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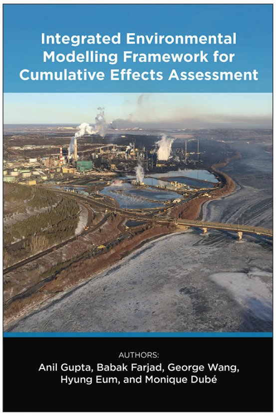

INTEGRATED ENVIRONMENTAL MODELLING FRAMEWORK FOR CUMULATIVE EFFECTS ASSESSMENT

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4.0 INTEGRATED ENVIRONMENTAL MODELLING

Integrated Environmental Modelling (IEM) allows the environment to be considered in a holistic way and provides a science-based system to explain (the past) and predict (the future) behavior of environmental systems in response to human and natural sources of stressors. IEM often requires integrating (spatial) data and computational models from a variety of disciplines (e.g., related to physical, biotic, social, and economic environments) and at different scales, to understand and to solve complex societal problems that arise from the interaction of humans and the environment, and to contribute in this way to establishing the foundation of sustainable development, to inform policy, and to support decision-making (Rothman, 1997; Parker, 2002).

Model integration is achieved by linking together stand-alone models or model components using various coupling approaches. Coupling approaches are defined from various perspectives, such as the degree and direction of linkage. Standard classifications and names have not yet been established. There are a variety of coupling approaches used in this review, which are classified based on the calculation order of model components:

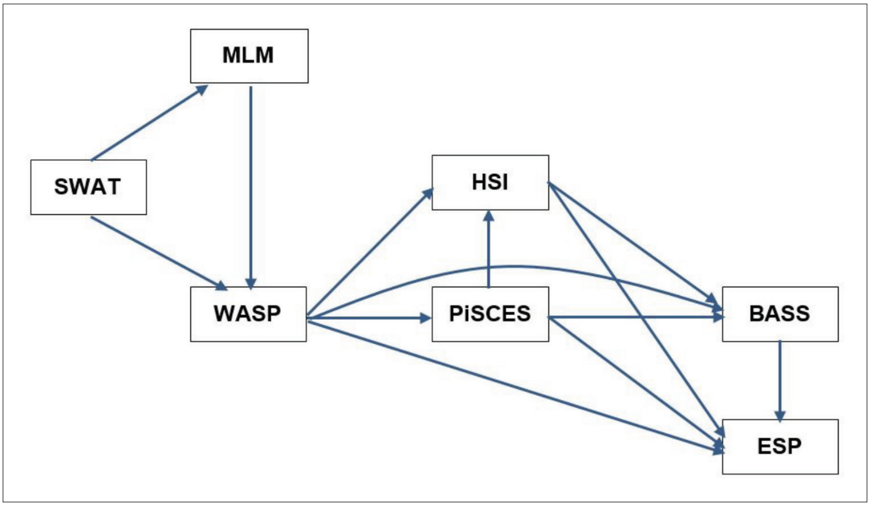
- *Fully coupling*: Equations governing all model components are solved simultaneously within a single monolithic code.
- *Dynamic coupling*: Two or more individual models are tightly coupled via the exchange of data dynamically during simulation at each timestep/predefined frequency.

- *Sequential coupling*: Two or more individual models are sequentially run and loosely coupled via the modelling output files by which the output of one model forms the input of the other.
- *Interactive coupling*: Two or more individual models are run in an alternative order following predefined time periods and loosely coupled via the modelling output files by which the output of one model forms the input of the other.
- *Iterative coupling*: Two or more individual models are loosely coupled by which one model is iteratively called as a slave to provide the output of simulation results to feed another master model.
- *Hybrid coupling*: Component models are integrated with two or more coupling approaches.

The key advantage of fully coupled models is there capacity to solve component models with concurrent feedbacks from each other without a delay in timesteps. There are fewer examples of fully coupled models at regional or watershed scales. The applications mentioned in literature are mainly for integrated subsurface and surface flow and solute transport models, such as MIKE SHE (Farjad et al., 2017a; Farjad et al., 2017b), HydroGeoSphere (Therrien et al., 2010), OpenGeoSys (Kolditz et al., 2012), and Parflow (Kollet & Maxwell, 2006). A dynamically coupled model transfers information at each simulation timestep and acts as a single model or framework component that communicates through feedback mechanisms, such as the MIKE SHE coupled with other models (e.g., MIKE 11) or a set of add-ons, including with DAISY and ECO Lab. Conversely, loosely coupled models lack feedback mechanisms during runs of component models and exchange information through file transfer mechanisms at or after each run of components.

Many stand-alone deterministic hydrological and water quality models are available. However, matching model capabilities with the complexities of natural and engineered systems is a challenge. In recent years, the difficulties in transferring information between models prompted the development of integrated modelling tools. General computer frameworks are available as integration tools for coupling component models, such as the Open Modelling Interface (OpenMI) developed by a consortium of European universities and private companies (Gregersen, Gijsbers, & Westen, 2007), the Object Modelling System (OMS) developed by the United States Department of Agriculture (Ahuja, Ascough II, & David, 2005), and FRAMES (Framework for Risk Analysis Multi-Media Environmental Systems) developed by the USEPA (Babendreier & Castleton, 2005). Figure 7 illustrates an ecological modelling system for assessing the impacts of multiple stressors on stream and riverine ecosystem services within river basins, utilizing FRAMES to combine component models. Although surface and subsurface flow systems are naturally connected, they are often divided into separate compartments due to computational burdens as well as different temporal and spatial scales of the processes involved. This applies to separation of flow between the unsaturated and saturated zone, as well as to surface (i.e., overland and channel) and groundwater flow. Although it sounds ideal to solve the different partial differential equations of all component models simultaneously at each timestep in a fully coupled system, it may be computationally inefficient, as feedback from some components to others is relatively slow. It is reasonable to simulate interactions between the unsaturated zone and the groundwater for a watershed with a shallow groundwater table by using dynamic coupling at certain timestep intervals. For a watershed with a deep groundwater table, where the roots of plants and agricultural practices cannot reach, there is no physical reason to go beyond sequential, interactive, or iterative coupling.

