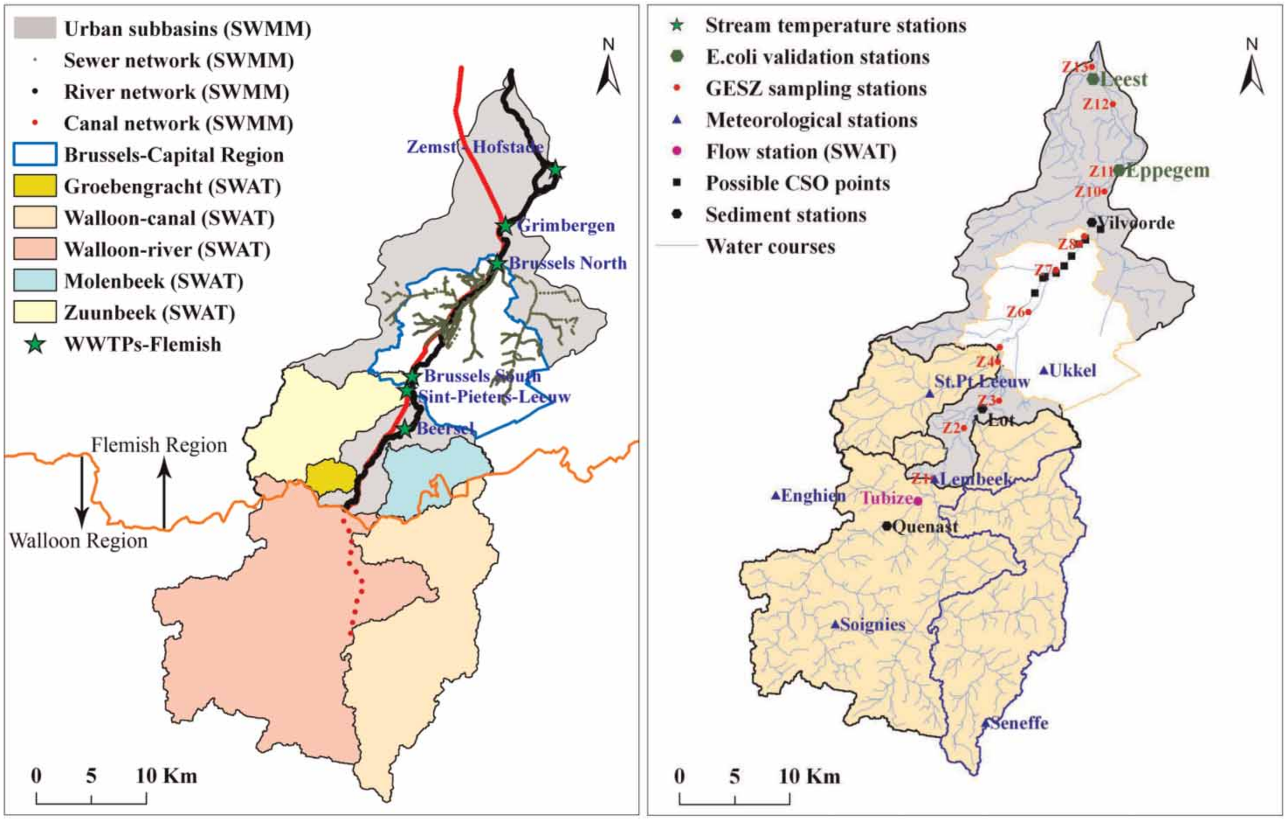


Figure 1 | The Zenne basin with the subbasins simulated with SWAT, the SWMM network for the river, the canal, the sewer systems and the major WWTPs (left); the hydro-meteorological, stream temperature, *E. coli* validation stations, the GESZ sampling stations and the possible CSO points (right).

Capital Region. Excess water in the canal can be discharged back into the river downstream from Brussels. About 1.5 million people are connected to the river, of which, more than 1 million people live in the Brussels Capital Region. The population density in the basin is about 1,260 inhabitants/km^2, which makes it the most densely populated basin of the Scheldt basin (van Griensven 2002). The land-use in the catchment is dominated by agriculture (51%) – mostly in the upstream part – and by urban regions (19%) in the downstream part. There are several small to large WWTPs in the basin. In the Brussels area, the river receives the sewage waters from the WWTP Brussels South (360,000 equivalent-inhabitants, in operation since 2000) and the WWTP Brussels North (1.1 million equivalent-inhabitants, in operation since 2007). The treatment at the WWTP Brussels South includes primary settling and an activated sludge treatment. The treatment at WWTP Brussels North also includes a tertiary treatment for the removal of nitrogen and phosphorus.

METHODS

With the aim of developing an OpenMI based integrated model to simulate faecal bacteria dynamics, the task was undertaken in the following steps and is discussed further below.

- Step 1: Processes and process interactions governing faecal bacteria dynamics were identified.
- Step 2: Suitable models to represent the processes were selected or developed.
- Step 3: Non-OpenMI compliant models were made OpenMI compliant.
- Step 4: All the required data to build-up, calibrate, and validate the models were sourced.
- Step 5: Several stand-alone and OpenMI integrated models were build-up, calibrated, and validated in sequential way as follows:

(a) SWAT (standalone).
(b) SWAT-SWMM (integrated).
(c) SWAT-SWMM-Temperature (integrated).
(d) SWAT-SWMM-Temperature-Sediment Transport (integrated).
(e) SWAT-SWMM-Temperature-Sediment Transport-Faecal Bacteria (integrated).

- Step 6: Goodness-of-fit statistics were chosen to track the accuracy of model calibration and validation. A final performance rating was calculated, based on the values of these statistics.

Processes governing faecal bacteria dynamics

Polluted surface waters can transport various pathogenic micro-organisms, e.g. bacteria, viruses, protozoa, etc. (Skraber *et al.* 2002; Servais *et al.* 2007a, b; Kamizoulis 2008; de Brauwere *et al.* 2011). As they cannot grow in natural aquatic environments (Edberg *et al.* 2000), the main origin of these micro-organisms is the release of faecal material from humans and animals (de Brauwere *et al.* 2011). Bacteria reach the river from point sources (WWTPs, CSOs, opportunistic discharges from industrial sites) and non-point sources (soil leaching, surface runoff) (Servais *et al.* 2007a). These inputs are highly variable (de Brauwere *et al.* 2011). The sanitary risks associated with the waterborne pathogens depend on their concentration and on the use of the water (Edberg *et al.* 2000; Servais *et al.* 2007a, b; Ouattara *et al.* 2011). Hence, modelling the fate and dynamics of faecal bacteria is essential for the assessment and management of water bodies.

Once released in rivers, the faecal bacteria are subjected to different processes leading to their disappearance (protozoan grazing, lysis, stress, settlement, solar radiation). These processes are commonly modelled by means of a temperature dependent rate of disappearance.

Besides mortality, most of the traditional modelling approaches of faecal bacteria also consider the settling of bacteria (Servais *et al.* 2007a, b; de Brauwere *et al.* 2009; de Brauwere *et al.* 2011). Regarding the latter process, it should be stressed that two fractions of bacteria should be distinguished: a free floating fraction and a sediment-adsorbed fraction (Matson *et al.* 1978; Wilkinson *et al.* 1995; Characklis *et al.* 2005). Although the modelling of these two – separate but interrelated – fractions has rarely been reported (Jamieson *et al.* 2004), the authors believe that doing so would allow for a better understanding of the faecal bacteria dynamics (Garcia-Armisen & Servais 2009). Also, it has been acknowledged that the sediment on the river bed can be a reservoir for such bacteria (Shiaris *et al.* 1987; Wilkinson *et al.* 1995; Crabill *et al.* 1999; Craig *et al.* 2002; Jamieson *et al.* 2005; Ouattara *et al.* 2011). Thus, the resuspension of the sediment in storm conditions could have serious implications on the degradation of the microbiological water quality (Crabill *et al.* 1999; Krometis *et al.* 2007), hereby increasing the sanitary risk (Craig *et al.* 2002).

