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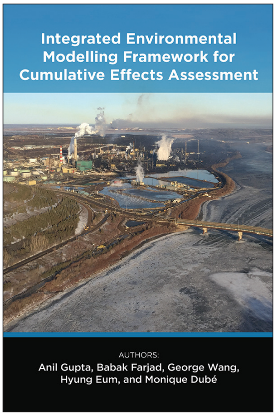

INTEGRATED ENVIRONMENTAL MODELLING FRAMEWORK FOR CUMULATIVE EFFECTS ASSESSMENT

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3.0 MODELLING APPROACHES FOR EACH COMPONENT

3.1 Hydrological models

Hydrological models are used to quantitatively analyze hydrological processes. They are applied to understand the dynamic interactions between the climate and land surfaces by simulating complex interaction processes in the hydrological cycle, which are subject to both normal and extreme climate conditions (Zhang, 2007) or to changes in the physical characteristics of a land surface.

The study of hydrological modelling dates back to the 1850s when Mulvany (1850) used a rational method to calculate the volume of runoff based on the percentage of rainfall and watershed area (Zhang, 2007). Sherman (1932) developed a unit hydrograph concept in which the runoff process was assumed to be linear and time invariant (Dawdy, 1983). The first runoff model based on physical processes was developed by Horton (1933) using the infiltration-excess runoff theory (Zhang, 2007). In the 1950s, Kalinin and Milyukov (1958) developed a channel routing method using linear analysis (Dawdy, 1983).

The classification of models helps to understand their capability and structure, while each class is an individual representation of the hydrological cycle. There is no universal model to simulate and characterize watershed hydrology; models are classified in different ways depending on the criteria of interest. Selection of these models is based on the spatial and temporal scale of the studies, the type of watershed, the modelling objective (Zhang, 2007), data availability, and economic constraints.

This current study distinguishes models that treat a watershed as a spatially variable system in three classes: lumped, semi-distributed, and distributed models.

3.1.1 Lumped models

Lumped models consider the watershed as one computational unit, with state variables representing average values of watershed characteristics, such as the total rainfall, soil moisture, or overland flow. The derivation of such variables depends on empirical relationships derived by various techniques, including curve fitting, using available monitoring data.

Lumped models rely on the techniques of systems analysis in relating inputs to outputs without reference to the internal and physical mechanisms of the watershed. Calibration of the model is based on the comparison between observed and simulated watershed outflows. There are different lumped models with different functional forms defined intuitively. These models are commonly called conceptual models in hydrology.

Generally, flow-routing mechanisms over the watershed area are ignored in lumped models (Beven, 2001). The discharge of lumped models is based on the global dynamics of the system. These models ignore infiltration of surface runoff and its connection with river flow since they are not physically based. They require many assumptions that increase the uncertainty of the models. For instance, precipitation is considered uniformly distributed over the watershed spatially and temporally. LULC, soil, and geology are also assumed uniform across a watershed (Reed, 2004). Although they have some advantages such as having a simple structure and easy setup, calibration, and use, they require long-term historical data for calibration and the parameter values may be potentially difficult to physically interpret.

Numerous studies have used different lumped models for hydrological studies. Four examples of lumped models are listed in Table 3 and described as follows:

IHACRES: Croke and Jakeman (2007) applied the IHACRES model that was originally designed for temperate climates to assess streamflow in three different climatic regions in Australia. They concluded that the model is suitable for arid and semi-arid catchments. However, they also suggested that the length of the calibration period should be increased to accommodate the lower frequency of streamflow events.

SRM: Kustas et al. (1994) used three different approaches for modelling snowmelt: 1) a degree-day model called the snowmelt runoff model (SRM); 2) a restricted degree-day model, characterized by a simple radiation component combined with the degree-day approach to improve estimates of snowmelt and reduce the need to adjust the melt factor over the ablation season; and 3) a daily energy balance model. They tested the three approaches using melt rates with lysimeter outflow measurements. The restricted degree-day and energy balance models produced better results than the snowmelt runoff model.

WATBAL: Yates (1996) investigated the impact of climate change on discharge in Arkansas. He selected two different basins to evaluate the range of the model's applicability; one (Mulberry River) in a humid climate that was dominated by winter rainfall and warm summers and a second one (East River) in a semi-arid region that was dominated by snowfall and colder temperatures. WATBAL as a water balance model combined with the Priestley-Taylor method were used to estimate potential evapotranspiration. The WATBAL model was originally designed as a simple model to assess the impact of climate change on a watershed. The parameters of the model are direct runoff, surface runoff, subsurface runoff, maximum catchment water-holding capacity, and baseflow. The results revealed that the model behaves fairly well, given its simplicity. The model showed the sensitivity to precipitation change in the Mulberry Basin. They suggested that WATBAL lacks seasonal parameters, as there was a strong seasonal variation in runoff in the Mulberry Basin.

USDAHL: England (1975) investigated soil moisture in two layers of soil in an Oklahoma basin. He simulated soil moisture for two arbitrary layers, 0 to 9 inches and 10 to 33 inches, and then compared the modelled results with observed data during a 15-month period. The results of the model simulation of soil moisture were very close to the observed data in layer 1, but there was a large deviation between simulated results and observed data in winter and spring for layer 2. He thereby concluded that the model is capable of simulating soil moisture continuously at a site.

Table 3. Lumped Models

Model	Provider	Reference	Description	Input data	Output
IHACREC	Center for Ecology and Hydrology (CEH) Wallingford, UK, and the Australian National University (ANU)	Jakeman et al., 1990	The model employs unit hydrograph (UH) and simulates steamflow either continuously or individually	Rainfall, temperature, evapotrans-piraton	Streamflow, wetness index
SRM	Swiss Snow and Avalanche Research Institute (SSARI)	Martinec, 1975	The model (simple degree-day) is designed for basins where snowmelt is a major runoff component	Precipitation, temperature, and elevation	Streamflow
WATBAL	University Helsinki, Finland	Yates, 1994	The model is a soil water balance model.	Precipitation, temperature, humidity, sunshine duration	PET, discharge
USDAHL	United States Department of Agriculture Hydrograph Laboratory	Holtan et al., 1975	The model is designed to simulate continuous streamflow predictions. It was useful to evaluate interactions between agricultural activities and hydrology of small rural watersheds.	Precipitation, temperature, evapotranspiration	streamflow, AET, soil moisture, groundwater recharge

3.1.2 Semi-distributed models

Semi-distributed models consider conceptual functional relationships for homogeneous sub-catchments as lumped units. These models discretize landscape based on common land use, soil, and slope characteristics of a watershed, known as hydrologic response units (HRUs). They include some of the important features of a watershed compared to the lumped models and require less data, and they have lower computational costs compared to distributed models (Orellana et al., 2008). However, HRUs are often spatially disconnected and routed directly to sub-basin outlets. Table 4 lists examples of semi-distributed models.

3.1.3 Distributed models

Distributed models consider catchments as finite geo-referenced computational units with different responses to forcing inputs. A grid-based hydrological model may not necessarily be a distributed model, unless grid cells can interact both vertically and horizontally with adjacent cells (within surface, unsaturated, or saturated zones) to simulate surface and/or subsurface processes. The main category of distributed models is physically based models, which are defined in terms of theoretically continuum equations based on physics. Although distributed models require large amounts of data for parameterization, they provide more detail of hydrological processes (Refsgaard, 1996) and imply a discrete grid system in which the spatial variations are aggregated over each grid. These models are used for: 1) flood studies – evaluation of volume and timing of peak flows; 2) yield studies – evaluation of the total flow obtained from rainfall within a watershed; 3) low flow studies – assessment of low flow in the watershed; and 4) water management studies – assessment of the impacts of the manmade water management infrastructure.

In a different classification, Refsgaard (1996) recognized four practical applications for using distributed physically based models:

1. *Watershed changes*: Distributed physically-based models are suited to estimating the influence of both natural and manmade changes on the hydrological cycle, since the parameters of the models have direct physical interpretation. Predictions by these models are based

Table 4. Semi-Distributed Models

Model	Provider	Reference	Description	Input data	Output
HBV-96	Swedish Meteorological and Hydrologic Institute (SHMI)	Lindström et al., 1997	The model is designed for runoff simulation and forecasting.	Precipitation, temperature, monthly ET	Daily flow, soil moisture
SLURP	National Hydrological Research Institute, Saskatoon, Canada	Kite, 1997	The model is a daily timestep hydrological model dividing a watershed into a number of units known as Aggregated Simulation Areas (ASAs).	Precipitation, temperature, albedo, snowmelt rate	Infiltration, overland flow, soil moisture
HEC-HMS	US Army Corps of Engineers (US-ACE) Hydrologic Engineering Center	Kumar & Bhattacharjya, 2011	The model is designed to simulate both event and continuous simulation over long periods of time.	Precipitation, temperature, evapotranspiration	Infiltration, soil moisture, runoff, flow in open channels
SWAT	USDA Agricultural Research Service at the Grassland, Soil and Water Research Laboratory in Temple, TX, USA	Preksedis et al., 2008	The model predicts the effect of management decisions on water, sediment, nutrient and pesticide yields with reasonable accuracy on large, ungauged river basins.	Precipitation, temperature, soil types	Surface and subsurface runoff, flow routing through drainage network, ET, soil moisture,
VIC	University of Washington	Liang et al., 1994; Wood et al., 2004; Zhao et al., 2013; Lievens et al., 2016	Variable Infiltration Capacity (VIC) is a semi-distributed, grid-based macroscale model designed for large-scale hydrological modelling.	Meteorological parameters (e.g., precipitation, air temperature, and wind speed) and soil	Runoff, soil moisture, ET, and infiltration

on parameter values and physical characteristics of a watershed, such as land use and soil.

2. *Simulations with intensive and short-term records*: In contrast to lumped models, which require long historical data for the assessment of the parameters, distributed models simulate hydrological processes in the watershed using short records.
3. *Prediction of the ungauged watershed*: In a well-gauged watershed, the model can be calibrated against observed discharge data with less uncertainty, but a prediction of flows in an ungauged watershed is complex, with a higher level of uncertainty regarding model output. The physical significance of the model parameters allows distributed physically-based models to predict the responses of an ungauged watershed.
4. *Spatial assessment*: Distributed models can use spatially variable inputs and predict outputs spatially. They provide necessary information such as movements of rainstorms, groundwater abstractions, and recharge, while lumped models can only consider average values in a watershed.

Table 5 lists four examples of distributed models identified in the literature. Some of the hydrological models have been used in combination with water quality modelling or have been integrated with groundwater models. A more detailed description of these hydrological model applications appears below:

> *WATFLOOD*: Toth et al. (2006) applied WATFLOOD model to investigate the hydrological regimes of the Peace and Athabasca watersheds under five different climate change scenarios (GCMs). Results revealed a significant shift towards an earlier melt season, a shift in the timing of peak flows, and small changes in the annual flow volumes.

CASC2D: Marsik and Waylen (2006) applied the two-dimensional, physically-based hydrologic model CASC2D to evaluate the influence of land-use/land cover change on hydrology from 1979 to 1999 in the Quebrada Estero in Costa Rica. The results showed increased peak discharges and above-threshold flood durations with changing LU/LC. This model was found to be well suited for operational use in tropical watersheds like the Quebrada Estero.

MIKE SHE/MIKE 11: Farjad et al. (2016) investigated seasonal and annual responses of hydrological processes to climate change in the 2020s and 2050s in the Elbow River watershed, southern Alberta, Canada. The MIKE SHE/MIKE 11 model was applied to simulate different hydrological processes under the GCM-scenarios of NCARPCM-A1B, CGCM2-B2(3), HadCM3-A2(a), CCSRNIES-A1FI, HadCM3-B2(b)). The model was set up based on a rigorous sensitivity analysis along with three different methods of calibration and validation to capture the complex watershed hydrology. Results indicated that future climate change is expected to progressively modify hydrological processes over the next 60 years.

HydroGeoSphere: Davison et al. (2018) assessed streamflow characteristics in the downstream and upstream of the Athabasca River Basin in Alberta. They found that forestlands and peatlands have a strong influence on the hydrology of the watershed.