Figure 7. Integrated Ecological Modelling System for the Coal River Basin (from Johnston et al., 2017).



Note: SWAT = Soil Water Assessment Tool, MLM= Mercury Loading Model, WASP = Water Quality Analysis Simulation Program, HSI = Habitat Suitability Index, PiSCES = Piscine Stream Community Estimation System, BASS = Bioaccumulation and Aquatic System Simulator, ESP = Ecosystem Services Processor.

4.1 Integrated surface water–groundwater quantity modelling

Understanding complex interactions between surface and groundwater hydrology is challenging due to the nonlinear hydrodynamic nature of surface and subsurface components, particularly in heterogeneous conditions. This can be even more complex when it comes to the mathematical representation of these interactions in a modelling system. There are a growing number of watershed models capable of simulating integrated surface and subsurface interactions, such as ParFlow, MIKE SHE, CATHY, HydroGeo-Sphere (HGS), PAWS, OpenGeoSys (OGS), PIHM, Cast3M, ATS, GEOtop, and tRIBS+VEGGIE. However, there are few intercomparison studies available in the literature involving regional scales (10^3 to 10^5 km^2). For example, Maxwell et. al. (2014) and Kollet et. al. (2017) conducted an integrated watershed intercomparison study on a series of benchmarking problems. Maxwell et al. (2014) compared several integrated watershed models: CATHY, HGS, OGS, PAWS, ParFlow, PIHM, and tRIBS+VEGGIE. The models simultaneously solved adapted forms of the Richards and shallow water equations based on three-dimensional or mixed (one-dimensional vadose zone and two-dimensional groundwater) formulations for subsurface flow and one-dimensional (rill flow) or two-dimensional (sheet flow) conceptualizations for surface routing. Kollet et al. (2017) used the same approach but a slightly different experiment using the MIKE SHE, ATS, CATHY, Cast3M, GEOtop, HGS, and ParFlow models. Overall, both studies found good agreement between models, especially for simple test cases, whereas some differences were identified that were mostly associated with mathematical and numerical representation or in the parameterization of physical processes. This intercomparison might not be valid for regional scales due to the heterogeneity of landscapes, topography, climatic, geomorphology, stream patterns, density, and geological units.

The Ontario Ministry of Natural Resources (2011) conducted an integrated watershed intercomparison study for regional scales of the most popular integrated models: GSFLOW, MIKE SHE, HydroGeoSphere, ParFlow, and MODHMS. The limitations of each model are summarized in the following section.

GSFLOW

- *Empirical water budget formulation*: While Precipitation-Runoff Modelling System (PRMS) includes a variety of methods for simulating surface water hydrologic processes, not all methods are enabled for integrating MODFLOW in GSFLOW. The GSFLOW implementation of PRMS represents the water interchange between the surface soil zone using three reservoirs: preferential flow, gravity flow, and capillary. The soil zone exchanges flow with the MODFLOW unsaturated zone, and the rate of interchange between these reservoirs is modelled empirically. However, identification of optimal parameters was found to be difficult when completing the case studies.

- *Restricted surface water time-stepping and hydraulic routing*: The GSFLOW implementation of MODFLOW and PRMS does not allow for the timesteps in a surface water model to be less than one day. This limitation may influence the simulation of hydrologic processes such as runoff or infiltration and snowmelt, all of which occur during shorter periods (i.e., sub-daily) within a day. Also, the model cannot represent overland flow routing and complex hydraulic structures, which are important to properly represent surface water flow events that occur during short time periods. Although GSFLOW may be calibrated to account for longer-term hydrologic trends, it should not be considered suitable for many short-term events.

MIKE SHE

- *Uniform Grid Resolution*: The overall capabilities of MIKE SHE would be more advanced if a variable resolution grid system were present. This would allow grid refinement near features of importance such as wells and surface water bodies as well as regions of highly variable topography. From a computational perspective, this would also be beneficial as it would allow for more efficient application of computing resources (e.g., fine model resolution within areas of interest and coarse resolution in surrounding regions).
- *Source code*: The source code is proprietary and not available for examination or modification.
- *Purchase price*: The purchase price of the code is considered to be high as compared to other alternatives. However, the experience gained when completing the case studies demonstrated that the purchase price of the code can be offset on a single project by the time savings realized by having the user interface available, as well as by the overall flexibility offered by MIKE SHE.

HydroGeoSphere

- *Computational effort*: HydroGeoSphere's simulation times may be on the order of weeks for a single scenario, which is not practical for many applications.
- *Surface water hydrologic processes and features*: HydroGeoSphere does not fully account for hydrologic processes such as snowmelt and hydraulic structures.
- *Lack of a graphical user interface*: While processing tools are available for components of the model (e.g., finite element mesh), there is not a single and complete graphical user interface available for HydroGeoSphere, which limits its ability to be cost-effective for most applications.