Hence, it is evident that the simulation should consider both free faecal bacteria and bacteria that are adsorbed to particulate matter, as well as the interactions between the bacteria and the particulate matter and the sediment transport. As such, a model to simulate water fluxes is evident; a model to simulate the stream water temperature is also needed as the disappearance rate of faecal bacteria is temperature dependent.

The models

To represent the different processes governing faecal bacteria dynamics in the riverine environment, different models are needed. To this end, we followed the so-called 'open source route', whereby the preference was given to open source tools that had previously been tested successfully in similar catchments. The reason for selection of SWAT for the simulation of the river basin processes has been stated above. SWMM was selected as a hydraulic model, as it allowed us to deal with all the different components of the system – including the sewer systems with their auxiliary structures. Having chosen these two core components, additional modules needed to be developed for the sediment, the faecal bacteria, and the temperature. In what follows, the different components are briefly described. Somewhat more emphasis is hereby put on the bacteria model that is the focus of this paper.

The hydrologic model: SWAT

SWAT is a physically based semi-distributed, hydrologic model that can operate at basin scale on different time steps. It has the capability to perform continuous simulations for a large group of processes (hydrology, nutrients, soil erosion, etc.) (Srinivasan *et al.* 1998; Santhi *et al.* 2001; White & Chaubey 2005; Jha *et al.* 2007; Lam *et al.* 2010). For modelling purposes, a watershed is divided into sub-basins that have a homogeneous area in terms of climatic conditions (Van Liew *et al.* 2005). Sub-basins are further subdivided into Hydrological Response Units (HRU), whereby each HRU has a unique combination of land use, soil type and slope (Arnold *et al.* 2011). The hydrological part of SWAT accounts for precipitation, evapotranspiration, surface runoff, lateral flow, return flow and deep groundwater losses (Neitsch *et al.* 2011). Soil erosion in SWAT is a hydrological driven process. The soil erosion and sediment yield from each HRU are modelled by the Modified Universal Soil Loss Equation (MUSLE) (Williams & Berndt 1977; Lal 2001). The channel sediment routing module uses the modified Bagnold's sediment transport method (Bagnold 1977).

The hydraulic model: SWMM

SWMM is a dynamic rainfall runoff model for computing the runoff quantity and quality (primarily) from urban areas. It can be used for both continuous and single event modelling (Rossman 2009). SWMM adopts a distributed non-linear reservoir concept to simulate the runoff from a specific sub-catchment after depression loss, infiltration and evaporation are satisfied. The one-dimensional flow routing is based on the full set of equations of Barré de Saint-Venant.

SWMM has provisions to build up any pollutant on the sub-catchment surface and for their subsequent wash-off. Once the pollutant is in suspension, there is no provision to allow for sedimentation or resuspension. This is important since some pollutants can be adsorbed to sediment particles and then start behaving as the sediments while being transported. Hence, there was a need for developing a new sediment transport model that complements SWMM.

The sediment transport model

The developed river sediment transport module is based on the concept of the critical shear stress and the related critical particle diameter for the initiation of motion of non-cohesive bed particles. Hence, it assumes a critical diameter that divides the sediment between a fraction in motion and a fraction without motion. The critical diameter is determined by solving an algebraic expression, proposed by Soulsby & Whithouse (1997), that closely fits Shields' curve (Shields 1936). Based on the critical diameter, the fate of sediment particles is determined. For this, the sediment is divided into number of classes according to its particle size distribution (PSD). A limitation on the transport capacity (on both sides) is imposed by using Velikanov's energy equation, as proposed by Zug *et al.* (1998):

$$\mathrm{CT}_{\min} = \eta_1 \frac{s\rho_{\mathrm{w}}}{(s-1)} \frac{u}{w_{\mathrm{s}}} S \tag{1}$$

$$\mathrm{CT}_{\max} = \eta_2 \frac{s\rho_{\mathrm{w}}}{(s-1)} \frac{u}{w_{\mathrm{s}}} S \tag{2}$$

where $\mathrm{CT}_{\max}$ is the critical erosion transport capacity (kg/m^3), $\mathrm{CT}_{\min}$ is the critical sedimentation transport capacity (kg/m^3), η_1 is the critical sedimentation efficiency coefficient (–), η_2 is the critical erosion efficiency coefficient (–), ρ_{w} is the water density (kg/m^3), s is the specific grain gravity (–), w_{s} is the settling velocity of grains (m/s) and u is the velocity of the water (m/s), S is the friction slope.

The authors recognise the simplicity of the approach for the modelling of the sediments. It is hereby important to consider that the aim of the tool is to perform long-term, continuous simulations, in view of the global assessment of alternative water quality management plans. In this perspective, a compromise had to be found between the complexity of the model on the one hand and, on the other hand, the availability of data regarding the sediments and their characteristics and the need for a fast and robust modelling tool that enables long-term continuous simulations.

The temperature model

To determine the stream water temperature, a regression model between air and stream water temperature is used. Such regression models are the simplest means to predict the stream temperature and are especially popular due to the fact that they only require readily available data on the air temperature and that they have a small calculation overhead but nevertheless proved to be quite accurate (Webb *et al.* 2003). A non-linear fit (Equation (3)) is used, as suggested by Mohseni *et al.* (1998):

$$T_s = \mu + \frac{\alpha - \mu}{1 + e^{\gamma(\beta - T_a)}} \tag{3}$$

where T_a and T_s are the air and the stream water temperature (°C), μ is the minimum stream temperature (°C); α is the maximum stream temperature (°C), γ is the steepest slope at the inflection point of the T_s function plotted against T_a (–) and β is the air temperature at the inflection point of the T_s function plotted against T_a (°C).

Studies have shown that stream temperatures tend to follow the air temperatures but with some time lag (Grant 1977; Stefan & Preud'homme 1993). Stefan & Preud'homme (1993) observed time lags to be related to stream depth and suggested a lag ranging from hours to days. Grant (1977) suggested predicting stream temperature with a time lag of 1 day. The temperature model developed for this study accounts for a time lag of 2 days (using the temperature of the same day and of the two previous days). Besides, thermal discharges from, for example, WWTPs can also be considered. As already depicted, at least 50% of the river flow downstream of Brussels consists of treated sewer discharges, mainly originating from the two WWTPs of Brussels (Garnier *et al.* 2012), their effect on thermal regime of the river could be significant because the effluents are discharged rather at a constant temperature throughout the year. Hence, consideration of such thermal discharge from the WWTPs is needed in the temperature model.

The faecal bacteria model

The model. We developed a faecal bacteria model that keeps track of both free and adsorbed faecal bacteria. It is assumed that when faecal bacteria enter the river, a part of the concentration is free and a part is adsorbed or attached to particles. The free bacteria do not settle down, but attached bacteria do. Once adsorbed to sediment particles, the attached faecal bacteria behave like sediment particles. Hence, the settlement (sedimentation) and resuspension of the attached faecal bacteria is governed by the sediment model. The decay of the both forms of faecal bacteria is modelled by a first order reaction as:

$$\frac{\mathrm{d(FC)}}{\mathrm{d}t} = -k_d \,\mathrm{FC} \tag{4}$$

where FC is the faecal bacteria concentration (#/l) and k_d is the mortality rate (h^{-1}).

Hereby, the free, attached and settled faecal bacteria may have different mortality rates: k_{d1}, k_{d2} and k_{d3}, respectively. The temperature dependence of the mortality rates is modelled by a sigmoid relationship, as suggested by Servais *et al.* (2007a, b):

$$k_{d,T_s} = k_{d,T_o} \frac{e^{\left(-\frac{(T_s - 25)^2}{400}\right)}}{e^{\left(-\frac{25}{400}\right)}} \tag{5}$$

where k_{d,T_s} is the mortality rate at stream temperature T_s (T_s in °C) and k_{d,T_o} is the mortality rate for a stream temperature of 20 °C.