Table 5. Distributed Models

Model	Provider	Reference	Description	Input data	Output
CASC2D	US Army Research Office (ARO) funded Center for Excellence in Geoscience at Colorado State University	Julien et al., 1995	Fully unsteady, two-dimensional, infiltration-excess (Hortonian) hydrologic model	Precipitation, temperature, ET	Soil moisture, infiltration, surface and channel runoff
WATFLOOD	University of Waterloo, Canada	Kouwen, 2001	The model is designed for real-time flood forecasting	Precipitation, temperature, ET	Surface flow, soil moisture, ET, Infiltration
MIKE SHE/ MIKE 11	DHI	Wijesekara et. al., 2012	The model is an integrated hydrological modelling system for building and simulating surface water flow and groundwater flow	Precipitation, temperature, ET	Overland flows, base flows, AET, soil moisture, Infiltration, groundwater table
HydroGeoSphere	Aquanty	Hwang et al., 2018	It is an integrated surface water and groundwater model to simulate major hydrological processes	Precipitation, temperature, ET	Streamflow, AET, Infiltration, groundwater table

3.2 Water quality models

Water quality is a complex subject and may involve interactions between surface water, groundwater, and coastal water systems. It is controlled by characteristics of watersheds and aquifers, including climate, land cover and land uses, geology, lithology, chemical reactions, and anthropogenic activities (Praskievicz & Chang, 2009; Tsakiris & Alexakis, 2012; Whitehead et al., 2009). Ever since Streeter and Phelps (1925) built the well-known Streeter-Phelps Oxygen Sag Formula (SP model) to describe the oxygen balance in the Ohio River, the development of water quality models has undergone tremendous improvements. Many water quality models have been developed to tackle various water quality problems or threats associated with growing populations, urbanization, and industrialization. Models have evolved from a primary stage (prior to 1965), characterized by simple BOD-DO bilinear systems considering point source pollution, to an improving stage (1965-1995), when two- and three-dimensional nonlinear system models were built to include non-point source pollution inputs, capacities of hydrodynamic, sediment, eutrophication simulation, and linkages to watershed models (Q. Wang et al., 2013). Thereafter, integrated modelling systems at various levels of sophistication have been developed where atmospheric deposition, climate and land use changes, and interactions between surface water, groundwater, and water resource management are considered in modelling to evaluate their impacts on water quality (Burian et al., 2002; Hesse & Krysanova, 2016; Hien et al., 2015; Panagopoulos et al., 2015; Wellen, Kamran-Disfani, & Arhonditsis, 2015).

Water quality models are effective tools to simulate and predict the transport and fate of pollutants in aquatic environments and support environmental impact assessment and planning. They can be classified according to their characteristics and intended purposes (Sharma & Kansal, 2013), for example:

- modelling purpose (simulation, optimization),
- development (generic, site specific),
- model type (physical, mathematical),
- application area (rivers, lakes, reservoirs, watershed, groundwater, estuaries, integrated),
- constituents of concern (sediments, salts, nutrients, metals, PAHs, etc.),
- nature (deterministic, stochastic),
- spatial variation (1-, 2-, 3-dimensional),
- spatial resolution (lumped, semi-distributed, distributed),

- temporal variation (steady state, quasi-dynamic, dynamic simulation), or
- solution method (analytical, finite difference, finite element, linear, nonlinear and dynamic programming, etc.).

There are already many attempts to review the development and applications of receiving water quality models (Bahadur, Amstutz, & Samuels, 2013; Tsakiris & Alexakis, 2012) and watershed water quality models (Booty & Benoy, 2009; K. H. Cho et al., 2016; Wellen et al., 2015). While most reviews are presented in brief articles for selected models, ASCE (2017) published a book offering a comprehensive review of 13 watershed models and 13 receiving water quality models, for total maximum daily load (TMDL) development. Building on these previous efforts, this book summarizes the advances in water quality modelling techniques with a focus on integrated modelling. It has been recognized that peer-reviewed journal literature no longer provides a representative picture of the subject of regional integrated environmental modelling, as modelling systems are becoming "too big to be published" or too pragmatic (Barthel & Banzhaf, 2016; Wood, 2012). Therefore, the existing reviews and water quality modelling studies reported in journal publications, conference proceedings, technical reports, and software manuals since 2000 have been searched and screened according to relevance to watershed and integrated water quality modelling. In the following subsections, water quality modelling approaches, along with the characteristics and applications of the models, are described.

3.2.1 Receiving Water Quality Models

The receiving water quality models commonly also include hydrodynamic models. Models vary widely as to their water quality modelling capacities, as they are developed with various temporal and spatial variables, types of receiving waters, contaminants of interest, and representations of processes (ASCE 2017).

Review of selected receiving water quality models are summarized in Table 6 according to key model characteristics or features, followed by a brief description about the source, capabilities, and applicability for each.

CE-QUAL-W2

CE-QUAL-W2 is a two-dimensional, longitudinal/vertical, hydrodynamic, and water quality model for stratified and non-stratified rivers, estuaries, lakes, reservoirs, and river basin systems. The model has been under continuous development since 1975. The original model was known as LARM (Laterally Averaged Reservoir Model) developed by Edinger and Buchak (1975). The first LARM application was on a reservoir with no branches. Subsequent modifications that allowed for multiple branches and estuarine boundary conditions resulted in the code known as GLVHT (Generalized Longitudinal-Vertical Hydrodynamics and Transport Model). Addition of the water quality algorithms by the Water Quality Modelling Group at the United States Army Engineer Waterways Experiment Station (WES) resulted in CE-QUAL-W2 version 1.0 (Environmental and Hydraulics Laboratory, 1986). The latest release is version 4.2.2, released in August 2020 and distributed by Portland State University. The model and source code are publicly available at http://www.ce.pdx.edu/w2/.

The CE-QUAL-W2 software directly links a hydrodynamic module and a water quality module using a dynamic coupling approach. In the model, the geometry of a waterbody is represented by a finite difference computation grid defined using layers of segments and cells. The module predicts water surface elevations, velocities (longitudinal and vertical), and temperatures. Temperature is included in the hydrodynamic calculations because of its effect on water density. The model can calculate onset, growth, and breakup of ice cover. Water quality computations are done after a hydrodynamic computation, allowing for feedback between water quality and hydrodynamic variables. The effects of salinity or total dissolved solids on density and thus on hydrodynamics is simulated only if it is set up as one of the state variables of the water quality module. The water quality algorithm is modular, allowing constituents to be easily added as additional subroutines. The model simulates eutrophication, alkalinity, and generic water quality processes in water column and sediment diagenesis processes in the sediment bed. Water quality variables include generic constituents, sediments, nutrients, multiple algal groups, epiphyton, periphyton, zooplankton, macrophytes, carbonaceous biochemical oxygen demand, dissolved oxygen, and dissolved and particulate labile/refractory organic matters. The generic water quality groups can be used to define any number of conservative tracers, water age or hydraulic residence time, coliform bacteria, and contaminants. Additionally, more than 60 derived variables, such as pH, TOC, DOC, TON, TOP, DOP, TP, TN, TKN, and turbidity, can be computed internally from the state variables and the output can be compared to measured data.

As the water surface elevation is solved implicitly, eliminating the surface gravity wave restriction on timestep, CE-QUAL-W2 permits larger timesteps during a simulation, resulting in decreased computational time. As a result, the model can easily simulate long-term water quality responses (Cole & Wells, 2017). Note that water quality can be updated less frequently than hydrodynamics, thus reducing computational requirements. However, water quality is not decoupled from the hydrodynamics (i.e., separate, standalone code for hydrodynamics and water quality), as output from the hydrodynamic model is stored on disc and then used to specify advective fluxes for the water quality computations. The CE-QUAL-W2 model is a powerful and widely used laterally averaged longitudinal/vertical two-dimensional model for simulating hydrodynamics and water quality in rivers, lakes, reservoirs, and estuaries (ASCE, 2017; Shabani, Zhang, & Ell, 2017). The model has been further enhanced to develop the Cumulative Environmental Management Association (CEMA) Oil Sands Pit Lake Model. This development incorporated a sediment diagenesis module, tailings consolidation, pore water release, biogenic gas production, bubble release, and salt rejection during ice formation within the CE-QUAL-W2 model Version 3.6 (Berger & Wells, 2014; Prakash, Vandenberg, & Buchak, 2015; Vandenberg, Prakash, & Buchak, 2014).

The assumption of the model, that lateral variations in velocities, temperatures, and constituents are negligible, may be inappropriate for large waterbodies that exhibit significant lateral variations in water quality. Whether this assumption is met is often a judgment call by the user and depends in large part on the questions that are being addressed.

EFDC-EPA

The Environmental Fluid Dynamics Code (EFDC) is a public domain, open source, surface water modelling system, which includes hydrodynamic, sediment and contaminant, and eutrophication modules fully integrated in a single source code implementation. EFDC was originally developed at the Virginia Institute of Marine Science (VIMS) by Dr. John M. Hamrick (Hamrick, 1992) in 1988 and was later enhanced by Tetra Tech for the USEPA (Tetra Tech, 2007). The model is currently maintained by Tetra Tech with support from the USEPA.

EFDC is a state-of-the-art hydrodynamic and water quality model that can be used to simulate aquatic systems in one, two, and three dimensions. EFDC uses stretched or sigma vertical coordinates and Cartesian or curvilinear-orthogonal horizontal coordinates to represent the physical characteristics of a waterbody. For one-dimensional applications, an optional cross-section description can be used. Two horizontal grid generation and preprocessing tools, GEFDC (GridEFDC) and VOGG (Visual Orthogonal Grid Generator), are also available. Based on a semi-implicit conservative finite volume solution scheme, EFDC's hydrodynamic component solves three-dimensional, vertically hydrostatic, free surface, turbulent averaged equations of motion for a variable-density fluid. Dynamically coupled transport equations for turbulent kinetic energy, turbulent length scale, salinity, and temperature are also solved. The EFDC model allows for drying and wetting in shallow areas by a mass conservation scheme. Additional capabilities include simulation of shoreline movement by drying and wetting, hydraulic control structures, vegetation resistance, wave-current boundary layers, and wave-induced currents.

The EFDC simulates multiple size classes of cohesive and non-cohesive sediments. A sediment processes function library allows the user to choose from a wide range of currently accepted parameterizations for settling, deposition, resuspension, and bed load transport. The sediment bed is represented by multiple layers and includes several armoring representations for non-cohesive sediment and a finite strain consolidation formulation for dynamic simulation of bed layer thickness, void ratio, and pore water advection. The sediment transport component can operate in a morphological mode with full coupling, with the hydrodynamic component representing the dynamic evolution of bed topography.

Table 6. Summary of Selected Receiving Water Quality Models

Model& Source	**Spatial Dimension**	**Type of Simulation**	**Simulated Processes**	**Simulated Parameters**	**GUI**	**Availability and Support**	**References**
CE-QUAL-W2 (Portland State Univ.)	2D laterally averaged rivers, estuaries, lakes, and reservoirs; includes hydraulic structures	Event and limited long-term simulations	Hydrodynamic and water quality (all pollutants except toxics and metals) for stratified and non-stratified systems	Water surface, velocity, temperature, nutrients, multiple algae, zooplankton, periphyton, macrophyte species, DO, pH, alkalinity, multiple CBOD, suspended solids, organic matters, and generic water quality groups	Yes	Public domain, open source	Berger & Wells, 2014; Cole & Wells, 2017; Shabani et al., 2017
EFDC (USEPA, VIMS, Tetra Tech, Inc.)	1D, 2D, and 3D rivers, estuaries, lakes, and coastal waters and hydraulic structures	Event and long-term simulations	Hydrodynamic, sediment transport, water quality (eutrophication, sediment diagenesis), toxics (adsorption, degradation)	Temperature, cohesive and non-cohesive sediments, COD/DO, nutrients, algae, salinity, metals, and other contaminants	Yes	Public domain	J. Craig et al., 2007; Hamrick, 1992; Hua & Zhang, 2017; Osmi, Ishak, Kim, Azman, & Ramli, 2016; Seo, Sigdel, Kwon, & Lee, 2010; Tetra Tech, 2007

Table 6. (*continued*)

EFDC-Plus (DSI)	1D, 2D, and 3D rivers, estuaries, lakes, and coastal waters and hydraulic structures	Event and long-term simulations	Hydrodynamic, sediment transport (added SEDZLJ approach), water quality (eutrophication, sediment diagenesis, rooted plant and epiphyte), toxics (adsorption, degradation, volatilization)	Temperature, cohesive and non-cohesive sediments, COD/DO, nutrients, algae, salinity, metals, and other contaminants	Yes	Proprietary for DSI multi-thread version; public open for DSI single thread version	DSI E. Cho, Arhonditsis, Khim, Chung, & Heo, 2016, 2017; Ji, 2017; Shen et al., 2014
HEC-RAS (USACE)	2D overland, 1D and 2D rivers, lakes, reservoirs, and inundated floodplains, and hydraulic structures	Event and long-term simulations	1D steady non-uniform and unsteady flows for WS profiles, floodways and floodplain determination, sediment and limited water quality. 2D capabilities are recently added	Bacteria, temperature, sediments, BOD/DO, salinity	Yes	Public domain	Brunner, 2016; Knebl, Yang, Hutchison, & Maidment, 2005; Patel, Ramirez, Srivastava, Bray, & Han, 2017; Wu & Fan, 2017; Xiong, 2011
MIKE 11 (DHI)	1D river reaches and hydraulic structures	Event and long-term simulations	River hydraulics and sediment transport; links to MIKE 21 for 1D and 2D flood and MIKE SHE & ECOLAB for water quality simulations	Sediment, temperature, BOD/DO, salinity, nutrients	Yes	Proprietary	DHI, 2017a; Liang et al., 2015; Patro, Chatterjee, Mohanty, Singh, & Raghuwanshi, 2009; Thompson, Sørenson, Gavin, & Refsgaard, 2004; Zhao, Zhang, James, & Laing, 2012