MODHMS

- *Application in cold regions*: The model does not include winter processes. Snowmelt is arguably one of the most important hydrological processes in cold regions.
- *Source code*: The source code is proprietary and not available to the public for examination or modification.
- *Flexibility*: The model is not flexible in terms of representing various hydrological processes at different levels of complexity (e.g., representing groundwater flow using a linear reservoir approach when subsurface data is sparse).

ParFlow

- ParFlow is primarily a research code that requires third-party software to visualize most of its output.
- ParFlow simulations cannot incorporate hydraulic structures (e.g., dams, weirs, etc.).

Besides the above-mentioned comparison of these models, the MIKE SHE/MIKE 11 model offers two specific benefits which are useful for CEA:

(i) MIKE SHE/MIKE 11 is capable of tracing water and pollutants from the ground surface, through the soil and groundwater, and back into the surface water, (ii) the MIKE package includes some other tools which can be linked to the integrated modelling system for a specific CEA application. For instance, MIKE ECO Lab and FEFLOW can be linked to the watershed model for ecological modelling and advanced localized groundwater quality simulation, respectively.

It should also be noted that while the MIKE SHE/MIKE 11 model is a useful tool for CEA in small to large scale (domain) regions, it might not be capable of supporting large regions when a high spatial resolution (grid size) configuration (e.g., < 200 m) is required. This is because, although MIKE SHE supports parallelized computations, the parallelized approach relies on a shared memory approach (OpenMP), which has limited opportunities for scaling. MIKE SHE's code can take advantage of multi-core processors, however, at a certain point (approximately eight multi-core processors) the cost of communication between parallel processes exceeds the benefits of additional processor cores. Furthermore, single model runs cannot be distributed across multiple computers. In this regard, high-resolution integrated models, called hyper-resolution models, have been developed. These models could enable more realistic process-level simulations that are critical for many important CEA applications at high spatial and temporal resolutions. Hyper-resolution modelling requires large parallel-clustered computing resources and solution algorithms that efficiently use these resources. While such systems are increasingly becoming available to scientists and modellers in many earth science disciplines (e.g., climate modelling) for continental/global scales, environmental modelling communities have been slow to utilize these computational resources for regional scales. Recently, a few studies (Kollet et al., 2010; Maxwell, 2013; Maxwell et al., 2015) have attempted to apply parallel and high-performance computing techniques to simulate surface water and groundwater interactions using high resolution models. For example, Kollet et al. (2010) used an integrated model (ParFlow) to simulate the interactions between land surface processes and variably saturated flow in a heterogeneous subsurface for a maximum number of approximately 8×10^9 grid cells. The parallel performance of the model was investigated based on a scaling assessment on the JUGENE massively parallel supercomputer. JUGENE is an IBM Blue-Gene supercomputer with a total of 294,912 processors and 144TB of memory capable of 0.825 PetaFLOPS (floating point operations per second) and is currently ranked the fourth fastest supercomputer in the world. They indicated that regional scale hydrologic simulations on the order of 103 km^2 are feasible at hydrologic resolution of ~10^0–10^1 m laterally and 10^{-2}–10^{-1} m vertically, with reasonable computation times, which had been previously assumed to be an intractable computational problem. The advantage of developing high-resolution integrated cumulative predictive models is not only motivated by the potential of coupling different environmental processes for cumulative effects assessment, but also because these types of models may be useful in serving as virtual laboratories or realities.

4.2 Integrated watershed and receiving water quality modelling

Although watershed models may have both hydrologic and water quality modules, their capacities to simulate hydrodynamic and water quality processes in receiving water bodies (e.g., rivers) are generally limited and often of one-dimensional and quasi-dynamic state. There is a need to take advantage of the capacities of existing receiving water models in simulating complex hydrodynamics and water quality processes by combining watershed and receiving water models. In such an integrated model, the watershed sub-model simulates and provides discharges (i.e., surface runoff) and loadings (i.e., non-point) to the receiving water quality model, coupled with either a dynamic or a sequential linkage. Some applications are summarized in Table 10 as examples.

For dynamic coupling, OpenMI is commonly reported as a tool for interfacing component models from different disciplines or domains. In the Pinios River catchment in Greece, approximately 10,500 km^2, two alternative integrated models were developed (Makropoulos et al., 2010) for water quality evaluation using OpenMI. The first consisted of the rainfall runoff NAM module of MIKE 11, the hydrodynamic model RISH–1D, and the water quality model RISQ–1D, while the second used NAM, the MIKE 11 hydrodynamic module, and the water quality model OTIS. The same

Table 10. Examples of Integrated Watershed and Receiving Water Quality Modelling Studies