Although it is clear that faecal bacteria exist in two forms (free and attached), the extent of the partitioning between them has not been reported in a unanimous way. Some studies suggest that the partitioning is positively correlated with the suspended particulate matter (SPM) concentration (Characklis *et al.* 2005; Garcia-Armisen & Servais 2009), while others suggest a constant partitioning (Characklis *et al.* 2005; Krometis *et al.* 2007). We assumed a reversible linear adsorption process (Equations (6) and (7)), as suggested by Chapra (1997) and as also used by other researchers, e.g. Bai & Lung (2005) and Russo *et al.* (2011), to represent the sorption of faecal bacteria to sediment.

$$F_f = \frac{1}{1 + K_p\, C_{SPM}} \tag{6}$$

$$F_a = \frac{K_p\, C_{SPM}}{1 + K_p C_{SPM}} \tag{7}$$

where F_f and F_a are the free and the attached fraction of the faecal bacteria, K_p is the partitioning coefficient (L/mg) and C_{SPM} is the SPM concentration (mg/L).

The indicator faecal bacteria. Usually, the level of microbiological pollution of water bodies is evaluated by the enumeration of FIB. FIB should be universally present in large numbers in the faeces of humans and animals, detectable by simple and inexpensive methods and not grow in natural environments (Edberg *et al*. 2000). Today, *E. coli* is the most commonly used FIB for evaluating microbiological water quality (Edberg *et al*. 2000). Recent regulatory guidelines, such as the EU directive on bathing waters (EU 2006), are also based on *E. coli* (along with intestinal enterococci) concentrations.

The models on the OpenMI platform

On the OpenMI platform, only OpenMI compliant components can be linked together to make an integrated model. Any existing (open-source) model can be migrated to the OpenMI platform, while new models can be developed in such a way that they directly become OpenMI compliant (Moore & Tindall 2005).

The migration of existing models to the OpenMI platform

The recommended practice for migrating an existing model engine to OpenMI is to construct a 'wrapper', i.e. an intermediate software component that makes the model engine addressable on the platform used by OpenMI (i.e. Microsoft .NET), according to the interface prescribed by the OpenMI standard. The concrete solution consists of three steps: (a) the existing engine code is compiled as a Windows Dynamic Link Library (DLL), (b) a basic .NET component employs the interoperability functionality of the .NET platform to make this DLL library accessible, and (c) another .NET component implements the OpenMI interface by interpreting the requests from OpenMI and translating them to the native functions of the model engine. As such, the execution of a simulation by the original model engine is triggered by the 'request-reply' mechanism of OpenMI. The OpenMI association provides a Software Development Toolkit (SDK) that contains auxiliary code to aid with step (c) of this process. We used accessories related to the OpenMI version 1.4 for this purpose.

For the SWMM OpenMI model the standard 'wrapping' approach has been adopted with one important modification to step (b). The standard SWMM5 code base already makes the basic functionality of the model engine available as a DLL library for the benefit of the SWMM graphical user interface. We extended this provision in the SWMM code base with a functionality to access the network elements (nodes and links) of a SWMM project and to inspect their basic hydraulic properties (such as flow, volume, depth, etc.) during simulation. More information on the SWMM OpenMI migration can be found in Shrestha *et al.* (2012a).

The SWAT OpenMI model is also a migration of an existing code base to OpenMI, using the standard 'wrapper' approach. More information on the SWAT OpenMI migration was provided by Betrie *et al.* (2011).

The development of new models for the OpenMI platform

The sediment transport, temperature and faecal bacteria models were directly conceived as OpenMI compliant model engines. They were written in C#, the predominant programming language for the .NET platform. These models carry out simulations over the same river trajectory as the SWMM project, using (dynamic) hydraulic variables that are provided from the SWMM simulation (velocity, water depth, etc.). Hereby, all modules use the (static) network configuration of the SWMM project (nodes and links, with their characteristics). This was achieved by a code base that is common to all model engines. By making use of a class hierarchy structure, the common code is shared and not duplicated. The latter code is placed in a separate .NET assembly (GESZ.SWMMNetwork, Figure 2). Appropriate OpenMI 'input exchange items' and 'output exchange items' were created for all the simulation parameters. At the level of the OpenMI, the exchange of physical quantities for an entire network (which may contain hundreds of nodes and links) requires some attention. When constructing an OpenMI composition, a 'link' is introduced for each exchange between the models. However, creating a separate link for each network element introduces a prohibitive work overhead (it is also inconvenient since OpenMI linking is usually a manual task in the graphical user interface). Fortunately, the OpenMI standard allows exchange items to transfer data values for multiple elements in a single operation using so

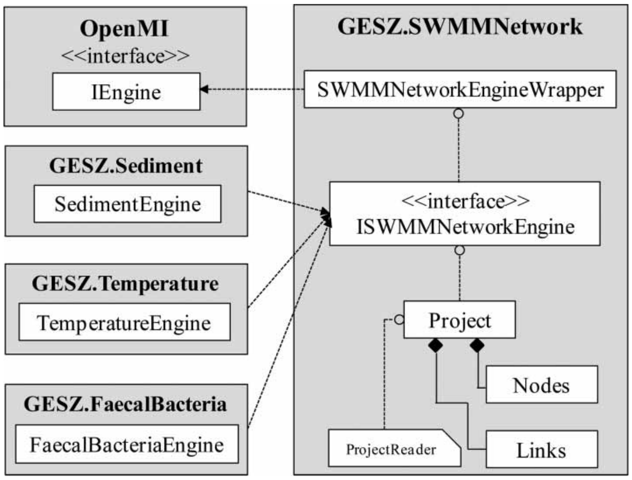


Figure 2 | The OpenMI wrapper design of the newly developed sediment, temperature and faecal bacteria models.

called 'element sets'. The different model components employ such element sets, which cover either all the nodes or all the links of the network.

Build-up, calibration, and validation of the models

Methodology

Different types of data were used for the build-up and calibration of the models (Table 1). While flow data and hydrometeorological data are monitored by different governmental agencies on an hourly or daily basis, physicochemical data are typically monitored with a frequency of one sample per month. Faecal bacteria are not even monitored at all. As the major of the WWTPs in the Brussels Capital Region became operational in 2006, data from before 2007 were also of little use to assess the actual condition of the river. To compensate for the lack of data, a series of sampling campaigns were set up in the framework of the GESZ project, over the period 2009–2011. These include the monitoring of longitudinal profiles for faecal bacteria and various physicochemical variables during dry weather conditions in different seasons (five campaigns). In addition, two campaigns were organised to gain information about the water quality during storm conditions, including a 24-h campaign. A dual procedure was therefore used for the build-up and calibration of the model parameters. Hereby, some parameters were derived based on the GESZ sampling campaigns, while other parameters were calibrated, based on time series provided by governmental agencies.

The modelling of the water quantity

SWAT model. As the SWAT does not need input from any other models, it was built, calibrated, and validated on a standalone basis.

The essential inputs for the SWAT model are a Digital Elevation Model (DEM), a soil map, a land-use map, and hydro-meteorological data such as rainfall, temperature, relative humidity, solar radiation and wind speed (Table 1 for data source and resolution). Figure 3 shows the land-use (left) and soil map (right) of the sub-basins simulated with SWAT. Altogether, we defined 30 sub-basins and 194 HRUs. For stream flow simulation, the SWAT model was built for the period 1988–2008. We used the years 1998–2008 for calibration and 1988–1997 for validation. We used daily stream flows recorded at Tubize (Figure 1) for both purposes. For sediment simulation, due to limited data, we used the years 1998–2008 for calibration and 1994–1997 for validation. For this, sediment concentrations measured at Quenast were used.