Table 6. (*continued*)

Model& Source	Spatial Dimension	Type of Simulation	Simulated Pro-cesses	Simulated Parameters	GUI	Availability and Support	References
QUAL2K/ QUAL2Kw (USEPA, Washington Department of Ecology)	1D rivers and streams divided into sub-reaches or computational elements	Event and long-term simulations	Quasi-dynamic simulations with steady (QUAL2K) or non-steady state (QUAL2Kw) state hydraulics, non-uniform steady flow, repeating diel conditions, and water-quality kinetics. Has auto-calibration and uncertainty analysis capabilities	Sediment, temperature, BOD/DO, salinity, pH and alkalinity, nutrients, algae, periphyton, pathogen	Yes	Public domain	Brown & Barnwell, 1987; Chapra & Pelletier, 2003; Pelletier & Chapra, 2005; Salvai & Bezdan, 2008
WASP (USEPA)	1D, 2D, and 3D rivers, lakes, reservoirs, estuaries, and coastal waters	Event and long-term simulations	With links to 1D, 2D, and 3D hydrodynamic models for dynamic flow inputs, it simulates water temperature, three types of sediments, biochemical oxygen demand, sediment oxygen demand, dissolved oxygen, nitrogen, phosphorus, multiple species of algae, detritus, periphyton, organic toxicants, mercury and other metals, pH and alkalinity, and pathogens	Bacteria, sediments, BOD/DO, nutrients, toxic organics, toxic metals, mercury, salinity, pH, and alkalinity	Yes	Public domain	Ambrose & Wool, 2009; Ambrose, Wool, Connolly, & Schanz, 1988; Di Toro, Fitzpatrick, & Thomann, 1983; J. M. Johnston et al., 2017; Z. Liu et al., 2008

The EFDC model includes a variable configuration eutrophication component for simulation of aquatic carbon, nitrogen, and phosphorus cycles. The kinetic processes included in the EFDC water quality model are derived from the US Army Corps of Engineers' CE-QUAL-ICM water quality model (Cerco & Cole, 1995), including sediment diagenesis. In contrast to earlier water quality models (such as WASP) (Ambrose & Wool, 2009), which use biochemical oxygen demand to represent oxygen demanding organic material, the EFDC water quality model is carbon-based and uses chemical oxygen demand (COD). The four algae species are represented in carbon units. The three organic carbon variables play an equivalent role to BOD. Organic carbon, nitrogen, and phosphorous can be represented by up to three reactive sub-classes, refractory particulate, and particulate and dissolved labile. In addition to the internal eutrophication model, EFDC can create hydrodynamic transport files formatted for WASP and CE-QUAL-ICM.

EFDC can also represent the transport and fate of an arbitrary number of contaminants, including metals and hydrophobic organics, sorbed to any of the sediment classes and dissolved and particulate organic carbon using a three-phase equilibrium partitioning formulation. Dissolved and particulate organic carbon can be represented as independent state variables, and pollutants of concern can be fractionally assigned to any of the sediment classes. A contaminant processes function library allows the representation of various degradation and transformation processes.

In addition to the grid generation tools, a windows-based model interface, EFDCView, which incorporates grid generation, pre-processing and post-processing tools, is available. The EFDC has been used for many modelling studies of rivers, lakes, estuaries, coastal regions, and wetlands internationally (Hua & Zhang, 2017; Huang, Falconer, & Lin, 2017; Osmi et al., 2016; Seo et al., 2010). Due to its range of applicability with respect to water body and pollutant types, EFDC has been a choice model for TMDL development in the United States, such as the Christina River (Merrill et al., 2002), Wissahickon Creek (Zou et al., 2006), Tenkiller Ferry Lake (P. M. Craig, 2006), Los Angeles Harbor (J. Craig et al., 2007), and Charles River (Peng et al., 2011).

EFDC-Plus (EFDC+)

The ongoing evolution of the EFDC model has been application-driven by a diverse group of EFDC users in the academic, government, and private sectors. Since 2002, Dynamic Solutions International, LLC (DSI) has been steadily improving and enhancing the original EPA version of the EFDC code. The improvements to the EFDC code had become so extensive that in 2016 the DSI version of EFDC was renamed as the EFDCPlus or EFDC+ model (DSI, 2017; E. Cho et al., 2016; 2017; Ji, 2017; Shen et al., 2014). The EFDC+ and its associated powerful graphical user interface, EFDC_Explorer, constitute the modelling system called the EFDC_Explorer Modelling System (EEMS), which supports integrated hydrodynamic, sediment, water quality, and toxics modelling for receiving water bodies.

Compared with EFDC-EPA, EFDC+ has many key enhancements, for example:

- *Dynamic memory allocation*: Dynamic memory allocation allows the user to use the same executable code for applications to different water bodies. Dynamic allocation eliminates the need to re-compile the EFDC code for different applications, because of different maximum array sizes required to specify the computational grid domain and time series input data sets. Dynamic allocation also helps prevent inadvertent errors and provides better traceability for source code development.
- *OpenMP - Multithreading*: OpenMP provides vastly improved model run times. The Intel® OpenMP* Runtime Library binds OpenMP threads to physical processing units. Depending on the machine topology, application, and operating system, thread affinity can have a substantial impact on the application speed. EFDC+ typically produces run time up to four times faster on a six-core processor than the conventional single-threaded EFDC model.
- *Sigma-Zed layering*: An improved version of the EFDC code helps deal with pressure gradient errors

that occur in simulations that have steep changes in bed elevation. The Sigma Zed code contrasts with the conventional EFDC code, which uses a sigma coordinate transformation in the vertical direction and uses the same number of layers for all cells in the domain. In the EFDC_SGZ model, the vertical layering scheme has been modified to allow for the number of layers to vary over the model domain. This approach is computationally efficient and provides significantly improved simulations of thermal stratification.

- *Hydraulic structures*: Equations governing hydraulic structures such as culverts, weirs, sluice gates, and orifices are implemented in EFDC+. This additional feature is different from the previous head lookup table used to describe the relationship between head and flow for a hydraulic structure.
- *Enhanced heat exchange*: Heat exchange options use equilibrium temperatures for the water and atmospheric interface and spatially-variable sediment bed temperatures.
- *Ice formation and melt.*
- *Lagrangian particle tracking*: This option is applicable to oil spill modelling and emergency response simulations.
- *Improved/simplified external wave model linkage.*
- *SEDZLJ toxics implementation*: The SEDZLJ sedflume model developed by Sandia National Laboratories has been adopted and greatly enhanced in EFDC+ in addition to the original approach used in the EPA version of EFDC for sediment transport modelling. A whole new toxic modelling capability has been implemented.
- *RPEM module*: A Rooted Plant and Epiphyte Model (RPEM) has been incorporated into EFDC to better

simulate water quality interactions with submerged aquatic vegetation (epiphytic algae and macrophytes).

- *Internal wind wave generation*: A wind-generated wave sub-model has been added to enable the computation of wind-generated wave bed shear stress on sediment resuspension and wave induced currents.
- *High frequency output*: These are new output snapshot controls for targeting specific periods for high frequency output within the standard regular output frequency.
- *Restart/continuation run options*: This application gives more options to run a model from the beginning or continue to run from the previous stop.
- *Streamlined code for quicker execution time*.
- *Model linkages*: This enhancement customizes linkage of model results for the Windows-based EFDC_Explorer graphical pre- and post-processor for EFDC+.
- *MHK linkage*: Incorporating the Marine and Hydrokinetic (MHK)-friendly module allows for the simulation of placement and potential effects of installing and operating turbines and wave energy converters in rivers, tidal channels, ocean currents, and other waterbodies. This code comes from Sandia National Laboratories modified Environmental Fluid Dynamics Code (SNL-EFDC) (Thanh, Grace & Carlton, 2008).

The aforementioned enhancements greatly improve the applicability of the EFDC model.

HEC-RAS

The Hydrologic Engineering Center River Analysis System (HEC-RAS) is a very powerful model for simulating one-dimensional, steady, non-uniform hydraulics, and one-dimensional, two-dimensional, and combined one-/two-dimensional unsteady flow through a full network of open channels, floodplains, and alluvial fans (Brunner, 2016). It evolved from the first FORTRAN version of HEC-2 released by the United States Army Corps of Engineers Hydrologic Engineering Center (HEC) in 1966.

The HEC-RAS system contains several river analysis components for: (i) steady flow water surface profile computations, (ii) one- and two-dimensional unsteady flow simulation, (iii) movable boundary sediment transport computations, and (iv) water quality analysis. In addition to these river analysis components, the system contains several hydraulic design features that can be invoked once the basic water surface profiles are computed. The steady flow water surface profiles component is intended for calculating water surface profiles for steady, gradually varied flow. The system can handle a full network of channels, a dendritic system, or a single river reach. The unsteady flow component can be used to perform subcritical, supercritical, and mixed flow regime (subcritical, supercritical, hydraulic jumps, and drawdowns) calculations in the unsteady flow computations module.

The sediment transport component of the modelling system is intended for the simulation of one-dimensional sediment transport/movable boundary calculations resulting from scour and deposition over moderate time periods (typically years, although applications to single flood events are possible). The sediment transport potential is computed by grain size fraction, thereby allowing the simulation of hydraulic sorting and armoring. Major features include the ability to model a full network of streams, channel dredging, various levee and encroachment alternatives, and the use of several different equations for the computation of sediment transport.

The water quality component of the modelling system is intended to allow the user to perform riverine water quality analyses. An advection-dispersion module is included with this version of HEC–RAS, adding the capability to model water temperature. This new module uses the QUICKEST-ULTIMATE explicit numerical scheme to solve the one-dimensional advection-dispersion equation using a control volume approach with a fully implemented heat energy budget. The transport and fate of a limited set of water quality constituents is available in HEC-RAS, including: dissolved nitrogen (NO_3-N, NO_2-N, NH_4-N, and Org-N), dissolved phosphorus (PO_4-P and Org-P), algae, dissolved oxygen (DO), and carbonaceous biological oxygen demand (CBOD).

HEC-RAS includes a user-friendly interface and has a variety of data storage, management, and graphics and reporting components. A companion program, HEC-GeoRAS, provides tools and utilities for processing geospatial data in ArcGIS using a graphical user interface (GUI) for preparation of geometric data for import into HEC-RAS.

The model is commonly used for simulating steady-flow water surface profiles or unsteady flow hydraulic and hydrodynamic simulations in support of hydraulic structure design, floodplain delineation, or floodway determination (Knebl et al., 2005; Patel et al., 2017; Xiong, 2011). Due to limited water quality capabilities, HEC-RAS is often used to generate hydraulic field inputs for other water quality models (Hosseini et al., 2016; Wu & Fan, 2017).

MIKE 11

MIKE 11 is a one-dimensional fully dynamic model for simulating flows, sediment transport, and water quality in estuaries, rivers, irrigation channels, and other water bodies (DHI, 2017a). The model is a part of the MIKE suite of water modelling software products developed by DHI Water and Environment.

The hydrodynamic (HD) module is the nucleus of the model, which solves the vertically-integrated equations for conservation of continuity and momentum, i.e. the Saint Venant equations. Advanced computational modules are included for the description of flow over hydraulic structures, including possibilities to describe structure operation. The primary feature of the MIKE 11 modelling system is the integrated modular structure with a variety of ad-on modules each simulating phenomenon related to river systems, including advection-dispersion, cohesive and non-cohesive sediment transport, and water quality.

The advection-dispersion (AD) module is based on the one-dimensional equation of conservation of mass of dissolved or suspended material, i.e. the advection-dispersion equation. Non-cohesive standard and advanced cohesive sediment transport modules are part of the AD module. The module requires output from the hydrodynamic module, in time and space, as well as in terms of discharge and water level, cross-sectional area, and hydraulic radius. The advection-dispersion equation is solved numerically using an implicit finite difference scheme which, in principle, is unconditionally stable and has negligible numerical dispersion. In association with DHI ECOLAB water quality analysis and simulation of fate and transport in riverine systems, it can be used to develop TMDL for a variety of constituents (Cabrejo, 2011; Liang et al., 2015). MIKE 11 can be dynamically linked to DHI software, MIKE 21, to perform two-dimensional river and floodplain simulaions (Patro et al., 2009), and MIKE SHE for surface-groundwater interactions (Thompson et al., 2004; Zhao et al., 2012).