Coupling	**Author**	**Region/watershed scale application**	**Watershed model**	**Receiving water quality model**	**Coupling tool & data exchanges**
Dynamic	Makropoulos et al., 2010	Pinios River catchment (10,500 km^2), Greece, integrated hydrologic, hydraulic, and water quality modelling	NAM	MIKE 11 & OTIS; or, RISH-1D & RISQ-1D	OpenMI, links for node connection, flow, water level, BOD concentrations.
	Shrestha et al., 2013	River Zenne, Belgium, integrated sediment transport modelling	SWAT	SWMM	OpenMI, SWAT output as upstream boundary condition for SWMM model.
	Mentzafou & Dimitriou, 2011	Evros river basin, 2,778km^2, Greece	MIKE SHE	MIKE 11	Add-on in single code, coupling flow, recharge, nitrate concentrations.
	Malek-Mohammadi et al., 2012	Upper East Fork Poplar Creek watershed, Tennessee	MIKE SHE	MIKE 11 + ECOLAB	Add-on in single code, coupling flow, recharge, TSS, and mercury concentrations.
Sequential	Michael Baker Jr. Inc. et al., 2015	Illinois River watershed, Oklahoma	HSPF	EFDC (3D)	User defined linkages via output and input text files. The HSPF model hourly results are used to provide streamflow, water temperature, suspended solids (TSS), organic carbon, nutrients (N, P), algae biomass, and dissolved oxygen as input data for the EFDC lake model.
	Sutula et al., 2016	Santa Margarita River Watershed, California, nutrient management	HSPF	EFDC + WASP (3D)	User-defined linkages via output and input text files, coupling hourly flow, nutrient loads.

Table 10. (*continued*)

Huang et al., 2017	Ribble catchment, Northwest England, 12,920 km^2	HSPF (rual area) + Infoworks (urban area) + DMHSF (for fecal indicator)	RMN 1D (river) + EFDC (2D estuary)	User defined linkages via output and input text files, coupling flow and E. coli.
Privette et al., 2015	Reedy River watershed, South Carolina	LSPC	WASP (3D)	User defined linkages via output and input text files, coupling hourly flow, total phosphorus, and total nitrogen.
Shabani et al., 2017	Devils Lake watershed, North Dakota	SWAT	CE-QUAL-W2	User-defined linkages via output and input text files, coupling daily flow and sulfate loads.
Yue & Derichsweiler, 2005	Cobb Creek Watershed, Oklahoma	SWAT	EFDC	User-defined linkages via output and input text files, coupling daily flow, Chlorophyll-a, CBOD, Nitrate, Organic N, Mineral P, and Organic P loads.
J. M. Johnston et al., 2011	Albemarle-Pamlico Watershed, North Carolina and Virginia	SWAT + WMM (watershed mercury model)	WASP	USEPA's FRAMES was used to define linkages, coupling daily flow, nutrients, and mercury.
Mankin et al., 1999	Melvern Lake watershed, Kansas	AGNPS	EUTROMOD	User-defined linkages via output and input text files, coupling annual flow and nutrient loads.

pollution loads for both diffusive and point sources were assumed in both integrated models, and the same BOD decay coefficient and dispersion coefficient were used in both RISQ-1D and OTIS. The comparative analysis of the two configurations illustrated the significant differences for two river nodes between model components and (consequently) model results, even when OpenMI was used as the integrating medium and the model schemes were set up for the same study area by collaborating modelling teams. It is suggested that this variation is therefore a measure of the uncertainty related to the input data discrepancies and different modelling techniques. The visualisation of this significant uncertainty may be very important for decision-making, including but not restricted to the identification of the required level of water treatment for local communities.

An OpenMI-based integrated model was developed for the purpose of simulating the sediment dynamics for the River Zenne in Belgium using SWAT to model water and sediment fluxes from rural areas and SWMM to simulate the hydraulics of the river, canal, and sewer systems in the downstream urban catchments (Shrestha et a., 2013). The SWAT model essentially formed the upstream boundary condition for the SWMM model.

MIKE SHE is fully and dynamically integrated with a channel flow, transport code MIKE 11, water quality, and the ecological module ECO Lab. The exchange of surface and subsurface water and the loadings between the two components take place during the whole simulation run. As the MIKE SHE/MIKE 11 system is a ready-to-use commercial package without a need for integration programming efforts, it can be directly applied to simulate groundwater, surface water, sub-subsurface interactions, receiving water hydrodynamics, and advection/dispersion processes, while the water quality kinetics are simulated using ECO Lab in a single model. For example, the system has been applied to analyze the mercury cycle in the environment and provide forecasting capabilities for the fate and transport of contamination within the Upper East Fork Poplar Creek watershed in Tennessee (Malek-Mohammadi et al., 2012) and the transport and fate of nitrate in the Evros River basin in Greece in a large area about 2,778km^2 (Mentzafou & Dimitriou, 2011).

In scientific and gray literature, many integrated watersheds and receiving water quality models developed using a sequential coupling approach have been reported. For integrated water quality modelling, HSPF and SWAT are the two most selected watershed models, while MIKE 11, EFDC, and WASP are frequently selected hydrodynamic and water quality models (Huang et al., 2017; Johnston et al., 2011; Mankin et al., 1999; Michael Baker Jr. Inc, Aqua Terra Consultants, & Dynamic Solutions LLC, 2015; Privette et al., 2015; Shabani et al., 2017; Sutula et al., 2016; Yue & Derichsweiler, 2005).

4.3 Integrated watershed and groundwater quality modelling

To evaluate the impacts of climate and land-use changes on water resources (surface and groundwater; quantity and quality) at a regional to watershed scale requires an integration of watershed, groundwater, and receiving water quality models which is capable of simulating all the important processes of hydrogeological cycle. Table 11 outlines several studies that attempted to integrate a watershed model with groundwater and receiving water quality models through a sequential coupling. Only few systems are reported with the dynamic coupling of all groundwater, watershed, and complex receiving water and transport models, including MIKE SHE/MIKE 11 model, which has been described in previous sections.