More information regarding the stream flow calibration/validation of the SWAT model can be found in Leta *et al.* (2011, 2012). Likewise, more information regarding sediment calibration/validation of the SWAT model can be found in Shrestha *et al.* (2013).

SWMM model. The SWMM model includes the Zenne river between the border of the Walloon – Flemish Region and the outlet of the Zenne – the river Dijle (Figure 1), the canal and its interconnections with the river, and the major collectors of the sewer systems (including the CSOs and the WWTPs). Also the urban storm flow for the Brussels Capital Region is modelled using SWMM. The SWMM model requires longitudinal and cross-section geometrical data as well as rainfall, temperature and evaporation data (Table 1 for data source and resolution). The SWMM model contains ca. 2,400 nodes/links and about 180 special structures (weirs, orifices, pumps, storage units, etc.).

As SWMM needs a rural catchment runoff which was modelled with SWAT, an integrated model in OpenMI

Table 1 | Model inputs for the different modules of the integrated faecal bacteria model

Input	Value/Resolution	Remarks/References
A: SWAT		
Digital Elevation Model (DEM)	30 × 30 m	ASTER GDEM[a], DHM-OC GIS Vlaanderen
Soil map (Figure 3, right)	20 × 20 m	Carte Numérique des Sols de Wallonie (CNSW)[b], VLM-OC
Landuse map (Figure 3, left)	20 × 20 m	Corrine (Walloon region), VLM-OC GIS Vlaanderen
Hydro-meteorological data (Rainfall, relative humidity, wind speed, solar radiation, temperature) (Figure 1, right)	Daily	Royal Meteorological Institute of Belgium (RMI), Direction Générale opérationnelle de la mobilité et des Voies Hydrauliques (DGVH)[c], Vlaamse Milieumaatschappij (VMM)[d]
B: SWMM		
River/Canal longitudinal profile and cross section geometry	ca. 100 m	Waterbouwkundig Laboratorium[e]
River longitudinal profile and cross section geometry	ca. 100 m	Waterbouwkundig Laboratorium[e]
WWTP-Brussels-North sewer system geometry	ca. 100 m	Translated from a hydraulic model HYSTEM-EXTRAN built
Rainfall	Hourly	Royal Meteorological Institute of Belgium (RMI)
Tide levels at outlet	30 minute	Waterbouwkundig Laboratorium[e]
Boundary flows at tributaries	Daily	SWAT simulated
C: Sediment transport model		
Particle size distributions, PSDs	–	Based on GESZ measurement[f], constant
Boundary sediment concentration at tributaries	mg/L	SWAT simulated
Sediment concentration at WWTP outlets	Daily	Observed series
Sediment concentration at CSO points	207 mg/L	Based on GESZ measurement, constant
Sediment concentration at outlet	8.1 mg/L	Based on GESZ measurement, constant
D: Temperature model		
Air temperature	Daily	Royal Meteorological Institute of Belgium (RMI)
Temperature of WWTP effluent	20 °C	Constant
Temperature of CSO points	15 °C	Constant
E: Faecal bacteria model		
Boundary *E. coli* concentration at tributaries	1.51E + 05 #/L	Based on GESZ measurement, constant
E. coli concentration at WWTP effluents	4.5–65.7E + 06 #/L[g]	Based on GESZ measurement, constant
E. coli concentration at CSO points	2.08E + 07 #/L	Based on GESZ measurement, constant
E. coli concentration at outlet	2.03E + 06 #/L	Based on GESZ measurement, constant
E. coli concentration from untreated sewage	1.23E + 08 #/L	Based on GESZ measurement, constant

[a] www.gdem.aster.ersdac.or.jp/search.jsp.
[b] cartographie.wallonie.be/NewPortailCarto/.
[c] voies-hydrauliques.wallonie.be/opencms/opencms/fr/hydro/Archive/annuaires/index.html.
[d] www.hydronet.be.
[e] www.watlab.be/nl.
[f] GESZ measurement: observed during GESZ sampling campaigns at different stations (Figure 1, right).
[g] Varies among the WWTPs.

was formed involving SWAT and SWMM. The input exchange items were 'stream flows' at SWAT sub-basin outlets, configured to the appropriate receiving SWMM nodes. While SWAT simulated stream flows in a daily time step which SWMM needed at every 5 seconds (routing time step), SWAT used a linear interpolation to reply to the requests sent by SWMM, which was indeed handled by an OpenMI data operation mechanism.

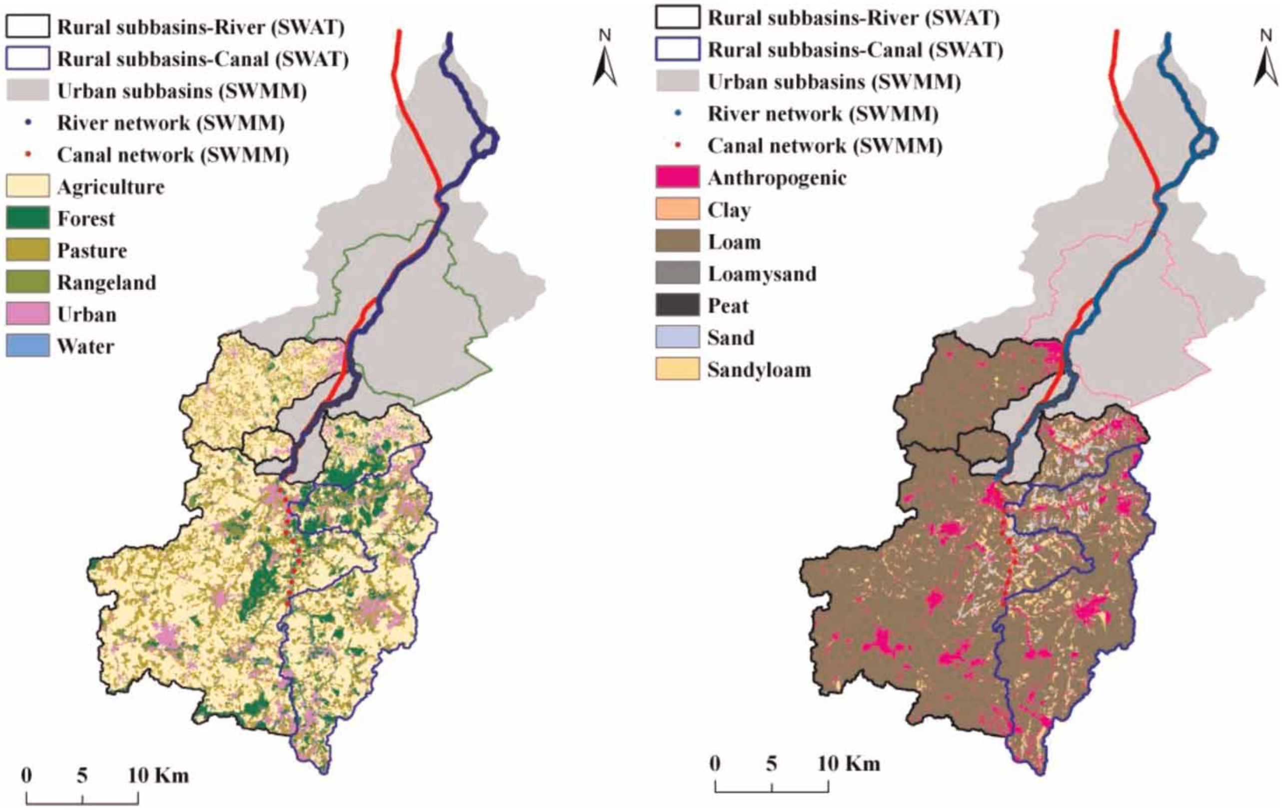


Figure 3 | Land use (left) and soil map (right) of the subbasins simulated with SWAT.