With its exceptional flexibility, speed, and user-friendly environment, MIKE 11 is an effective modelling tool to support detailed analysis, design, management, and operation of channel systems. MIKE 11 has been used in numerous applications around the world for flood plain analysis and mapping, real-time flood, inflow and water quality forecasting, analysis and design of hydraulic structures, sediment transport, dredging impact and channel restoration alternative analysis, water quality analysis, issues related to TMDL and ecosystem restoration, and integrated groundwater and surface water analysis. In many aspects, MIKE 11 is very similar to HEC-RAS, with added benefits: direct linkage with the watershed and groundwater flow components of MIKE SHE to allow integrated hydrologic, hydraulic, and hydrogeological modelling; a soft linkage to ECOLAB to allow water quality analysis and TMDL development; and a hard linkage to MIKE 21 (MIKE FLOOD) to allow a combination of one-dimensional and two-dimensional flood simulations.

DHI introduced MIKE HYDRO River as the new-generation river modelling software and as a successor to MIKE 11 (DHI, 2017b). The release of MIKE 2017 includes both MIKE 11 and MIKE HYDRO River. MIKE HYDRO River includes most features and add-ons available in MIKE 11.

QUAL2K

QUAL2K (or Q2K) (Chapra & Pelletier, 2003) is a one-dimensional, river and stream water quality model (Brown & Barnwell, 1987). The QUAL2K code is distributed by the USEPA. A variation of QUAL2K is distributed as QUAL2Kw (Pelletier & Chapra, 2005) by the Washington Department of Ecology, and includes versions with auto-calibration and Monte Carlo simulation.

The QUAL2K model is an extremely powerful model based on many of the same assumptions as QUAL2E (an earlier version of QUAL2K), such as a one-dimensional system with steady-state, non-uniform flows and hydraulics, which allows simulation of diel variations in water quality. It simulates a wide variety of conventional pollutants as well. Enhancements over QUAL2E include algorithms for slow and fast carbonaceous biochemical oxygen demand, periphyton and detritus (in addition to sediment diagenesis), pH and alkalinity, and other advanced features. The model input and output are in the form of user-friendly Excel spreadsheets, with underlying VBA routines to write and read files for use in a FORTRAN executable code.

QUAL2K is applicable to waste-load allocation (WLA) and TMDL studies (Salvai & Bezdan, 2008) of rivers, streams, and some estuaries, using tidally averaged dispersion coefficients for conventional pollutants such as pathogens, nitrogen, phosphorus, dissolved oxygen, biochemical oxygen demand, sediment oxygen demand, phytoplankton, benthic algae, and pH. It is not applicable to toxics or metals and is limited to simulation of steady time-invariant flow, while time variations in water quality are only over diel cycles but constant otherwise.

In the recent version 6 of QUAL2Kw, the model has been updated into a dynamic water quality model which simulates non-steady, non-uniform flow using kinematic wave flow routing. Continuous simulations can be run with time-varying boundary conditions for periods of up to one year, with the option to use repeating diel conditions with either steady or non-steady flows.

Water Analysis Simulation Program (WASP)

WASP is a general dynamic mass balance framework for contaminant fate and transport in surface water aquatic systems, including both the water column and the underlying benthos. The model has been continuously supported by the USEPA and enhanced since its original development in the 1980s (Ambrose & Wool, 2009; Ambrose et al., 1988; Di Toro et al., 1983).

Based on the flexible compartment modelling approach, WASP can be applied in one, two, or three dimensions with advective and dispersive transport between discrete physical compartments or segments. WASP is designed to permit easy substitution of user-written routines into the program structure to form different water quality modules.

The WASP code can simulate water temperature, three types of sediments, biochemical oxygen demand, sediment oxygen demand, dissolved oxygen, nitrogen, phosphorus, multiple species of algae, detritus, periphyton, organic toxicants, metals, pH and alkalinity, and pathogens. The software includes a data preprocessor to format input datasets from simple 'cut and paste' to detailed queries from a database. A post-processor (MOVEM) provides an efficient method for reviewing simulations with field data for calibration and confirmation testing. Simulations can be transferred to spreadsheets as *.CSV files and plotted or animated two-dimensionally.

WASP is one of the most widely used water quality models in the United States and throughout the world. Because of the model's capacity to handle multiple pollutant types, it has been widely applied in the development of TMDLs. WASP has the capability of linking with hydrodynamic and watershed models, which allows for multi-year analysis under varying meteorological and environmental conditions (J. M. Johnston et al., 2017; Z. Liu et al., 2008).

3.2.2 Watershed Water Quality Models

Most of the watershed models were either designed for hydrologic modelling to support soil and water management, or for general watershed and other resource management. Water quality modelling capabilities are limited or absent in most of the existing watershed models. Watershed models have been applied to predict non-point pollutant loadings through surface runoff and provide inputs to receiving water quality models. The review herein is simply a screening of existing watershed models capable of conducting daily and/or sub-daily water quality modelling for potential inclusion in integrated modelling system.

A review of selected watershed water quality models is summarized in Table 7 using eight model characteristics/features, followed by brief descriptions about the source, capabilities, and applications of the models.

Watershed water quality models commonly require extensive input data, including topography, hydrography with reach geometry, LULC, soils, meteorology, agricultural practices (e.g., crop rotation, schedules, tillage practices, fertilizer applications, pesticide and herbicide applications).

AnnAGNPS

The Annualized Agricultural Non-Point Source Pollution Model (AnnAGNPS) is a watershed-scale continuous simulation model, which is an expansion of the capabilities developed in the single event model AGNPS. The model is freely available from the US Department of Agriculture (USDA).

On a daily timestep, AnnAGNPS simulates quantities of surface water, sediment, nutrients, and pesticides which are leaving the land areas, as well as their subsequent travel through the watershed. In the model, a watershed is subdivided into homogenous land areas with respect to soil type, land use, land management, and climate. Areas can be of any shape including hydrologically-based or square grid. The soil profile is divided into two layers. The top 200 mm is used as a tillage layer whose properties can change (bulk density, etc.). The remaining soil profile comprises the second layer whose properties remain static. A daily soil moisture water budget includes applied water (rainfall, irrigation, and snowmelt), runoff, evapotranspiration, and percolation. Runoff is calculated using the Soil Conservation Service runoff curve number equation but is modified if a frozen, shallow surface soil layer exists. Curve numbers are modified daily based upon tillage operations, soil moisture, and crop stage.

Overland erosion of sediment is determined using the revised Universal Soil Loss Equation (RUSLE). Special components are included to handle concentrated sources of nutrients (feedlots and point sources), ephemeral gully sources, concentrated sediment sources (classical gullies), added water (irrigation), and the impacts of riparian buffers and wetlands. The model partitions soluble nutrients and pesticides between surface runoff and infiltration. Soluble nutrients from feedlots are also transported with runoff. Sediment-transported nutrients and pesticides are also determined. The sediment generated from the land areas and gullies is subdivided into particle size classes (clay, silt, sand, small aggregate, and large aggregate) before being added to the stream system. Particle sizes

Table 7. Summary of Selected Watershed Water Quality Models

Model & Source	Spatial Representation	Type of Simulation	Simulated Processes	Simulated Parameters	Management Operations	BMP Measures	GUI	Availability and Support	References
AnnAGNP (USDA-ARS)	Any shapes of homogenous land areas, channels	Event and continuous (daily)	Hydrology, snowmelt, plant growth, land management, erosion, pollutant loadings, fate, and transport	Surface runoff, subsurface lateral flow, sediments, nutrients, chemical oxygen demand, and pesticides	Irrigation, pumping	Agricultural BMPs	Yes	Public domain	Bingner, Theurer, & Yuan, 2015; Yasarer et al., 2017
HEC-HMS (US Army Corps of Engineers)	Sub-watersheds, reaches, and junctions	Event and continuous	Precipitation, snow accumulation and melting, direct runoff (overland flow and interflow), baseflow, flow routing, infiltration, evapotranspiration	Surface and subsurface flows, snow melt, sediment, nitrogen, phosphorus, algae, dissolved oxygen (DO), and carbonaceous biological oxygen demand	Reservoir operations	No (indirectly reflected vis the topographic factor describing the influence of plant cover on surface erosion)	Yes	Public domain	Pak, Fleming, Scharffenberg, Gibson, & Brauer, 2015; Scharffenberg, 2016

Table 7. (*continued*)

Model & Source	Spatial Representation	Type of Simulation	Simulated Processes	Simulated Parameters	Management Operations	BMP Measures	GUI	Availability and Support	References
HSPF (USEPA and USGS)	Catchments with pervious and impervious areas, channels, and reservoirs	Event and continuous	Hydrology, snowmelt, erosion, pollutant loadings, fate, and transport	Surface and subsurface flows, snow melt, conservatives, sediment, temperature, DO, biochemical oxygen demand, pH, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, organic phosphorous, phytoplankton, zooplankton, fecal coliforms, and pesticides	Land-use management practices, and water management operations	Yes, moderate level of analysis; some limitations. Explicit BMP representation in version 12.4 to release	Yes	Public domain	ASCE, 2017; Bicknell, Imhoff, Kittle, Jobes, & Donigian, 2005

Table 7. (*continued*)

LSPC (Tetra Tech Inc.)	Catchments with pervious & impervious areas, channels, and reservoirs	Event and continuous	Hydrology, snowmelt, erosion, pollutant loadings, fate, and transport	Surface and subsurface flows, snow melt, conservatives, sediment, temperature, DO, biochemical oxygen demand, pH, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, organic phosphorous, phytoplankton, zooplankton, fecal coliforms, and pesticides	Land-use management practices, and water management operations	Yes, moderate level of analysis; some limitations	Yes	Public domain	Tetra Tech, 2009

Table 7. (*continued*)

Model & Source	**Spatial Representation**	**Type of Simulation**	**Simulated Processes**	**Simulated Parameters**	**Management Operations**	**BMP Measures**	**GUI**	**Availability and Support**	**References**
MIKE SHE (DHI	2D overland, 1D channels, 1D-unsaturated, and 3D-saturated zones	Event and continuous	Precipitation, snow accumulation and melting, overland and channel flow, unsaturated zone, saturated zone, exchanges between aquifers and rivers, crop growth and nitrogen processes in root zone, geochemical processes, advection and dispersion of solutes, soil erosion	Surface and subsurface flows, sediments, nutrients, pesticides, and other water quality parameters with link to ECOLAB	Irrigation, plumping, water control structures	No, needs add-on modules	Yes	Proprietary	DHI, 2017c, 2017d; Graham & Butts, 2005

Table 7. (*continued*)

SWAT (USDA-ARS)	Subwatersheds, channels, and ponds	Event and continuous (daily, sub-daily)	Precipitation, snowmelt, surface runoff, interflow, groundwater flow, infiltration, percolation, evapotranspiration, soil temperature, crop growth, soil erosion, nutrients, pesticides	Weather, surface and subsurface flows, sediment, soil temperature, crop growth, nutrients, pesticides, and agricultural managements	Irrigation, plumping, reservoir	Agricultural BMPs	Yes	Public domain	Arnold, Williams, Srinivasan, King, & Griggs, 1994; Neitsch, Arnold, Kiniry, & Williams, 2011; Pignotti, Rathjens, Cibin, Chaubey, & Crawford, 2017; Sood & Ritter, 2010; White & King, 2003
SWMM (USEPA)	Catchments, stream & sewer network, & ponds	Event and continuous	Surface and subsurface flows, urban storm and sanitary sewer flows, sediment, water quality	Surface runoff, subsurface flow, dynamic flow routing in stream, subsurface drainage network and sanitary sanitary sewers, and loadings for up to ten pollutants	Stormwater and sewer water management	Low impact development	Yes	Public domain (proprietary PCSWMM, XPSWMM)	Alamdari, Sample, Steinberg, Ross, & Easton, 2017; Bhowmick, Irvine, & Jindal, 2017; Ricks, 2015; Rossman, 2015

are routed separately in the stream reaches. A Windows-based interface provides capabilities to subdivide the watershed into hydrologically derived cells, an input editor assisting in preparation of AnnAGNPS input data, and a processor that can calculate output loads at any point in the watershed.

AnnAGNPS can be used to evaluate non-point source pollution from agricultural watersheds and to compare the effects of implementing various best practices over time within the watershed (Yasarer et al., 2017). Cropping and tillage systems for sheet and rill and ephemeral gully erosion, fertilizer, pesticide, irrigation application rates, point source loads, feedlot management, riparian buffers, and wetland management can be evaluated. However, there are several limitations that might restrict the application of the model for certain purposs: (i) all runoff and associated sediment, nutrient, and pesticide loads for a single daily event are routed to the watershed outlet before the next day simulation; (ii) there is no tracking of nutrients and pesticides attached to sediment deposited in stream reaches from one event to the next event; and (iii) point sources are limited to constant loading rates (water and nutrients) for the entire simulation period.

HEC-HMS

The Hydrologic Modelling System (HEC-HMS) is designed by the United States Army Corps of Engineers Hydrologic Engineering Center to simulate the complete hydrologic processes of dendritic watershed systems (Scharffenberg, 2016). The model is available to the public, with versions on Windows, Linux, and Solaris platforms.