Klammler et al. (2013) implemented a sequential coupling of the one-dimensional unsaturated water flow and nitrate transport model SIMWASER/STOTRASIM with the two-dimensional saturated approach of FEFLOW to simulate the nitrate leaching from the soil zone into the aquifer Westliches Leibnitzer Feld in Austria to evaluate the impact of agricultural practices on groundwater quality. The results of the unsaturated water model (water and nitrate flux) are provided as the upper time series boundary condition to the FEFLOW model.

Narula and Gosain (2013) applied SWAT, MODFLOW, and MT3DMS to model hydrology, groundwater recharge, and non-point nitrate loadings in the Himalayan Upper Yamuna basin in India. The groundwater recharge and nitrate (NO_3) loads simulated by the SWAT model are linked to the groundwater flow model (MODFLOW) and the multi-species transport model (MT3DMS). The hydrologic terms simulated by SWAT for each sub-basin were transformed to the system of units specified for MODFLOW's simulation. Grid cells of MODFLOW were associated with the geographical extent of sub-basins simulated by SWAT. Groundwater limits for the model correspond to those of the surface water basin. These boundaries were designated as no flow boundaries. A similar integrated modelling framework was developed by Pulido-Velazquez et al. (2015) for the integrated assessment of the impact of climate and land use changes on groundwater quantity and quality in the Mancha Oriental system in Spain by sequentially coupling a watershed agriculturally based hydrological model (SWAT) with a groundwater flow model developed in MODFLOW, and with a nitrate mass-transport model in MT3DMS. SWAT model outputs (mainly groundwater recharge and pumping, considering new irrigation needs under changing evapotranspiration and precipitation) were used as MODFLOW inputs to simulate changes in groundwater flow, storage, and impacts on stream-aquifer interactions. SWAT and MODFLOW outputs (the nitrate load from SWAT and groundwater velocity field from MODFLOW) are used as MT3DMS inputs for assessing the fate and transport of nitrate leached from the topsoil.

Ameli and Creed (2017) developed a linked subsurface–surface model to assess the continuum of time and distance variations of hydrologic connectivity of wetlands in the Beaverhill watershed, Alberta, characterized by the high density of geographically isolated wetlands. A three-dimensional steady-state groundwater-surface water interaction model was used to simulate watershed-scale subsurface flow and velocity fields as well as to calibrate the infiltration rate. These model results were then used to map watershed-scale subsurface connections. The two-dimensional transient fill-and-spill surface flow routing approach within the numerical, physically based HydroGeoSphere model was linked to the output of the groundwater model and used to simulate the watershed-scale surface water level and overland flow routing, and ultimately to determine the surface connectivity of wetlands using a transient water particle tracking scheme. The performance of the model was also assessed using chemical (Ca, Mg, EC and TDS) and isotopic (^{18}O and ^{2}H) tracer data.

Table 11. Examples of Integrated Watershed and Groundwater Quality Modelling Studies

Coupling	**Author**	**Application region/ watershed**	**Watershed model**	**Groundwater model**	**Coupling tool & data exchanges**
Sequential	Klammler et al., 2013	Westliches Leibnitzer Feld, Austria, 44 km^2	SIMWASER/ STOTRASIM	FEFLOW	A specific add-in module for FEFLOW is developed to link recharge and nitrate concentration.
	Narula & Gosain, 2013	Himalayan Upper Yamuna basin, India, 11,600 km^2	SWAT	MODEFLOW + MT3DMS	User-specified transform and coupling for recharge and nitrate concentration.
	Pulido-Velazquez et al., 2015	Mancha Oriental system, Spain	SWAT	MODEflow + MT3DMS	User-specified transform and coupling for recharge, pumping flow, and nitrate concentration.
	Ameli & Creed, 2017	Beaverhill watershed, Alberta	A 3D groundwater–surface water interaction model	HGS	User-specified transform and coupling for recharge, pumping flow, and chemical and isotopic tracer concentrations

4.4 Integrated groundwater and receiving water quality modelling

There is a transition zone where groundwater and surface water interact. This is an ecologically active zone where contaminants from upland areas that are transported by groundwater can be retained within sediments and transported to the receiving surface water. Similarly, contaminants discharged to the surface water can be a source of contamination to groundwater if the surface water recharges the underlying aquifer. Both sediments and surface water provide a pathway by which contaminants can enter to the groundwater systems. The transition zone is strongly influenced by the dynamic exchanges between groundwater and surface water and changing biogeochemical conditions (Bobba, 2012).

Traditional approaches to model groundwater–surface water interactions often focus on representing one hydrological system in detail and the other as a boundary condition without explicitly considering the effects of feedback between the two systems. Models in this category are integrated using a sequential coupling approach. For example, to simulate pit lake water quality, modelling knowledge from different scientific domains such as groundwater, lake circulation, hydrochemistry, and limnology needs to be combined. The modelling system MODGLUE couples the groundwater flow and transport model PCGEOFIM with the lake circulation water quality model CE-QUAL-W2 and the hydrochemical model PHREEQC (Müller et al., 2008). Jia et al. (2015) developed a linked surface water and groundwater simulation model to assess the impact of a trans-basin water diversion project on the groundwater. By using results of the surface water simulation as input for the groundwater simulation, a surface water quality WASP and a groundwater model MODFLOW plus MT3 were sequentially coupled to simulate the water levels and four contaminants (NH3-N, COD, Mn, F, As).