The integrated model was calibrated and validated using daily and hourly stream flows observed for the years 2007 and 2008 at two locations along the river (Lot and Vilvoorde; Figure 1). We used the stream flow data of 2007 to calibrate the model and 2008 to validate the model.

The temperature model. Firstly, we calibrated the five parameters of the temperature model (Equation (3)) as a stand-alone application using air temperatures recorded at Ukkel (Figure 1) by the Royal Meteorological Institute of Belgium (RMI) and stream water temperatures recorded by Flemish Environmental Agency (VMM) at four locations upstream of Brussels. These (upstream) stations were selected in order to limit the effect of thermal fluxes from the big WWTPs that discharge in the Brussels.

Once the parameters of the temperature model were determined, an integrated temperature model was set up consisting of three models: SWAT, SWMM, and the temperature model itself. In building up the integrated temperature model, the temperature for the WWTP effluents was assumed to be 20 °C, while a temperature of 15 °C was assumed for the CSOs (Table 1). The results of the integrated temperature model were validated using stream water temperatures at two locations along the river (Lot and Vilvoorde) for the years 2007 and 2008, recoded by VMM.

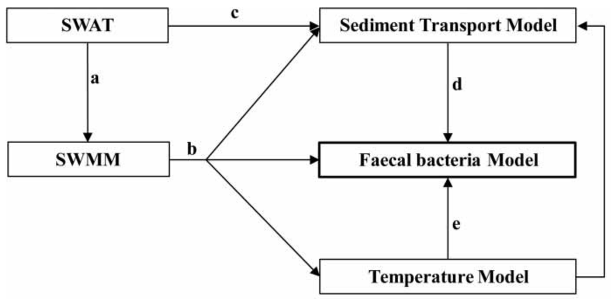
The sediment transport model. An integrated sediment model was built, consisting of SWAT, SWMM, the temperature model and the sediment model. SWAT provided flow and sediment flux boundary conditions for the upstream rural areas. More information regarding the calibration of SWAT for the sediment fluxes can be found in Shrestha *et al.* (2013). The (fixed) PSDs for the sediments in the tributaries were based on sampling campaigns during the GESZ project.

Sediment concentrations for the WWTP effluents were based on daily observations. The (fixed) PSDs for these sediments were based on sampling campaigns during the GESZ project. As the sewer models in SWMM only contain a simplified representation of the systems, it was not possible to model the sediment settlement/resuspension processes in these systems. An average sediment concentration of 207 mg/L and PSDs, as measured during GESZ sampling campaigns, were used to characterise the sediment fluxes at CSOs. At the downstream boundary, being the confluence of the river Zenne with the (tidal) river Dijle, a constant concentration of 8.1 mg/L was imposed.

We calibrated three parameters (s, η_1, and η_2) of the integrated sediment transport model by means of manual calibration. For this, the sediment concentration measured at two locations (Lot and Vilvoorde) for the year 2007 was used. The integrated model was then validated using the observations from 2008. More information regarding the sediment model calibration and validation can be found in Shrestha *et al.* (2013).

The faecal bacteria model. Finally, an integrated faecal bacteria model was built by adding the faecal bacteria component to the sediment transport model. Exchanged quantities included the sediment concentration (provided by the sediment transport model), stream water temperature (provided by the temperature model), and various hydraulic variables (provided by SWMM). The element-sets for each data were all SWMM nodes and links. The faecal bacteria model was also configured to use SWMM routing time, such that the exchange quantities provided by SWMM, temperature, and sediment transport model were directly compatible. The time step difference between the SWAT model (daily) and SWMM model (5 seconds) as well as the sediment model (5 seconds) was handled by the OpenMI data operation using linear interpolation. The different model components and the information regarding data exchange are shown in Figure 4. As already depicted, *E. coli* is taken as indicator faecal bacteria in this study.

E. coli can enter a river domain by point sources (WWTP effluents, CSO) and as diffuse sources (surface runoff, soil leaching). Many studies have, however, indicated that the point sources are predominant for a highly urbanised catchment like the Zenne, as most inhabitants are connected to sewer systems (Garcia-Armisen & Servais 2007; Servais *et al.* 2007b; de Brauwere *et al.* 2011; Ouattara *et al.* 2011). As the value of the concentrations of the diffuse sources is thus not critical for our case, we considered a constant concentration (1.51×10^5 #/L) for all the natural tributaries, based on measurements for the GESZ project. For the modelling



Exchange item	Element set	Quantity	Time step
a	Nodes	Runoff*	5 seconds
b	Nodes/Links	Flow, volume, depth, velocity, shear velocity	5 seconds
c	Nodes	Sediment concentration	5 seconds
d	Nodes/Links	Sediment concentration	5 seconds
e	Nodes/Links	Water temperature	5 seconds

Figure 4 | Model components of the integrated model and their data flow.

of the CSOs, a constant *E. coli* concentration (2.08×10^7 #/L) was considered, based on (a limited number of) observations made during the GESZ project. *E. coli* input from raw sewage was also considered, based on number of inhabitant equivalents and the capacities of the WWTPs. We also considered an illicit sewer connection of 50,000 inhabitant equivalents in the Brussels region, an estimate based on the observation by Petrovic *et al.* (2012). The downstream part of the river experiences a tidal influence of the river Dijle. During the flood phase, the concentrations in the tidal reaches of the river Zenne are therefore determined by the concentration in the river Dijle. As no data about the evolution of these concentrations are available, a constant *E. coli* concentration (2.03×10^6 #/L) was imposed as a downstream boundary condition. The latter value is based on the GESZ sampling campaign.

The decay rates for three fractions of *E. coli* (free, attached and settled) were set, based on observations made by Servais *et al.* (2007a, b) on the river Seine (France) and by Garcia-Armisen & Servais (2009) on the rivers Seine, Meuse (Belgium) and Scheldt. Hence, a first order decay rate of 45×10^{-3} h^{-1} at 20 °C is considered for free *E. coli*, while a lower mortality rate (22.5×10^{-3} h^{-1} at 20 °C) is used for the attached and for the settled *E. coli*. One remaining parameter of the integrated model, the partitioning coefficient, was calibrated using a heuristic approach based on the faecal bacteria concentrations at 13 GESZ sampling stations during DWF conditions. The integrated model was then validated for a long period that also included storm conditions. For the DWF situation, data obtained during five sampling campaigns at 13 selected stations along the river (Figure 1) were used. For the long-term analysis, data obtained in the framework of the TIMOTHY project (www.climate.be/TIMOTHY/) were used. From March 26, 2007 to June 13, 2008, monthly samples were taken at two monitoring stations (Figure 1): Eppegem (ca. 15 km downstream from Brussels), and Leest (ca. 25 km downstream from Brussels; under tidal influence) (Ouattara *et al.* 2011).

In the sampling campaigns, samples were collected in sterile 2 L bottles, kept at 4 °C and analysed within 12 h. *E. coli* concentrations were enumerated by plate count on Chromocult agar (CC) (Merck) after membrane filtration (0.45 μm-pore-size, 47-mm-diameter sterile cellulose nitrate filters, Sartorius) or spread plating depending on their abundance. *E. coli* colonies were enumerated after 24 h incubation at 37 °C, following the manufacturer's instructions.