The hydrologic forecasts are based on a physical description of watersheds, obtainable from geographic information systems combined with meteorological information and model parameters. The physical representation of a watershed is accomplished with a basin model formulated as a dendritic network which connects hydrologic elements such as subbasin, reach, junction, reservoir, diversion, source, and sink. Computation for runoff processes proceeds from upstream elements in a downstream direction. A variety of methods are available for simulating hydrological processes, such as: (i) infiltration losses – initial constant, Soil Conservation Service (SCS) curve number, exponential, Green Ampt, Smith Parlange, deficient and constant, and soil moisture accounting methods; (ii) surface runoff – Clark, modified Clark, Snyder, SCS and user-specified unit hydrograph methods, and the kinematic wave method; (iii) baseflow – recession, bounded recession, constant monthly, linear reservoir, and non-linear Boussinesq methods; (iv) open channel flow – kinematic wave, lag, modified plus, Muskingum, Muskingum-Cunge, and Straddle Stagger methods; (v) water impoundments – a user-entered storage-discharge relationship, pumps, and physical spillway and outlet structures; and (vi) diversion structures – user-specified function, lateral weir, pump station, and observed diversion flows.

Sediment and water quality are simulated in an optional component in the basin model of the HEC-HMS. Sediment yields are estimated from land surface erosion and channel and reservoir transport. Sediment transport simulations define the non-cohesive sediment carrying capacity of flow in channels and reservoirs by grain-size distribution. The basin model solves the advection-diffusion equation using the QUICKEST scheme. The channel reaches and the reservoir's mass balances simulate nitrogen (as organic, ammonia, nitrite, and nitrate), phosphorus, algae, dissolved oxygen (DO), and carbonaceous biological oxygen demand.

While the HEC-HMS model has been applied for hydrologic and flood studies, only few applications for water quality purposes are reported in the literature. The HEC-HMS model has been applied to simulate soil erosion and sediment transport in the Upper North Bosque River Watershed (UNBRW).The HEC-HMS results matched the observed TSS at five gauge locations across the UNBRW (<1% error at all gauges) during model calibration, and maintained modest residuals (-31 to 12% error) during the validation period (Pak et al., 2015).

HSPF

The Hydrologic Simulation Program–Fortran (HSPF) model developed in the 1960s (supported by both the USEPA and the USGS) has a long history of development and applications. In the 1990s, HSPF was selected as the core watershed model in the BASINS (Better Assessment Science Integrating Point and Non-point Sources) modelling system (K. Borah & Bera, 2004). USEPA is expected to release version 12.4 with a number of enhancements including explicit Best Management Practice (BMP) representation and modelling, dynamic wave channel flow routing, and wetland modelling capabilities (ASCE 2017).

HSPF is a process-based semi-distributed watershed model capable of simulating a single event, as well as continuous water quantity and quality, in urban and rural watersheds. It uses sub-basins as hydrologic response units and represents the landscape as pervious, impervious, and water body reach segments (Bicknell et al., 2005). The model has three basic modules: (i) PERLND (Pervious Land Upland Loading Module) represents hydrologic and water quality processes that are specific to pervious surfaces, (ii) IMPLND (Impervious Land Module) represents processes specific to impervious surfaces, and (iii) RCHRES (Reservoir Routing Module), which is a one-dimensional stream model that serves as the receiving water model. The PERLND module has upper, lower, and active groundwater zones. It uses simple storage-based equations for one-dimensional flow routing. The HSPF uses meteorological input time series data and computes hydrology and water quality time series data. The model simulates interception, soil moisture, surface runoff, interflow, base flow, snowpack depth and water content, snowmelt, evapotranspiration, groundwater recharge (flux to deep aquifer), dissolved oxygen, biochemical oxygen demand, temperature, pesticides, conservative constituents, fecal coliform, sediment detachment and transport, sediment routing by particle size, channel routing, reservoir routing, constituent routing, pH, total nitrogen, total phosphorus, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, organic phosphorus, phytoplankton, and zooplankton. The model operates on any timestep from one minute to one day. Because inputs for many parameters are needed to characterize the lumped hydrologic response units at sub-basin level, calibrating a comprehensive HSPF model is generally a challenging task.

HSPF has been used for a variety of applications such as assessing the impact of land-use change, reservoir operations, point or non-point source pollution management, flow diversion and water withdrawal impact assessment studies, and setting TMDLs for water quality-impaired water bodies (ASCE, 2017). It can model areas from one square meter to thousands of square kilometers at user-specified timesteps. These capabilities enable model users to evaluate the impact of BMPs over many years through wet and dry cycles and the dynamic evaluation of pollutant loadings to receiving water bodies. Although HSPF is a comprehensive and highly flexible model, the current version of the model has limited abilities to explicitly represent and simulate BMPs such as detention basins and infiltration trenches.

LSPC

The Loading Simulation Program in C++ (LSPC) is a watershed modeling system that includes streamlined HSPF algorithms for simulating hydrology, sediment, and general water quality on land, as well as a simplified stream fate and transport model (Tetra Tech, 2009). LSPC was originally developed by Tetra Tech for the USEPA Region 3 in the early 2000s to determine watershed-scale TMDLs. The code is publicly available from the USEPA.

The primary difference between the LSPC and the HSPF is the programming architecture. The LSPC uses C++ to use common data management software (i.e., Microsoft Access) and to avoid inherent limits on data array size and spatial and temporal resolution. To streamline interpretation for each simulation, the LSPC automatically generates comprehensive sub-watershed files for all land-layers, reaches, and simulated modules using hourly or daily intervals. The software also calculates the TMDL and allocates the source reductions.

Because of its C++ programming architecture, which has no inherent limits on array size and spatial/temporal resolution associated with model setup, LSPC overcomes many of the difficulties experienced with large-scale watershed simulation. LSPC is frequently used for watershed applications and can be readily linked to receiving water models such as EFDC, WASP, and CE-QUAL-W2 for complex waterbody TMDL development.

MIKE SHE

MIKE SHE is a distributed and physically based integrated surface and subsurface hydrological and water quality modelling system for simulating the entire land phase of a hydrologic cycle. It is a proprietary model developed and maintained by the Danish Hydraulic Institute (DHI, 2017c, 2017d).

In the model, the study area is divided into polygons based on land use, soil type, and precipitation region. The polygons are then assigned identification numbers. Model input files can be generated by overlaying the model input parameters with a grid network. Most of the data preparation and model set-up can be completed using an external GIS software or MIKE SHE's built-in graphic preprocessor. The system has no limitations regarding watershed size. It can be implemented as a single event or as a long-term continuous simulation model using different time intervals for processes in different zones (overland hydrology, river hydraulics, groundwater, and water quality).

MIKE SHE simulates the entire land phase of the hydrologic cycle from rainfall to stream flow and various flow processes, such as evapotranspiration from vegetated land cover and evaporation from water bodies, overland flow, infiltration into soils, unsaturated zone flow, groundwater flow, and interaction between groundwater and surface water bodies (interflow and base flow). MIKE SHE offers several different approaches for hydrologic processes ranging from simple, lumped, and conceptual approaches, to advanced, distributed, and physically-based approaches. With distributed physically based approaches, overland flow is routed using a two-dimensional finite difference solution of the diffusive wave approximation of the Saint Venant equation. Flow in the unsaturated zone is solved using a one-dimensional finite difference solution of the Richards equation, and flow in the saturated zone is solved using a three-dimensional finite difference solution for Darcy's law. MIKE SHE can be coupled with MIKE 11, a one-dimensional hydraulic model based on the one-dimensional solution for the Saint Venant equations, to conduct integrated watershed and receiving water modelling. The model also simulates water use and management operations including irrigation systems, pumping wells, and various water control structures. A variety of agricultural practices and environmental protection alternatives may be evaluated using other add-on modules, such as MIKE SHE DAISY, the crop yield and nitrogen consumption module (Booty & Benoy, 2009).

A generic ecological modelling tool called MIKE ECO Lab can be coupled to a MIKE SHE hydrologic model to allow for the representation of a range of water quality and ecological processes with respect to the river, surface water, soil, and groundwater systems. MIKE ECO Lab relies on other models to calculate flow and transport processes. With existing or customized MIKE ECO Lab water quality templates, MIKE SHE can be applied to simulate the fate and transport of different substances (such as sediments, nutrients, and pesticides) across all hydrologic and hydraulic model components. MIKE SHE can simulate fully integrated solute transport between surface water and the subsurface, including decay, sorption, precipitation, and selective plant uptake. More complex, multispecies, and kinetic reactions comprising all aspects of eco-hydrology can also be set up with MIKE ECO Lab.

As one of the first commercially available, distributed, and physically-based hydrologic models (El-Nasr et al., 2005), MIKE SHE has been used in a wide range of research and application projects, including surface water and groundwater quality assessment and remediation, impacts of land use and climate changes on long term water availability and quality, and impacts of agricultural management practices (e.g., irrigation, drainage, sediments, nutrients, and pesticides) (Graham & Butts, 2005). In the United States, most of the applications have been in Florida, where there are strong interactions between surface water and groundwater aquifers because of high water table conditions and extensive lakes and wetlands. For example, MIKE SHE and MIKE ECO Lab have been used to establish a water quality model for TMDL development in the city of Kissimmee in Central Florida. The model was calibrated with historical data and then used to identify significant pollutant load areas for the implementation of specific corrective measures to reduce quantities of loadings entering the receiving water bodies.

SWAT

The Soil and Water Assessment Tool (SWAT) is a semi-distributed, conceptual and continuous-time river basin or watershed-scale model developed at the United States Department of Agriculture Agricultural Research Service (Arnold et al., 1994; Neitsch et al., 2011). The model is open source, has multiple geographic information system interfaces such as ArcSWAT and QSWAT for creating input files, and has user-friendly tools for model calibration. SWAT is included in the USEPA BASINS for non-point source simulations on agricultural lands.

SWAT was developed to predict the impacts of land management practices on water, sediment, and agricultural chemical yields in large complex watersheds with varying soils, land use, and management conditions over long periods of time. In SWAT, a watershed is portioned into sub-watersheds, and each sub-watershed is further divided into a number of hydrologic response units (HRU). An HRU represents a lumped land area having unique soil, land cover, and land management characteristics. A channel network can be delineated at a chosen scale of interest with a watershed containing at least one main channel or reach and a tributary channel. Ponds, wetlands or reservoirs, and point sources can be added as additional subunits.

SWAT is capable of simulating physical, chemical, biological, and physiological processes of watersheds. The model simulates water flow and water quality in uplands, in subsurface water, in stream channels, and in open water bodies (ponds, wetlands, and impoundments). SWAT is a process-based model which conserves water and constituent mass. For example, the land phase of the hydrologic cycle is based on the water balance equation. The model uses a modification of the SCS curve number method or the Green and Ampt infiltration equation to compute surface runoff volume for each hydrologic response unit. Evapotranspiration is calculated from potential evapotranspiration, which is estimated by the Penman-Monteith, Priestly-Taylor, or Hargreaves method. Peak runoff is estimated using a modification of the rational method. Flow is routed through channels using either a variable storage coefficient method or the Muskingum routing method. The water balance for the simulated shallow aquifer is expressed in terms of a linear flow balance equation, which is solved to yield a simple algebraic relationship for base flow. Similarly, mass conservation of snowmelt, sediment, nutrients, carbon, bacteria, pesticides, and dissolved oxygen are all formulated in terms of simple algebraic relationships akin to the explicit finite difference approximation of ordinary differential equations. A mass balance in vegetative filter strips, grassed waterways, wetlands, ponds, and impoundments or reservoirs is described by a similar numerical approach. As a management tool, SWAT simulates crop management, conservation, and agricultural best management practices, as well as water management. It can also be adapted to simulate management practices that are not explicitly represented in the model.

Due to its open source nature and an active development community, SWAT is constantly being improved and augmented with new process representations since it was created in the early 1990s. The model is best suited for long-term continuous applications. Most of the applications of SWAT have been on a daily timestep, although a recent addition to the model includes the Green and Ampt infiltration equation, using rainfall input at any time increment and channel routing at an hourly timestep. SWAT is ideally suited for addressing a wide array of issues related to climate change, land use change, bioenergy crops, blue and green water availability, sediment transport, nutrient cycle and contaminant loads, BMPs, and TMDL studies (Sood & Ritter, 2010; White & King, 2003).

While the HRU approach provides a simple, computationally efficient framework, processes modelled on HRUs are lumped and therefore spatially disconnected, as they are routed directly to sub-basin outlets. This was identified as a key weakness of the model (Douglas-Mankin, Srinivasan, & Arnold, 2010). This lack of definition of landscape position makes implementation of spatially targeted management measures difficult to incorporate into the model. To overcome the spatial limitations of the HRU approach, a grid-based version of the SWAT model, SWATgrid (Rathjens et al., 2015), was developed to perform landscape simulations on a regularized grid by employing a modified landscape routing algorithm. However, SWATgrid remains largely untested, with little understanding of the impact of user-defined model spatial resolution (Pignotti et al., 2017).