In cases where relatively large, dynamic, bidirectional exchanges are anticipated, the interfacial processes cannot be adequately represented by using an uncoupled interaction to represent surface water in a groundwater model or with a source term to represent groundwater flux in a surface water model. Although the existing ready-to-use integrated subsurface and surface water and solute transport models such as HGS and MIKE SHE are capable of simulating groundwater–surface water interactions, they do not appear to provide a full representation of sediment/benthic processes. Mugunthan et al. (2017) developed an interface module that holistically simulates fate and transport by dynamically coupling two commonly used models, AQFATE and SEAWAT, to simulate surface water and groundwater hydrodynamics, while providing an enhanced representation of the processes in the transition zone. AQFATE is an enhanced version of the EFDC model (Connolly et al., 2000). SEAWAT is a groundwater model developed by USGS which combines MT3DMS's solute transport capabilities with MODFLOW to simulate density effects on groundwater flow

(Langevin et al., 2008). The interface code is developed in FORTRAN, the same language used in the original SEAWAT and AQFATE models. At each groundwater sub-model timestep, the modelling framework represents the surface water body as a boundary condition. Constituent concentrations (temperature, salinity, or contaminants) are passed to SEAWAT. Upon completion of the first and subsequent groundwater sub-model timesteps, the AQFATE sub-model is simulated for the corresponding period with the flows and mass fluxes calculated by SEAWAT at the interfacial grid cells passed to AQFATE through intermediate variables in the interface module code. The modelling framework was tested with a published test problem and applied to evaluate field-scale two- and three-dimensional contaminant transport. The model accurately simulated concentrations of salinity from a published test case. Table 12 lists some examples of integrated groundwater and receiving modelling studies.

Table 12. Examples of Integrated Groundwater and Receiving Water Quality Modelling Studies

Coupling	**Author**	**Application region/ watershed**	**Groundwater model**	**Receiving water quality model**	**Coupling tool & data exchanges**
Dynamic	Mugunthan et al., 2017	A former oil refinery site in Western Canada	SEAWAT	AQFATE (an enhanced version of EFDC)	User-developed interface module, coupling flow, and concentrations
Sequential	Müller et al., 2008	Several mine pit lakes in Germany	PCGEOFIM	CE-QUAL-W2 PHREEQC	User-developed interface, coupling flow, water level, and water quality parameters
	H. Jia et al., 2015	Chaobai River alluvial plain, Beijing, China	MODFLOW + MT3D	WASP	User defined text files, coupling flow, water level, concentrations of NH3-N, COD, F, As

4.5 Integrated atmospheric deposition and water quality modelling

Atmospheric wet and dry deposition can be important non-point-source contributors to total pollutant loadings to water bodies, both through direct deposition to water bodies and deposition to watersheds with subsequent transport into water bodies. In a study of the nitrogen budgets of 16 catchments in the northeastern United States, atmospheric deposition was found to be the largest source of nitrogen input to the catchments, contributing about 31% to the overall budget (Boyer, 2002). Atmospheric deposition can affect ecosystems in numerous ways including acidification and eutrophication. Acidification of lakes and streams is primarily caused by the atmospheric deposition of sulfur (S) and reactive nitrogen (N) to watersheds, with some impact from direct deposition to lakes. The deposited chemicals undergo subsequent biogeochemical cycling and the transfer of chemicals to surface water systems (Paerl, Dennis, & Whitall, 2002; Sullivan et al., 2008).

Quantification of the atmospheric deposition is important to water quality studies. Watershed-scale fate and transport models such as SWAT and HSPF use this information to estimate loadings to rivers and watersheds, for use in TMDL developments and other water quality assessment and management plans. However, obtaining good estimates of atmospheric wet and dry depositions can be challenging. Direct measurement of deposition, particularly dry deposition, can be difficult and very expensive to monitor at several sites in a watershed (Schwede, Dennis, & Bitz, 2009). Atmospheric deposition models, generally classified as Eulerian and Lagrangian models, can be used to fill in spatial or temporal holes left by a monitoring program and predict future conditions due to growth or regulatory changes (NEIWPCC 2017). Eulerian models perform calculations of atmospheric chemistry, transport, and deposition of pollutants based on grids. Eulerian models are effective for capturing the complex nonlinear chemistry necessary to model ozone, nitrogen, sulfur, and mercury accurately. Examples of Eulerian models include the Regional Acid Deposition Model (RADM), the Regulatory Modelling System for Aerosols and Deposition (REMSAD), and the Community Multiscale Air Quality (CMAQ) model. Lagrangian models generally work well for toxic compounds that have simple decay or linear atmospheric chemistry. These models track emission plumes that spread out toward some receptors, such as an estuary, where deposition is taking place, based on the receptor's chemical and physical parameters and meteorology. Examples of Lagrangian models include the Regional Lagrangian Model of Air Pollution (RELMAP) and the California Puff Model (CALPUFF).

For integrated air and water quality management, there have been significant advances in the development of integrated airshed, watershed, and water body modelling and analysis technologies. A sequential coupling approach is generally used to link the output of a deposition model to watershed and receiving water quality models. In the United States, models of the Chesapeake Bay airshed, watershed, and tidal waters have been created and linked to model daily atmospheric deposition loading and the impacts on bay water quality and resources (e.g., underwater grasses, benthic communities, pelagic fish habitats) (Ackermann, 1997). In particular, the Regional Acid Deposition Model (RADM) has been used to delineate the airshed contributing nitrate to the Chesapeake Bay watershed and water surface (Dennis, 1997). Burian et al. (Burian et al., 2002) developed an integrated modelling framework composed of a CIT urban air chemistry model, a SWMM urban runoff model, and a WASP water quality model. The models were linked to simulate the fate and transport of air emissions of nitrogen compounds in the air, urban watersheds, surface water runoff, and a coastal receiving water body. The model linkage is demonstrated by evaluating the potential water quality implications of reducing NOx emissions by 32%, volatile organic compound emissions by 51%, and ammonia emissions by 30%, representing changes from the 1987 levels to the proposed 2000 target levels in Los Angeles, California.