Goodness-of-fit statistics

The quality of the different models was assessed using the percentage bias (PBIAS, Equation (8)), the ratio of the root mean square error to the standard deviation of the measured data (RSR, Equation (9)) – as purposed by Moriasi *et al.* (2007) and the Nash–Sutcliffe efficiency (NSE, Equation (10)) (Nash & Sutcliffe 1970).

$$\mathrm{PBIAS} = \frac{\sum_{i=1}^{N}(X_{\mathrm{sim},i} - X_{\mathrm{obs},i})}{\sum_{i=1}^{N}(X_{\mathrm{obs},i})} \times 100 \tag{8}$$

$$\mathrm{RSR} = \frac{\sqrt{\sum_{i=1}^{N}(X_{\mathrm{sim},i} - X_{\mathrm{obs},i})^2}}{\sqrt{\sum_{i=1}^{N}(X_{\mathrm{obs},i} - \overline{X_{\mathrm{obs}}})^2}} \tag{9}$$

$$\mathrm{NSE} = 1 - \frac{\sum_{i=1}^{N}(X_{\mathrm{sim},i} - X_{\mathrm{obs},i})^2}{\sum_{i=1}^{N}(X_{\mathrm{obs},i} - \overline{X}_{\mathrm{obs},i})^2} \tag{10}$$

where X_{sim} is the simulated quantity, X_{obs} is the observed quantity, σ_{sim} is the standard deviation of simulated quantities, σ_{obs} is the standard deviation of observed quantities and N is the total number of observations.

Four performance ratings (very good, good, satisfactory and unsatisfactory) are used to provide a qualitative description of the model simulation accuracy. They are based on the values of the above mentioned statistical indicators, as formulated by Moriasi *et al.* (2007). Table 3 shows the range of statistical indicator values associated with a particular performance rating. Once the performance ratings based on each statistical indicator was assigned, a global performance rating was determined. For this, each category was assigned with an integer from 4 (very good) to 1 (unsatisfactory), and an average performance was calculated. For example, if the performance rating for a variable was very good (score = 4) according to PBIAS and RSR, and unsatisfactory (score = 1) according to NSE, then the global performance rating would be good (9/3 = 3).

RESULTS AND DISCUSSION

Table 2 shows the calibrated parameters of the component-models of the integrated faecal bacteria model. The parameters of SWAT and SWMM are not presented here and referred to Leta *et al.* (2012). Table 3 shows different goodness-of-fit statistics used in this study, and a final performance rating based on the statistics. The goodness-of-fit statistics illustrate good quality of the water quantity modelling as well as temperature modelling. For the sediment model, Table 3 shows that the results at Lot, upstream of Brussels, are 'Good' (for the calibration period, and for the validation period). Downstream of Brussels, at Vilvoorde, however the model quality indicators point to a 'Satisfactory' quality of the model. While the very small number of observations (12) has to be taken into account in this assessment, it is probable that (too) simplified representation of the in-sewer processes and, consequently, of the CSO emissions of sediments are at the cause of the mismatch. To complement the goodness-of-fit statistics (Table 3), results of stream flow, temperature, and suspended sediment is presented for Vilvoorde (Figure 5). Following sections discuss the results of faecal bacteria results in detail.

Table 2 | Model parameters

Parameter name and description	Value	Remarks/ references
A. SWAT and SWMM model (water fluxes)		
More information regarding parameter related to water fluxes can be found in Leta *et al.* (2012)		
B. SWAT (sediment)		
More information can be found in Shrestha *et al.* (2013)		
C. Sediment transport model		
Sediment particle specific gravity, s (–)	2.6	Weighted average
Critical sedimentation efficiency coefficient, η_1 (–)	0.007	Calibrated
Critical erosion efficiency coefficient, η_2 (–)	0.009	
D: Temperature model		
Minimum stream temperature, μ (°C)	2	Calibrated
Estimated maximum stream temperature, α (°C)	30	
Steepest slope (infection point) of T_s function, γ (–)	0.1	
Air temperature at this infection point, β (°C)	19	
Lag period (days)	2	
E: Faecal bacteria model		
Decay rate for free *E. coli* (–) at 20 °C	0.045	Taken from Garcia-Armisen & Servais (2009)
Decay rate for attached *E. coli* (–) at 20 °C	0.0225	
Decay rate for sedimented *E. coli* (–) at 20 °C	0.0225	
Partitioning coefficient (L mg^{-1})	0.015	Calibrated

Faecal bacteria model result

The dry weather flow (DWF) simulations

Figure 6 shows that the model represents the variation of the *E. coli* concentration along the river well. This is also shown by the statistical indicators (Table 3), although the PBIAS indicates a slight underestimation of the *E. coli* concentrations. The performance rating was calculated to be 'Very Good'. Between the samplings stations Z1 (the upstream boundary of the model) and Z3, there is no major source of *E. coli* pollution, except some small WWTPs. Hence the *E. coli* concentration tends to decrease in this reach, by mortality and sedimentation. At station Z4, a significant increase of the *E. coli* concentration is observed due to the input from the Beersel WWTP (50,000 IE). The increase of the concentration at Z5, by a factor of ca. 100, is due to the release of the treated effluents of Brussels-South WWTP (360,000 IE), which is known not to function in an optimal way (Brion *et al.* 2012) and to the confluence with a contaminated tributary, the Zuunbeek, which also receives the effluents of the Sint-Pieters-Leeuw WWTP (30,000 IE). The concentration in the Brussels region (Z5–Z9) then gradually decreases. As opposed to the WWTP Brussels South, the WWTP Brussels-North (1.1 million IE and situated just before station Z9) tends to dilute the concentration. With an average removal of 2.6 Log units, the removal of faecal bacteria in this WWTP is quite efficient. Downstream of the border of the Brussels region, no major source of *E. coli* input exists, except from the effluents from the WWTPs Grimbergen (100,000 IE, upstream of Z10) and Zemst-Hofstade (5,000 IE, upstream of Z12). The stations downstream of Z11 are affected by the diurnal tide; hence larger variations of the measured concentration are observed, especially at station Z13. The underestimation at Z13 can be attributed to the lack of robust information regarding the boundary *E. coli* concentration at the outlet.

Figure 7 shows the variation of the free and attached *E. coli* fractions at different GESZ sampling stations during DWF conditions. As expected, the free fraction of *E. coli* dominates in the total *E. coli* population for most of the stations. In general, it can be observed that the free fraction tends to dominate for the stations which are located at considerable distance from a pollution source, presumably as most of the attached *E. coli* have been settled there. Similarly, the attached fraction tends to be about 50% at stations that are located near to a pollution source that discharges high *E. coli* amounts and high suspended matter concentrations, as the latter favour higher adsorption. Hence, the stations, Z2 and Z3, have a dominant free *E. coli* fraction while stations Z4 to Z7 have attached *E. coli* as a slightly higher fraction. At Z8, the free fraction dominates again. The effluent of the Brussels North WWTP is characterised by low *E. coli* and suspended matter concentrations. Hence, the free fraction dominates at Z9. The dominance of the free fraction decreases at stations Z10 and Z11, as the effluent of the WWTP Grimbergen and some untreated sewage is discharged in the river reach. In the tidal reach of the river (stations Z12 and Z13), the free fraction of *E. coli* dominates

Table 3 | Goodness-of-fit-statistics

Variable	Station	Model	Period	Time span	Sample size	PBIAS (%)	RSR	NSE	Performance rating[a]
Stream flows	Tubize	SWAT standalone	Calibration	1998–2008	4,018	– 7.58	0.46	0.79	Very good
			Validation	1994–1997	2,873	3.00	0.59	0.65	Good
	Lot	Integrated SWMM	Calibration	2007	8,760	– 6.16	0.50	0.75	Very good
			Validation	2008	8,784	– 6.02	0.60	0.64	Good
	Vilvoorde	Integrated SWMM	Calibration	2007	8,760	4.62	0.64	0.59	Good
			Validation	2008	8,784	7.12	0.62	0.61	Good
Temperature	U/S Brussels	Standalone	Calibration	1996–2000	133	0.37	0.83	0.84	Very good
	Lot	Integrated temperature	Validation	2007–2008	24	12.23	0.76	0.77	Very good
	Vilvoorde		Validation	2007–2008	26	– 0.41	0.87	0.82	Very good
Sediment[†]	Quenast	SWAT standalone	Calibration	1998–2008	140	– 5.20	1.03	– 0.07	Satisfactory
			Validation	1994–1997	49	– 18.82	1.28	– 0.63	Satisfactory
	Lot	Integrated sediment	Calibration	2007	12	2.98	0.51	0.74	Good
			Validation	2008	12	10.96	0.68	0.54	Good
	Vilvoorde	Integrated sediment	Calibration	2007	12	– 12.58	0.97	0.05	Satisfactory
			Validation	2008	12	– 26.74	1.47	– 1.16	Satisfactory
Faecal bacteria	GESZ stations	Integrated faecal bacteria	Calibration	2009–2010	13	– 24.84	0.48	0.77	Very good
	Eppegem		Validation[b]	2007–2008	16	– 6.19	1.04	– 0.09	Satisfactory
	Leeste		Validation[b]	2007–2008	16	– 3.49	1.13	– 0.28	Satisfactory

[†]Sediment concentrations were ln-transformed before calculating statistics.