SWMM

The Storm Water Management Model (SWMM) is a comprehensive hydrologic and hydraulic model used for single event or long-term (continuous) simulation of runoff quantity and quality primarily from urban areas. SWMM was originally developed by the USEPA in 1971 and has undergone several major upgrades (Rossman, 2015). SWMM is included in the BASINS and is publicly available. Two widely used proprietary software packages derived from SWMM are PCSWMM (Bhowmick et al., 2017) and XP-SWMM (Ricks, 2015), which have additional graphic user interface functions and capabilities.

The EPA SWMM has been widely used throughout the world for planning, analysis, and design related to storm water runoff, combined sewers, sanitary sewers, and other drainage systems in urban areas, with many applications in non-urban areas as well. The current edition, version 5.1, is a complete rewrite of the previous release and provides an integrated environment for editing data, running hydrologic, hydraulic, and water quality simulations. The runoff component of SWMM operates on a collection of sub-catchment areas that receive precipitation and generate runoff and pollutant loads. The routing portion of SWMM transports this runoff through a system of pipes, channels, storage/treatment devices, pumps, and regulators. SWMM accounts for various hydrologic processes that produce runoff from urban areas, including nonlinear reservoir routing of overland flow, and capture and retention of rainfall/runoff with various types of low impact development practices. SWMM also contains a flexible set of hydraulic modelling capabilities used to route runoff and external inflows through a drainage system network of pipes, channels, storage/treatment units and diversion structures. SWMM can also estimate pollutant loads associated with runoff. The following processes can be modelled for any number of user-defined water quality constituents

- dry weather pollutant build-up over different land uses,
- pollutant wash-off from specific land uses during storm events,
- direct contribution of rainfall deposition,
- reduction in dry-weather build-up due to street cleaning,
- reduction in wash-off load due to BMPs,
- entry of dry weather sanitary flows and user-specified external inflows at any point in the drainage system,
- routing of water quality constituents through the drainage system, and
- reduction in constituent concentration through treatment in storage units or by natural processes in pipes and channels.

The SWMM software has been used in thousands of studies worldwide, including storm water master planning, sewer master planning, floodplain management, water quality and TMDL modelling, and BMP and LID evaluations (Alamdari et al., 2017).

3.3 Groundwater models

Besides groundwater quantity, the quality of groundwater is equally important as a wide variety of contaminants can be found in groundwater, both organic and inorganic, including synthetic organic chemicals, hydrocarbons, inorganic cations and anions, pathogens, and radionuclides. The groundwater models focus on changes in storage and fluxes within the saturated zone and can be classified into physical, analogue, and mathematical models to simulate groundwater movement and contaminant transport. Physical models can be developed in the laboratory to study specific problems of groundwater flow or contaminant transport. Analogue models are based on equations (e.g., Ohm's law/Darcy's law) which describes groundwater flow in isotropic homogenous porous media. Mathematical models rely on groundwater flow (differential) equations which can often be solved only by approximate methods using a numerical method. The most widely used numerical methods are finite element and finite difference methods. With the advancements in computing technology, sophisticated groundwater models have been developed that can be interfaced with GIS or coupled with other models. A selective list of popular groundwater numerical models is presented in Table 8.

MODFLOW

MODFLOW (Modular Three-Dimensional Finite-Difference Groundwater Flow) was developed by the United States Geological Survey (USGS) for simulating steady-state and/or transient saturated groundwater flow under confined and unconfined conditions (Harbaugh, 2005). The model and source code are publicly available on the USGS website, along with many customized versions and utility programs.

The model simulates three-dimensional groundwater flow through a porous medium, using a finite difference method originally documented by McDonald and Harbaugh (McDonald & Harbaugh, 1984). The model domain is discretized into rectangular grid cells, and spatial derivatives are approximated based on the difference between the values of groundwater head at neighboring nodes and the spatial distance between the nodes. The groundwater flow can then be reconstructed based on the potentiometric heads. Numerous MODFLOW versions have been developed as a result of growing interest in surface and groundwater interactions, solute transport, and saltwater intrusion (Christian D. Langevin et al., 2017). The customized packages include enhanced capabilities to simulate processes related to evapotranspiration, rivers, lakes, and multi-node wells (Jones & Mendoza, 2012). Public domain and commercial Graphical user interfaces (GUI) are available for MODFLOW set up, execution and results post-processing, including the MODELMUSE maintained by the USGS.

MODFLOW is the most widely used modelling tool in the world for simulating groundwater flow, with numerous applications by studies on surface and groundwater interactions (Barthel & Banzhaf, 2016; Golden et al., 2014; Guzman et al., 2015), climate change impacts (Chunn, Faramarzi, Smerdon, & Alessi, 2019), solute transport (Zhang et al., 2013),including Alberta Oil Sands environmental impacts assessment ((R. Thompson, Mooder, Conlan, & Cheema, 2011).

MT3D-USGS

MT3D-USGS (Bedekar et al., 2016) is a USGS updated release of the groundwater solute transport code MT3DMS (Modular Transport, 3-Dimensional, Multi-Species model) version 5.3 (Zheng & Wang, 1999). MT3D-USGS includes new transport modelling capabilities to accommodate flow terms calculated by MODFLOW packages that were previously unsupported by MT3DMS, and to provide greater flexibility in simulation of solute transport and reactive solute transport. MT3D-USGS is available in the public domain.

MT3D-USGS uses simulated hydraulic heads, intercell flows, and source and (or) sink terms from the MODFLOW output in the solution of the advection dispersion equation. MT3D-USGS capabilities and features include

- unsaturated-zone transport,
- transport within streams and lakes, including solute exchange with connected groundwater,
- capability to route solute through dry cells that may occur in the Newton-Raphson formulation of MODFLOW (that is, MODFLOW-NWT),

- chemical reaction option that includes the ability to simulate interspecies reactions and parent-daughter chain reactions,
- pump-and-treat recirculation that enables the simulation of dynamic recirculation with or without treatment for combinations of wells that are represented in the flow model, mimicking the above-ground treatment of extracted water,
- reformulation of the treatment of transient mass storage to improve conservation of mass and yield solutions for better agreement with analytical benchmarks,
- separate specification of partitioning coefficient (Kd) for mobile and immobile domains,
- capability to assign prescribed concentrations to the top-most active layer,
- ability to ignore cross-dispersion terms, and
- ability to specify an absolute minimum thickness rather than the default percentage minimum thickness in dry-cell circumstances.

MT3DMS has been an industry standard, accepted by practitioners and researchers and applied in thousands of studies worldwide (Ghoraba, Zyedan, & Rashwan, 2013; H. Zhang, Xu, & Hiscock, 2013). Like MT3DMS, MT3D-USGS is designed as a generalized groundwater solute transport code for use with any block-centered finite-difference groundwater flow model such as MODFLOW. MT3D-USGS can be used to simulate changes in concentrations of contaminants in groundwater considering advection, dispersion, and chemical reactions. The chemical reaction package options available in the model include equilibrium-controlled linear or nonlinear sorption, first-order irreversible decay or biodegradation, interspecies reactions, and parent-daughter chain reactions.

SUTRA

SUTRA (Saturated-Unsaturated Transport) is a finite element simulation model for two-dimensional or three-dimensional saturated-unsaturated, fluid-density-dependent groundwater flow with energy transport or chemically-reactive single-species solute transport model (C. I. Voss & Provost, 2010). The original version of SUTRA was released in 1984, and the latest version, SUTRA 3.0, was released in 2019.

The model employs a two-dimensional or three-dimensional finite-element and finite-difference method to approximate the governing equations that describe the two interdependent processes that are simulated: fluid-density-dependent saturated or unsaturated groundwater flow and either (a) transport of a solute in the groundwater, in which the solute may be subject to equilibrium adsorption on the porous matrix and both first-order and zero-order production or decay, or (b) transport of thermal energy in the groundwater and solid matrix of the aquifer. SUTRA tracks the transport of either solute mass or energy in flowing groundwater through a unified equation, which represents the transport of either solute or energy. Solute transport is simulated through a numerical solution of a solute mass balance equation where the solute concentration may affect fluid density. The single solute species may be transported conservatively, or it may undergo equilibrium sorption (through linear, Freundlich, or Langmuir isotherms). In addition, the solute may be produced or decayed through first-order or zero-order processes. Energy transport is simulated through a numerical solution of an energy balance equation. The solid grains of the aquifer matrix and fluid are locally assumed to have equal temperature, which may affect fluid density and viscosity.

As the primary calculated result, SUTRA provides fluid pressures and either solute concentrations or temperatures, as they vary with time, everywhere in the simulated subsurface system. SutraGUI is a public domain computer program designed to run with the proprietary Argus ONE package, which provides two-dimensional Geographic Information System (GIS) and meshing support (Winston & Voss, 2004).

SUTRA's modular design allows straightforward modifications to the code. Eventual modifications, for example, are the addition of non-equilibrium sorption (such as two-site models), equilibrium chemical reactions or chemical kinetics, or the addition of overburden and underburden heat loss functions, a wellbore model, or confining bed leakage. The USGS's SUTRA code is the most widely used simulator for seawater intrusion and other variable density groundwater flow problems based on solute transport or heat transport (C. Voss, 1999). It has also been widely used for many other types of problems (Tsanis, 2006).

HGS

HydroGeoSphere (HGS) is a three-dimensional control-volume finite-element simulator which is designed to simulate the entire terrestrial portion of the hydrologic cycle based on a rigorous conceptualization of the hydrologic system consisting of surface and subsurface flow regimes in fractured or unfractured porous media (Aquanty, 2015). Originally, it was known as FRAC3DVS. HGS is developed by Aquanty Inc. in Canada.

In order to accomplish integrated analysis, HydroGeoSphere utilizes a rigorous, mass conservative modelling approach that fully couples the surface flow and transport equations with the three dimensional, variably saturated subsurface flow and transport equations. This approach is significantly more robust than previous conjunctive approaches that relied on the linkage of separate surface and subsurface modelling codes. HGS uses a globally implicit approach to simultaneously solve two-dimensional diffusive wave equations and the three-dimensional form of Richards' equation based on unstructured finite element grids. For each timestep, the model solves surface and subsurface flow, and solute and energy transport equations simultaneously, and provides a complete water and solute balance. HGS has the following features for surface and subsurface water modelling:

- surface domain represented as two-dimensional overland flow;
- subsurface domain consisting of three-dimensional unsaturated/saturated flow;
- surface/subsurface domains interacting through physically based fluid exchange;
- temporally and spatially varying evapotranspiration based on land use;

- impact of snowmelt on hydrologic regime;
- delineation and tracking of the water table position;
- handling of non-ponding or prescribed ponding recharge conditions and seepage faces;
- representation of fractured geologic materials with arbitrary combinations of porous, discretely fractured, dual-porosity, and dual-permeability media for the subsurface;
- accommodation of storage, solute mixing and variable flow distribution along wellbores; and
- density-dependent flow and transport.

The capabilities of the mass and heat transfer module of HGS include:

- capability of modelling non-reactive and reactive chemical species transport in the associated surface and subsurface flow fields, including solute interactions between the surface and subsurface flow regimes;
- calculation of temperatures in the surface and subsurface flow regimes as driven by air temperature and incoming solar radiation, accounting for land surface-atmospheric thermal interactions;
- handling of fluid and mass/thermal energy exchanges between fractures and matrices, including matrix diffusion effects and solute/thermal energy advection in the matrix; and
- straight or branching decay chains representing degradation reactions.

HGS is written in FORTRAN and is being continuously developed. It runs on all versions of Windows and Linux systems. HGS does not currently have a graphical user interface (GUI). All model parameters, grid structures, material properties, or numerical parameters are written in text files. A preprocessor (called GROK) prepares the input files for HGS.

The main input file is an instruction-driven text file that only requires a text editor. HGS has a post-processing program called HSPLOT to convert the output data to a format that can be read by third-party visualization packages such as TECPLOT or GMS (Aquanty, 2015). HGS has been used for simulating variably saturated groundwater flow and reactive solute transport, such as nitrate (Koh, Lee, & Lee, 2016).

FEFLOW

The Finite Element subsurface FLOW system (FEFLOW) is a two-dimensional/three-dimensional finite-element model for simulating groundwater flow, solute, and heat transfer in porous media and fractured media (DHI, 2016).

FEFLOW uses finite-element-based analysis to solve the groundwater flow equation of both saturated and unsaturated conditions as well as reactive multi-species solute and heat transport, including fluid density effects and chemical kinetics for multi-component reaction systems. Contaminant transport processes include advection, hydrodynamic dispersion, linear and nonlinear sorption isotherms, and first-order chemical, non-equilibrium, kinetic reactions between species. FEFLOW is available for Windows systems as well as for different Linux distributions. FEFLOW is a completely integrated package from simulation engine to user interface. The option to use and develop user-specific plug-ins via the programming interface (Interface Manager IFM) allows for the addition of external code or even external programs to FEFLOW.