Sequential coupling requires post-processing the dry and wet deposition outputs from a deposition model into an input format required by watershed and receiving water quality models. For example, a tool called the Watershed Deposition Tool was developed for providing the linkage between air and water quality modelling and for analyzing related non-point-source impacts on the watershed. Using a gridded output of atmospheric deposition from the CMAQ model, the tool calculates the average per unit area and total deposition to selected watersheds and sub-watersheds (Schwede et al., 2009).

4.6 Integrated load allocation and water quality modelling

Load allocation is the distribution of pollutant loadings among point and non-point sources in a watershed such that the receiving water body is ensured to be compliant with water quality standards. In the United States, Section 303(d) of the *Clean Water Act* established the total maximum daily load (TMDL) approach to water quality management. A TMDL is the maximum loading rate of a pollutant that can be sustained in a water body without water quality impairments. It also specifies the maximum amount of a pollutant that a waterbody can receive and still meet water quality standards and allocates pollutant loadings among point and non-point pollutant sources. A TMDL is the sum of the individual waste-load allocations (WLAs) for point sources, load allocations (LAs) for non-point sources, and the natural background with a margin of safety (USEPA, 2008).

In most load allocation analyses or TMDL developments, load reduction scenarios are evaluated through trial and error (TAE) simulations, using a process-based watershed water quality model. However, the TAE simulation method does not necessarily generate cost-effective, reliable, and equitable load allocations (Y. Jia & Culver, 2006). To overcome the limitation of TAE scenario analysis, coupled simulation-optimization models have been built and recommended to develop optimal load allocations (USEPA, 2008). One of the challenges of applying optimal management strategies for load allocation is defining an appropriate objective function, decision variables, and constraints. Potential objectives may be maximization of equity among sources, minimization of total load reduction, maximization of total net benefit, or minimization of total cost. For example, the same percentage reduction in load contribution could be applied to sources of similar types, or the maximum difference in percentage reduction among sources can be defined as constraints. Although it may be desirable to maximize the benefit or minimize the cost of load reductions, this requires substantial site-specific information about the types of management alternatives and associated costs and benefits. Multiple objective optimization (Allam et al., 2016) and game theoretical models (Nikoo, Beiglou, & Mahjouri, 2016) have often been developed for load allocation in order to take into account stakeholders in the negotiation processes.

The water quality constraints are generally based on simulated receiving water quality and water quality guidelines or limits. The optimization-simulation load allocation model is essentially an iteratively coupled model, which requires repeated calls of the water quality model to solve the optimization model. For instance, multiple objective models were developed and applied to the Gharbia drain in the Nile Delta in Egypt during both the summer and winter seasons of 2012 through the integration of a water quality model QAUL2Kw and a genetic algorithm, by considering the total waste load abatement and the inequity among waste dischargers. The steady water quality model was directly coupled and iteratively run to produce BOD_5 concentrations for a particular arbitrary treatment level during the process of optimization.

To reduce the prohibitive computational resources often required by the iteratively coupled model, an indirect simulation-optimization framework utilizing a response matrix approach is commonly used to replace the iterative calls of the water quality model (Y. Jia & Culver, 2006). In this approach, output of the water quality model runs are used to derive a linear response matrix (Y. Jia & Culver, 2006), load delivery factors (Shortle et al., 2016), transfer coefficients (Nikoo et al., 2016; Zolfagharipoor & Ahmadi, 2016), or nonlinear stressor-response relationships (F. Zhou et al., 2015), which are then read by the optimization model to find the solution. Therefore, an iterative coupled optimization-simulation problem is transformed into a sequentially coupled simulation-optimization model. A robust optimization approach to minimize total load reduction was successfully developed by Jia and Culver (2006) using sequential coupling with a response matrix and applied to the fecal coliform TMDL study in the Moore's Creek watershed located in Albemarle County, Virginia, USA. The response matrix was defined with elements representing temporal changes in water quality with unit load reduction for each source derived based on water quality simulation time series results. One advantage of the robust formulation of TMDL allocations is that the uncertainty of the watershed simulation model, HSPF, is incorporated into the load allocation optimization model by introducing the probability of acceptable parameter sets of the watershed model and corresponding simulated baseline

Table 13. Examples of Integrated Load Allocation and Water Quality Modelling Studies