[a]Performance rating calculated based on Moriasi *et al.* (2007).

[b]*E. coli* values were log-transformed before calculating statistics.

Performance rating	PBIAS (%) for stream flows	PBIAS (%) for water quality variables	RSR	NSE	Colour scheme
Very good	< ±10	< ±15	0–0.5	0.75–1	
Good	± 10 to ±15	± 15 to ±30	0.5–0.6	0.65–0.75	
Satisfactory	± 15 to ±25	± 30 to ±55	0.6–0.7	0.5–0.65	
Unsatisfactory	> ±25	> ±55	> 0.7	< 0.5	

because the flow velocity in the tidal reach is too low to keep the attached fractions in suspension.

From a management point of view, it should be mentioned that the *E. coli* concentrations in the river Zenne during dry weather conditions are well above EU level for bathing water (900 *E. coli*/100 mL), even for the river reaches upstream of Brussels. Despite the construction of the wastewater treatment plants, the *E. coli* concentrations in the Brussels region (Z5–Z9) remain very high.

The long-term simulations

Figures 8 and 9 show the simulated and measured *E. coli* concentrations (daily maximum and minimum) at Eppegem and Leest respectively, over a period of 14 months. The simulated *E. coli* concentrations are generally in good agreement with the measured concentrations, although some of the peak concentrations do not match well, especially at Leest. This is also reflected by the statistical indicators (Table 3). For both cases, the performance ratings were found to be 'Satisfactory'. The negative values of PBIAS indicate that the model tends to underestimate the *E. coli* concentrations, as was already observed for the DWF simulation (Figure 6). The mismatch at Leest may again be due to the limited information regarding the downstream boundary condition. The higher variation at Leest than at Eppegem is due to the tidal influence. The figures clearly show the increase – up to a factor 100 – of the faecal bacteria concentration during storm events. The latter may be explained by several factors

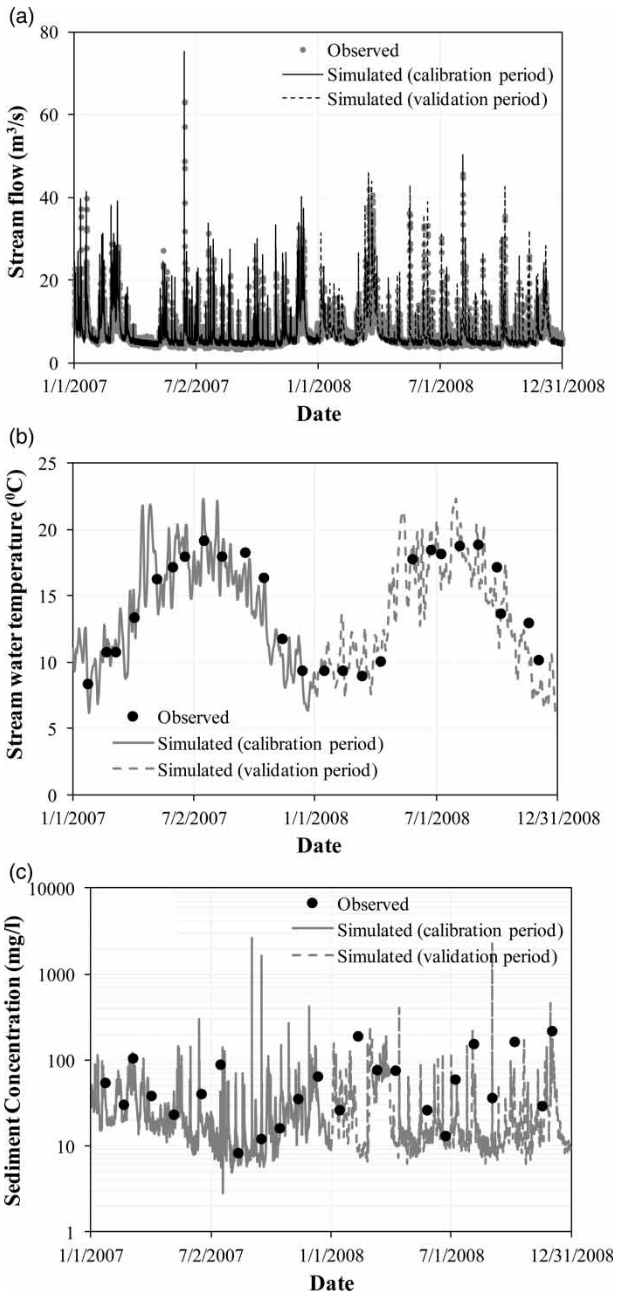


Figure 5 | Plots of (a) stream flow, (b) stream water temperature, and (c) sediment concentration at Vilvoorde.

such as CSOs or, more importantly, higher concentrations in WWTPs effluents during storm events. Unfortunately, no measurements of faecal bacteria concentrations are available for the CSO structures and at the WWTPs in storm conditions. The authors believe that the resuspension of previously settled bacteria during storm events also plays an important role with regard to this phenomenon. The latter has serious implications with regard to the way the bacteria should be modelled: while most of the bacteria models only account for the free-form bacteria and for a one directional disappearance of the bacteria (considering settling only) in addition of mortality, the results shown here indicate that the bottom sediment constitutes a reservoir for bacteria and that resuspension needs to be accounted for.

Calculation time overhead

While the OpenMI based integration ensures the dynamic data exchange between the model components, thereby reducing the cumbersome and error-prone task of data extraction and conversion, it comes at the price of a substantial calculation time overhead. We found the increase of the calculation time to be around 9-fold in the OpenMI integrated sediment transport model (106 h per simulated year on a dual core PC with 3 GHz processer and 3.83 GB RAM) as compared to a SWMM standalone application (about 15 h). The SWMM model is hereby taken as reference as the other modules would require, in a stand-alone run, a negligible computation time as compared to SWMM. As other authors, e.g. Castronova & Goodall (2013), found that the run time communication does not induce a significant overhead, it should be investigated if, in our case, the overhead might not be caused by the way we linked the model components, i.e. by means of sharing the static SWMM network as in Figure 2.