Since its birth in 1979, FEFLOW has been continuously extended and improved. It is consistently maintained and further developed by a team of experts at DHI-WASY. FEFLOW is used worldwide as a high-end groundwater modelling tool at universities, research institutes, government agencies, and consulting companies. FEFLOW can be efficiently used to describe the spatial and temporal distribution and reactions of groundwater contaminants (Regnery et al., 2017), to model geothermal processes, to estimate the duration and travel times of chemical species in aquifers, to plan and design remediation strategies and interception techniques, and to assist in designing alternatives and effective monitoring schemes.

Table 8. Summary of Selected Groundwater Quality Models

Model & Source	**Spatial Representation**	**Type of Simulation**	**Simulated Processes**	**Simulated Parameters**	**GUI**	**Availability and Support**	**References**
MT3D-USGS (USGS)	3D finite difference grid	Steady-state or transient solution	Advection, dispersion, and chemical reactions (sorption, first-order decay, interspecies reactions, and parent-daughter chain reactions) of contaminants in groundwater systems coupled with MODFLOW. Transport within streams and lakes, including solute exchange with connected groundwater.	Reactive and non-reactive contaminants	Yes (public domain and propriety)	Public domain	Bedekar et al., 2016; Zheng & Wang, 1999
SUTRA (USGS)	2D/3D finite element grid	Steady-state or transient solution	Saturated-unsaturated, fluid-density-dependent groundwater flow with energy transport or chemically-reactive (sorption, first-order decay) single-species solute transport.	Reactive and non-reactive, single species	Yes (partially publicly available, partially propriety)	Public domain	Tsanis, 2006; C. Voss, 1999; C. I. Voss & Provost, 2010

Table 8. (*continued*)

HydroGeo-Sphere (Aquanty)	3D finite element grid	Steady-state or transient solution	Entire terrestrial portion of the hydrologic cycle; uses a globally-implicit approach to simultaneously solve the 2D diffusive-wave equation and the 3D form of Richards' equation.	Reactive and non-reactive contaminants	No	Propriety	Aquanty, 2015; Koh et al., 2016
MIKE SHE (DHI)	Square finite difference grids: 2D overland, 1D channels, 1D-unsaturated, and 3D saturated zones	Steady-state or transient solution	Entire hydrologic cycle, including groundwater and solute transport with simplified reaction processes (desorption, degradation, plant uptake, multi-species kinetics). Finite difference method for saturated groundwater flow, several representations of unsaturated flow, including the 1D Richards equation, MIKE 11 for flow in river and stream networks, and the 2D diffusive-wave approach for overland flow.	Reactive and non-reactive contaminants	Yes	Propriety	DHI, 2017c, 2017d; Refsgaard, Thorsen, Jensen, Kleeschulte, & Hansen, 1999

Table 8. (*continued*)

Model & Source	Spatial Representation	Type of Simulation	Simulated Processes	Simulated Parameters	GUI	Availability and Support	References
FEFLOW (DHI)	2D/3D finite element grid	Steady-state or transient solution	Saturated and unsaturated density dependent flow, transport of mass (multiple solutes, desorption, degradation, kinetic reactions between species), and heat	Reactive and non-reactive contaminants	Yes	Propriety	DHI, 2016; Regnery et al., 2017

3.4 Land use/land cover models

Land use/land cover (LULC) modelling helps to explain and/or predict LULC change processes (Pontius & Schneider, 2001) to understand the linkage between socioeconomic processes associated with land development and natural resource policies (Brown et al., 2000) and the causes and consequences of changes in the spatial and temporal patterns of land conversion (Irwin & Geoghegan, 2001). Furthermore, the models represent a simplification of the complex behavior of the socioeconomic and physical environments, and ecological changes. Such models are used to explore future land-use changes under different scenarios and conditions (Veldkamp & Verburg, 2004). According to Lambin et al. (2000), LULC change modelling can address at least one of the following:

1. Socioeconomic and environmental variables that mostly explain land-cover changes.
2. The locations that are affected by land-cover change.
3. The rate at which land-cover changes progress.

In terms of modelling, LULC deals with a complex structure of linkages and feedbacks to analyze the dynamics of LULC practices in the past, with the intention of determining trajectories of change and projecting possible future changes.

The first generation of LULC models dates from the 1940s. The models considered an entire land system as a static entity. Land uses and activities were simulated at a cross-section in time, and their dynamics were considered as trending toward self-equilibrium. These models were criticized because they had no spatial structure (Silva & Wu, 2012). Later on, the models started to take the spatial dimension into account with cellular automata (CA) models (Fredkin, 1990), and also to use GIS for data integration and spatial analysis, such as the California Urban Futures Model (CUF) (Landis, 1995).

Many LULC change models have been developed for different applications, such as deforestation (Kaimowitz & Angelsen, 1998), agricultural intensification (Lambin et al., 2000), land-use based on economic theory (Bockstael & Irwin, 2000), and urban studies (Mitasova & Mitas, 1998).

Table 9. Land Use/Land Cover (LULC) Change Models

Model	**Reference**	**Description**	**Watershed studies**	**Study area**
Land-use change scenario kit (Luck)	Ott & Uhlenbrook, 2004	This model executes LULC change scenarios based on the characteristics of each grid cell and its relationships to neighboring cells. It has three modules for simulation of urbanization, agriculture, and forest LULC change. Luck includes the topography, soil, river network, and axes of infrastructural development. The spatially averaged, large-scale trend of LULC development must be provided as an external input, the so-called "scenario target."	Quantified the impact of LULC changes at the event and seasonal time scale.	Dreisam basin in southwest Germany
Land Transformation Model (LTM)	Tang et al., 2005	A LULC forecasting model that employs a set of spatial interaction rules and machine learning using artificial neural network to identify the nature of spatial interactions of driving forces based on the historical data to forecast future LULC change.	Assessed the impacts of future LULC change on long-term runoff and non-point source pollution.	Muskegon River watershed, in the eastern coast of Lake Michigan
Conversion of Land Use and its Effects (CLUE)	Lin et al., 2007	This model is based on the spatial allocation of demands for different LULC types to individual grid cells. It combines biophysical and human LULC drivers in space and time (Veldkamp and Fresco, 1996). The model is an empirical model which begins with the evaluation of relationships between land use and its driving factors and continues with the addition of dynamic simulation of interactions between the spatial and temporal dynamics of land use systems.	Used the CLUE-s model (which is a modified version of CLUE) to simulate various future land use scenarios based on driving factors with spatial and non-spatial policies to assess the impact of future LULC change on hydrological processes.	Wu-Tu watershed in northern Taiwan

Table 9. (*continued*)

Urban growth model Slope, Land use, Excluded land, Urban extent, Transportation, and Hillshading (SLEUTH)	Lin et al., 2008	The model is a cellular automata class model, which is a probabilistic model that uses Monte Carlo routines to generate multiple simulations of urban growth.	Applied SLEUTH and CLUE-s models to to analyze the effects of future urban sprawl on the LULC patterns and hydrological processes.	Paochiao watershed in Taipei County, Taiwan
Urban Development Simulation Model (UrbanSim)	Cuo et al., 2011	UrbanSim incorporates the interactions between land use, transportation, the economy, and the environment.	A land cover change model (LCCM), UrbanSim, and biophysical site and landscape characteristics were used to investigate the potential impacts of projected future land cover and climate change on the hydrology.	Puget Sound basin, Washington
"What if?"	McColl & Aggett, 2007	An easy-to-use GIS-based planning support system that can be used to explore the most important and difficult aspects of the land planning process: conducting a land suitability analysis, projecting future land use demand, and allocating the projected demand to suitable locations.	Integrated a land-use/cover forecasting model with an event scale, rainfall-runoff model to improve LULC policy formulation in the study area.	Kittitas County, Washington
Cellular Automata (CA)	Wijesekara et al., 2012	CA is a rigorous modelling approach for characterizing complex spatial systems through a bottom-up simulation of local interactions between neighboring cells.	Investigated the impact of future (20 years) land-use changes on the hydrological processes using a LULC cellular automata (CA) model and the distributed physically-based MIKE SHE/MIKE 11 hydrological model.	Elbow River watershed in southern Alberta
NERC/ESRC Land Use Programme (NELUP)	Dunn & Mackay, 1995	The model applies a general system framework for organizing the large amounts of information that are relevant to decision-making in land use.	Evaluated the potential impacts of land use change on evapotranspiration.	Tyne River basin, UK

However, little attention was paid to simulate future land-use/cover changes for hydrological studies at a watershed scale. Most of them have considered historical LULC maps as static input for land-related parameters in their simulations. In the recent past, very few studies have reported developing LULC modelling to forecast future LULC to analyze the effect of LULC changes on the catchment water balance (Wijesekara et. al., 2011; Cuo et al., 2011; Lin et al., 2007; Tang et al., 2005). Table 9 lists the widely used LULC models in the literature.

In this report, we classify LULC models into two broad groups: empirical models and simulation integrated models.

3.4.1 Empirical models

Empirical models consider the statistical/mathematical relationship between LULC classes, and external driving factors, such as physical characteristics (biodiversity, soil functions, and water resources), population, and technological development. However, they do not consider the interactions among LULC classes over time and the human behavior that can lead to the spatial process/outcome of land-use changes. The models can be implemented based on different statistical methods. For example, multivariate regression models (Braimoh & Vlek, 2004) and logit regression models (Turner et al., 2001) have been used to evaluate the possible exogenous contributions of causal factors (Yu et al., 2011). They can also use some assumptions of possible future land developments to project future land-use patterns such as 'what if' scenarios (Braimoh & Vlek, 2004).

Empirical models can be spatial or spatially explicit models (Yu et al., 2011). Spatial models have been primarily developed by economists to describe spatial patterns of land use (Yu et al., 2011). These models are mostly based on the concept of distance to driving factors, and they ignore other important features of the landscape.

According to Agarwal et al. (2002), there are two groups of spatially explicit models: spatially representative and spatially interactive. However, only spatially representative models belong to empirical models in our classification. These models deal with data in two or three spatial dimensions (for example, northing, easting, and elevation). These models cannot examine topological interactions between geographical features at each of the timesteps. However, the value of each feature can change or stay constant independent of neighboring features. (Spatially interactive models, which incorporate spatial relationships and interactions between neighboring units over time, belong to the simulation integrated models class described in the next section.)

3.4.2 Simulation integrated models

Simulation integrated models are capable of conducting integrated simulations of LULC dynamics of landscape influenced by several factors. Integrated models represent “the relationships, interactions, and feedbacks between spatial and non-spatial components of a LULC system, such as human and economic activities, and physical and environmental characteristics of the landscape. On the other hand, simulation models are mathematical models that use computational resources to simulate the dynamics of land surface. However, in terms of modelling technique, Wilson (1974) explains that they are:

> a set of rules which enable a set of numbers to be operated upon, usually in the computer, although the rules and the consequences of applying them cannot be written down as a set of algebraic equations. . . . Sometimes, the simulation technique lends itself naturally to a problem. This happens, for example, when the underlying theory consists of a set of statements involving conditional probabilities. . . . We resort to simulation techniques for situations which are too complicated to be handled by more straightforward algebraic techniques.

The meaning of simulation methods of modelling was clarified by Batty (1976) as:

> Analytic methods of modelling use mathematical analysis to reach at explicit equations representing the behavior of the system while simulation methods are used to derive the behavior of the system when the system is too complex to be modeled using the more direct analytic approach.

In general, simulation integrated models derive the behavior of a complex system, and simulate the change of the land's attributes using a set of rules based on the interactions, relationships, and linkages arising between components of land use either internally (the number of LULC classes and their interactions among neighborhood units) or externally, with the overall intent to capture the dynamics of land and reproduce its patterns over time.

3.5 Climate models

Climate models are important for improving our understanding and ability to predict climate behavior as a result of natural variability and change and human activity, as well as understanding the impacts of climate change and variability on environmental processes (Farjad et al., 2019). Climate models are mathematical methods and computer programs which simulate interactions between land, and/or atmosphere, and/or ocean, and/or ice by incorporating physical system processes. They are run using powerful computers to capture the complex influence of internal processes and/or external forcing on the climate system. They range from simple energy balance models to complex Earth Systems Models (ESMs). To keep it simple, climate models could be divided into three categories: simple models, general circulation models, and intermediate complexity models.

3.5.1 Simple models

These are the earliest and most simplified version of climate models developed based on the concept of energy balance. The simple linear relaxation model (usually referred to as an Energy Balance Model) is the simplest climate model in this category and is time dependent. These models can range from zero- to two-dimensional models. Zero-dimensional models assume a balance between incoming solar radiation and outgoing long-wave radiation, resulting in a uniform temperature over the land surface. One-dimensional models assume different latitudinal zones cover land surfaces with different incoming solar energies. However, two-dimensional models assume variations in two directions.