Coupling	Author	Application region/ watershed	Load allocation model	Water quality model	Coupling tool & data exchanges
Iterative	Allam et al., 2016	Gharbia catchment, Egypt, 2940 km^2	Minimize total waste abatement; minimize inequity among wastewater dischargers	QUAL2Kw	Direct coupling steady water quality model (BOD5/ DO) with optimization model
Sequential	Y. Jia & Culver, 2006	Moore's Creek watershed, VA	Minimize total weighed load reduction	HSPF	Response matrix for instream fecal coliform concentrations to 1% reduction of loads
	Nikoo et al., 2016; Zolfagharipoor & Ahmadi, 2016	Zarjub River, Iran	Non-cooperative and cooperative game theoretic multiple-pollutant waste load allocation models	QUAL2Kw	Transfer coefficients and trading ratios, determined based on the results of a calibrated QUAL2Kw model for BOD/DO and TN
	Zhou et al., 2015	Swift Creek Reservoir, Chesterfield County, VA	Enhanced-interval linear programming for nutrient TMDL allocation	CE-QUAL-W2	Nonlinear stressor-response relationships
	Shortle et al., 2016	Chesapeake Bay watershed, MD	Cost minimization static and dynamic optimal models	Chesapeake Bay Watershed Model (CBWM)	Delivery factors, land areas, and baseline nutrient loadings based on watershed modelling

source load contributions into the objective function and water quality constraints, respectively. A total of 381 acceptable parameter sets for the Moore's Creek HSPF model were established using the Monte-Carlo-based generalized likelihood uncertainty estimation (GLUE) approach with 50,000 HSPF runs (Beven & Binley, 1992; Y. Jia & Culver, 2008). The likelihood value of each of these is calculated using a fuzzy logic procedure. The robust optimization model was then solved using a genetic algorithm. Some of the integrated load allocation and water quality modelling studies are listed in Table 13.

4.7 Integrated water allocation and water quality modelling

Water allocation is the combination of actions that enable water users to take or to receive water for beneficial purposes according to a recognized system of rights and priorities (UN-ESCAP 2000). Water allocation is central to the management of water resources, which often engages multiple stakeholders with conflicting interests. Dinar et al. (1997) discuss four basic institutional mechanisms for water allocation: user-based allocation, marginal cost pricing, public allocation, and water markets allocation. Water allocation models have been developed for different purposes such as water rights allocation (Labadie, 1995; L. Wang, Fang, & Hipel, 2007), economic optimal water allocation (McKinney, 1999), and cooperative, fair, efficient, and sustainable water allocation (L. Wang, Fang, & Hipel, 2008). Although the inseparable interaction of water quantity and quality clearly exists in all river basins, most water allocation models focus on water quantity with interactions, if any, accounted for by superficial trial and error processes. This trial and error water allocation with consideration of water quality is achieved based on a simple sequential coupling, i.e., a water allocation model is run to provide flow inputs for subsequent water quality modelling (Salla et al., 2014). To eliminate the limitations of the trial and error approach, water quality models have been directly linked to optimal water allocation models and are iteratively called to run for each potential water allocation. One typical iteratively coupled water allocation model is the MODSIMQ model developed by Dai and Labadie (2001). The

Table 14. Examples of Integrated Water Allocation and Water Quality Modelling Studies

Coupling	**Author**	**Application region/ watershed**	**Water Allocation model**	**Water quality model**	**Coupling tool & data exchanges**
Iterative	Dai & Labadie, 2001	Arkansas River Basin, CO	MODSIMQ	QUAL2E	Frank-Wolfe nonlinear programming algorithm, coupling salinity concentrations
	D. Liu et al., 2013	Northwest Pearl River Delta, China	Multi-objective Water quantity and waste load allocation model: minimize water shortages, maximize economic interest, maximize waste load discharges subject to water quality targets	1D advection–dispersion water quality model	Non-dominated sorting GA-II (NSGA-II) algorithm, coupling COD concentration
Sequential	Salla et al., 2014	Araguari River basin, Brazil	SIMGES module of AQUATOOL	GESCAL module of AQUATOOL	Text files, coupling oxygen, biochemical oxygen demand, organic nitrogen, ammonia, nitrate, and total phosphorus
	Tavakoli et al., 2014	Dez River, Iran	An optimization model based on equitable allocation of water to users in proportion to their water demands	Soil,Water, Atmosphere, and Plant (SWAP) simulation model	Iterative linear programming (ILP), coupling 5 meta-models, each zone representing the relationships between quantity and quality (TDS) of return flow versus the allocated water
	Heydari et al., 2016	Zayanderood river basin, Iran	Multi-Objective Optimization Model: minimize relative water deficit, minimize annual groundwater level changes, minimize the groundwater quality change	MODFLOW and MT3DMS models	Two surrogate models, namely an Artificial Neural Network model for groundwater level simulation and a Genetic Programming model for TDS concentration prediction were coupled with NSGA-II

MODSIM river basin water rights planning model developed at Colorado State University is extended by MODSIMQ, integrating with the Frank-Wolfe nonlinear programming algorithm to directly include conservative routing of water quality constituents, maintenance of salinity load mass balance, and the imposition of constraints on water quality concentrations. Water quality constraints can be imposed based on (i) quality standards for certain river reaches, (ii) irrigation water quality control, (iii) water quality preference for demand nodes, and (iv) groundwater quality rehabilitation. An iterative procedure between MODSIMQ and QUAL2E assures convergence to solutions that satisfy water right priorities, while attempting to maintain minimum streamflow and water quality requirements. In the literature, there are a few studies on simultaneous water resources and waste load allocation in river basins, in which waste loads are also included as decision variables and objective functions (D. Liu et al., 2013).

Generally, integration of a nonlinear simulation model in a management model is difficult and computational time to achieve the optimal solution may be a constraint (Singh, 2014). The required computational time can be reduced via approximations of the simulation model by using simplified response matrixes or surrogate models as alternatives to actual complex numerical models (Heydari, Saghafian, & Delavar, 2016; Tavakoli et al., 2014). The actual complex water quality models are sequentially coupled to water allocation models through the approximate relationship or surrogate models between water quality and quality. Table 14 lists some examples of integrated water allocation and water quality modelling studies.