CONCLUSIONS

In the light of growing realisation of the need for an integrated approach to holistic water resources management, any new methodologies, tools and frameworks that support the essence of integrated modelling should be tested and tried sufficiently in different use cases and environments so as to boost the confidence of practitioners. The OpenMI has the potential to become a standard model linking interface. OpenMI has been tested and tried for some time now. At the same time, it is important that we create

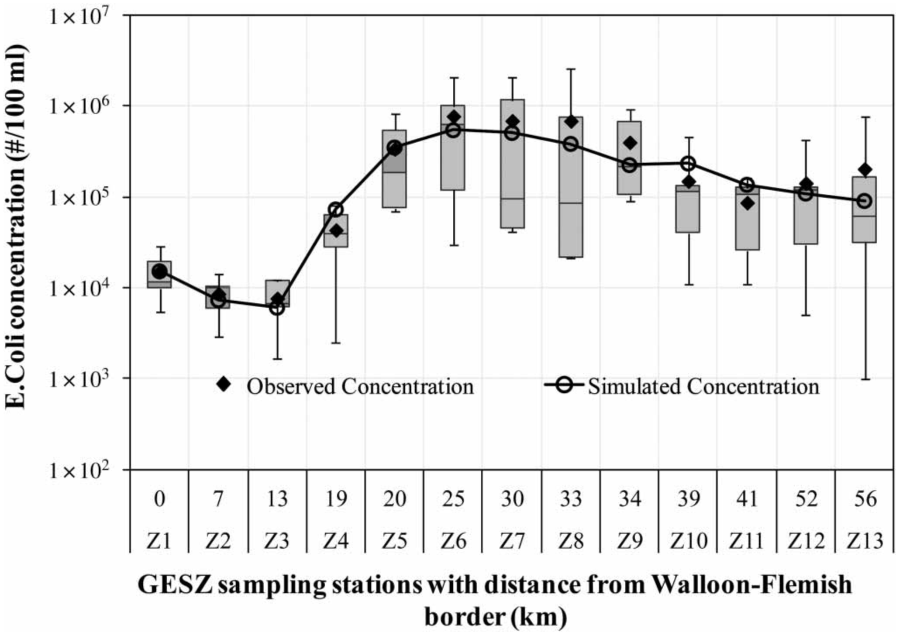


Figure 6 | Measured and simulated *E. coli* concentrations at different GESZ sampling stations (DWF period).

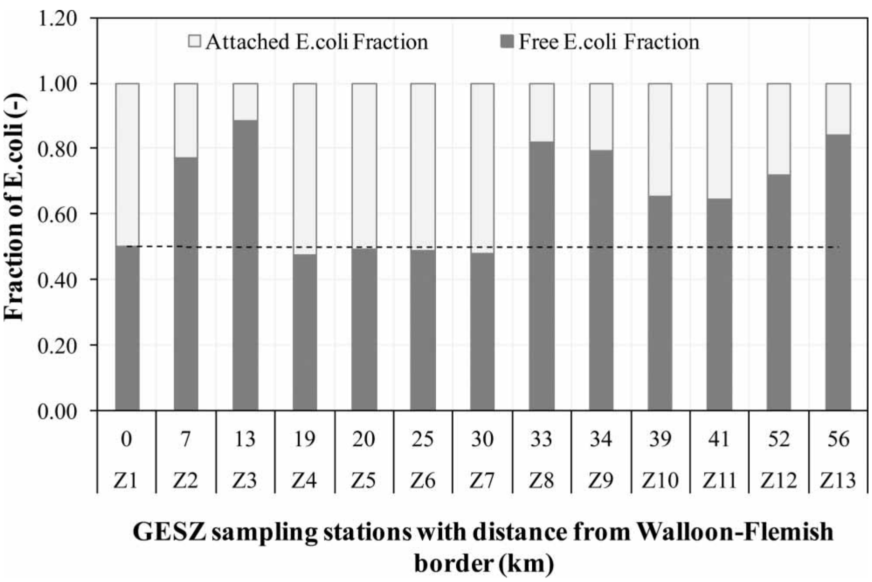


Figure 7 | Free and attached *E. coli* fractions at different GESZ sampling stations for DWF period.

a sufficiently large pool of OpenMI linkable components. Then, practitioners could simply pick and plug the most ‘suitable’ components to form an integrated modelling chain.

Our research has contributed in this respect by making SWMM OpenMI-compliant and developing three other OpenMI components. Additionally, we demonstrated the usefulness and feasibility of employing the OpenMI to

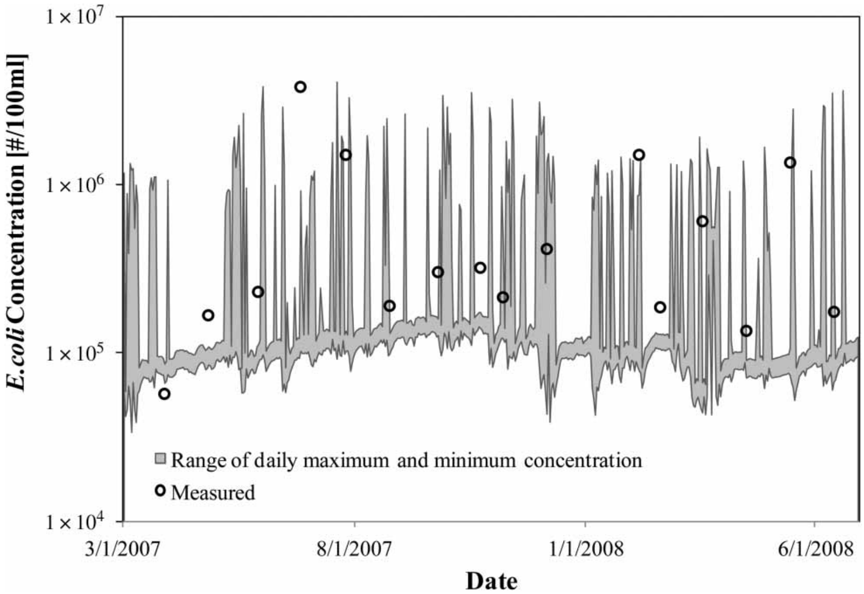


Figure 8 | Simulated and measured *E. coli* concentration at Eppegem.

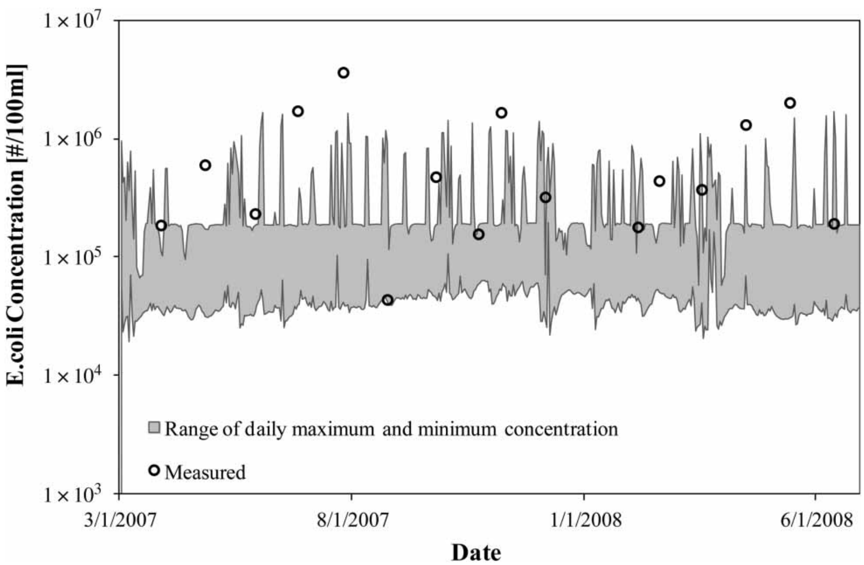


Figure 9 | Simulated and measured *E. coli* concentration at Leest.

perform an integrated simulation using SWAT, SWMM, and newly developed sediment, temperature and faecal bacteria models. We tested this integrated model in terms of the river Zenne in Belgium to simulate faecal bacteria dynamics, with *E. coli* as indicator bacteria.

The results showed that the integrated model can simulate the dynamics of *E. coli* concentrations with 'Very Good', and 'Satisfactory' accuracy for DWF, and long-term simulations, respectively. We are confident that such an integrated approach, which makes use of the best suitable models to build an integrated one for the river basin, can be very useful for supporting integrated river basin management. We also found that the calculation time overhead of the OpenMI-based integrated model is a major drawback of this approach. Hence, solutions for optimising the efficiency of the computer hardware and software, such as grid computing or parallel computing, need to be explored.

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