3.5.2 General circulation models

General circulation models, also known as Global Climate Models (GCMs), are numerical models used to simulate the complex interaction of the processes and feedbacks in the climate (M. Wang et al., 2012). They are developed based on physical laws of climate dynamics, and they are solved by mathematical equations or sometimes empirical relations. For example, atmospheric GCMs numerically solve the equations of physics, such as dynamics, radiative transfer, or thermodynamics, as well as chemistry applied to the atmosphere and its constituent components. Whereas in more primitive GCMs only the thermodynamic role of the ocean was considered, GCMs today typically include the dynamics of the ocean and its interactions with the atmosphere and are therefore known as Atmosphere-Ocean GCM (AOGCM) or coupled atmosphere-ocean models. The term Global Climate Models (GCMs) is typically used to refer to climate models that reflect both atmospheric and oceanic processes and feedbacks. The current generation of GCMs includes the hydrological cycle (which couples terrestrial, atmospheric, and ocean reservoirs of water and the flows between these reservoirs), terrestrial biosphere, continental ice sheets, and the ocean's carbon cycle and its interactions with the atmosphere and the ocean. As a result, a variety of climate components are included such as atmospheric and ocean circulation, atmospheric temperature profiles, snow and ice distribution, and wind patterns.

General circulation models are numerical models used to simulate the complex interaction of the processes and feedbacks in the atmosphere (M. Wang et al., 2012). They are developed based on physical laws of climate dynamics of the atmosphere, and they are solved by mathematical equations or sometimes empirical relations. Primitive GCMs prescribed the physical characteristics of the earth's surface (e.g., sea-surface temperature, land temperature, and soil wetness) as boundary conditions. Subsequently, coupled atmosphere-ocean models have been developed to reflect interactions between the atmosphere and the ocean. The term Global Climate Models (GCMs) is typically used to refer to climate models that reflect both atmospheric and oceanic processes and feedbacks. GCMs today typically include the dynamics of the ocean and its interactions with the atmosphere and are therefore known as Atmosphere-Ocean GCM (AOGCM) or coupled atmosphere-ocean models. For example, atmospheric GCMs numerically solve the equations of physics, such as dynamics, radiative transfer, or thermodynamics, as well as chemistry applied to the atmosphere and its constituent components. The current generation of GCMs includes the hydrological cycle (which couples terrestrial, atmospheric, and ocean reservoirs of water and the flows between these reservoirs), terrestrial biosphere, continental ice sheets, and the ocean's carbon cycle and its interactions with the atmosphere and the ocean. As a result, a variety of climate components are included such as atmospheric and ocean circulation, atmospheric temperature profiles, snow and ice distribution, and wind patterns.

Further, a subset of climate modelling involves Integrated Assessment Models (IAMs) by incorporating socioeconomic aspects to understand how societal factors influence the climate (for example, how population, economic growth, and use of fossil energy influence the climate on earth). Therefore, IAMs produce scenarios of future greenhouse gas emissions, and these scenarios are then run through various Earth System Models (ESMs) to generate future climate projections, used for assessing the impact of climate change to develop adaptation and mitigation strategies and policies for sustainable growth and environmental stewardship for future generations.

GCMs provide coarsely scaled outputs in spatial and temporal resolutions, as they are computationally intensive. Therefore, these scales are nearly inadequate for direct use in environmental models (S. Tripathi et al., 2006; Sunyer et al., 2012), and so the outputs of a low-resolution climate model need to be downscaled to a finer suitable scale (Teng et al., 2012), which can be dynamical or statistical (Sunyer et al., 2012). Downscaling methods are an important tool in assessing the impact of future climate change on environmental processes at both regional and local scales. In fact, downscaling methods bridge the gap between the resolution of climate models and environmental models (Fowler et al., 2007). Various studies have used downscaling methods to produce the required meteorological variables for environmental modelling (X.-C. Zhang, 2005; Chen et al., 2010; Willems & Vrac, 2011; Li et al., 2012; Farjad et al., 2015). Dynamical downscaling refers to the use of process-based regional climate models (RCMs) to provide climate data within boundary conditions prescribed by a GCM, through regional-scale atmospheric simulations, at a finer spatial and temporal resolution than GCMs (Phatak et al., 2011). On the other hand, statistical downscaling relies on the statistical relationships between large-scale climate model variables (GCMs or RCMs) and local-scale climate variables (Sunyer et al., 2012).

3.5.3 Intermediate complexity models

Intermediate complexity models strike a balance between simple energy balance models and GCMs, in terms of degree of complexity. These models are also known as Earth Models of intermediate Complexity (EMICs). In terms of dynamics and resolution, these models are simpler than GCMs, but they are more comprehensive than simple models, in terms of the number of components and processes (e.g., LOVECLIM). Some of these models are built for specific purposes with a specified range of atmospheric components, but most of them include sea ice, dynamic vegetation, land surface processes, and ice sheet models. LOVECLIM1.2 incorporates atmosphere, land surface, ocean and sea ice, ice sheets/icebergs, and the carbon cycle.

3.6 Ecological models

Ecological models are mathematical models for biological and biophysical processes (which can be analytic or simulation-based) to understand ecological processes and capture changes in ecosystems. Most ecological models are generally integral parts of core system analyses or watershed models. For example, the AQUATOX model is an integral part of the BASINS system with links to the watershed models SWAT and HSPF, whereas ECO Lab is an integral part of MIKE SHE/MIKE Hydro. The widely used ecological models are described as follows:

3.6.1 AQUATOX model

The AQUATOX model simulates the fate of sediments, organic chemicals, and nutrients, and their influence on the ecosystem (such as fish, invertebrates, or aquatic plants) and thus is capable of integrated modelling of ecology/biology and water quality. For example, Bingli et al., (2008) used the AQUATOX model to simulate the environmental fate and aquatic ecological impacts of a nitrobenzene concentration in the Songhua River, China. They conducted a sensitivity analysis to determine the key processes that influence the nitrobenzene concentration levels and found significant changes in biomass for diatoms and mussels. Other typical applications of the AQUATOX model are:

- calculating recovery time of contaminated fish tissues to safe levels when pollutant loads are reduced,
- evaluating impacts of pesticides and other toxic substances,
- developing numeric nutrient targets based on desired biological endpoints,
- evaluating effects of multi-stressors on biological systems, and
- measuring the impact of climate change on the ecosystem.

3.6.2 Mike ECO Lab

MIKE ECO Lab is a generic ecological modelling tool for simulating processes related to water quality and ecological systems. One of the advantages of the MIKE ECO Lab compared to other ecological models is that it can be linked to the range of one-dimensional, two-dimensional, and three-dimensional MIKE modelling systems to address a variety of complex ecological issues. In addition, MIKE ECO Lab not only contains a generic equation solver, but it can also be applied as a generic post-processor of hydrodynamic results, for instance, calculating flood risk indices or a scour risk formula. Santos et al. (2015) used the MIKE ECO Lab linked with Mike Hydro Basin model for water quality assessment, such as the dissolved concentration of phosphorus, in a river basin with recurrent wildfires in northern Portugal. They found a positive correlation between the occurrence of forest fires and the concentration of phosphorus in the water. Other typical applications of the MIKE ECO Lab model include:

- study of simple and complex ecological systems,
- water quality modelling related to surface/subsurface, rivers, wetlands, lakes, reservoirs, estuaries, coastal waters, and the sea,

- modelling of ecosystem response spatially, and
- impact and remediation assessment.

3.6.3 BASS

Bioaccumulation and Aquatic System Simulator (BASS) is used to simulate the bioaccumulation of chemical pollutants and dynamics, and the population of fish assemblages under chemical and non-chemical stressors. BASS is a process-based model that can simulate ecological, physiological, and toxicokinetic processes, and can address the limitations of simple bioaccumulation factor (BAF) approaches for predicting concentrations of extremely hydrophobic chemicals and metals. Knightes et al. (2009) used BASS to model fish mercury-intake as a function of gill exchange and dietary ingestion. The model partitions mercury internally to water, lipid, and non-lipid organic materials. Knightes et al. estimated a physiologically based carrying capacity for zooplankton and phytoplankton based on projected oxygen consumption and prevailing dissolved oxygen content. Typical applications of the BASS model are:

- simulating fish methylmercury bioaccumulation,
- estimating lag times of mercury residues in fish in response to mercury load reductions,
- simulating time dynamic bioaccumulation when simple steady-state methods (e.g., BSAFs or BAFs) are not considered sufficient, and
- evaluating responses of fish community composition, production, biomass, and PCB/mercury bioaccumulation potential to changes in climate, LULC, and fisheries management scenarios.

3.6.4 SERAFM

SERAFM is a process-based (steady-state) mercury cycling model used to estimate mercury concentrations in the water column, fish tissue, and sediment for the species Hg0, HgII, and MeHg. Sub-modules of SERAFM consist of mercury loading (watershed and atmospheric deposition), abiotic and biotic solids balance (soil erosion, settling, burial, and resuspension), equilibrium partitioning, water body mercury processes, and wildlife risk calculations. S. Brown et al. (2007) used the SERAFM model to estimate unfiltered and dissolved total mercury concentration, as well as MeHg, in the water column in Steamboat Creek in Nevada. They highlighted the capability of the SERAFM model of estimating mercury concentration in arid western environments. Typical applications of the SERAFM model are:

- mercury deposition impacts on a water body,
- estimating steady-state mercury cycling in a river, lake, and watershed,
- wildlife risk prediction exposed to mercury-contaminated sediments, and
- evaluating sensitivity of model parameters and processes to pollution.

3.6.5 Physical Habitat Simulation System (PHABSIM)

The Physical Habitat Simulation System (PHABSIM) model is used to simulate relationships between river flow and physical habitat for a variety of life stages of a species of fish or a recreational activity. PHABSIM integrates a river model with a biological model of habitat (based on habitat suitability criteria) to estimate changes in a habitat index (weighted usable area) as a function of river discharge. Some of applications of the PHABSIM model are:

- predicting the micro-habitat conditions in rivers and the relative suitability of those conditions to aquatic life,
- understanding the impact of mining-derived sediment on aquatic physical habitat,
- determining the utility of a reconnaissance-level physical habitat suitability, and
- examining the trade-off between the value of water used instream with the water used out-of-stream.

3.7 Air quality models

Understanding the impact of emitted air pollutants from natural or manmade sources is a challenging topic in CEA studies.

There are many approaches to quantify air pollution, and they can be categorized as dispersion, photochemical, and receptor models, as well as geospatial-based models. Different factors are considered in the literature for selecting a proper approach, such as availability of data, temporal and spatial scale, acceptable level of uncertainty, type of the pollutant, and type of the activity (biomass burning, traffic-based pollution). Here, the most commonly used approaches to investigate air pollution are explained.

3.7.1 Dispersion modelling

Dispersion models are mathematical models that predict the concentration of pollutants at specified ground level receptor locations. These models use emissions and meteorological variables as inputs. The most common dispersion models are AERMOD and CALPUFF. The AERMOD model incorporates air dispersion based on a planetary boundary layer turbulence structure and scaling concepts while, the CALPUFF model simulates the effects of space- and time-varying meteorological conditions on pollution transport, transformation, and removal. Other common dispersion models are CALINE3, BLP, CAL3QHC/CAL3QHCR, OCD, and CTDMPLUS.

3.7.2 Photochemical modelling

Photochemical models simulate atmosphere pollutant concentrations using a set of mathematical equations characterizing the chemical and physical processes over large spatial scales. The most common photochemical models are the Community Multiscale Air Quality model (CMAQ), the Comprehensive Air quality Model with extensions (CAMx), and the Regional Modelling System for Aerosols and Deposition (REMSAD).

3.7.3 Receptor modelling

Receptor models are mathematical or statistical procedures that use the measured physical and chemical characteristics of gases/particles (not pollutant emissions and meteorological data, unlike photochemical and dispersion models) to identify and quantify the source of pollutants at receptor locations. The most common receptor models are the Chemical Mass Balance (CMB) model, Unmix model, and Positive Matrix Factorization (PMF) model.

3.7.4 Geospatial-based modelling

These models typically generate the spatial distribution of pollutants and can be categorized as:

3.7.4.1 Proximity-based models:

These models are GIS based and are used for assessment of exposure to air pollution when the density of spatial monitoring stations is sparse. These models use simple approximate measurements such as 'buffering' to assess the exposure, which results in severe limitations on their usefulness.

3.7.4.2 Interpolation-based models:

Spatial interpolation models have been developed to estimate values at unknown locations based on known values (i.e., measurements) by using deterministic and stochastic geostatistical techniques. The interpolation of values between monitor locations is an approach that can be completed entirely within GIS. These models use different geostatistical interpolation techniques. One conventional technique is inverse distance-weighted interpolation (IDW). For any given location in the study area (i.e., a residential address or postal code), a weighted average concentration is developed, with the highest weight given to the nearest monitors, thereby producing a continuous pollution surface. These methods assume a stronger correlation among points that are close together versus those that are farther apart.

The most popular interpolation-based model used in air pollution studies is Kriging, an optimal interpolation technique that makes the best linear unbiased estimate of the variable's value. Interpolation models use pollution measurements, which offer primary advantages over the proximity models. However, the main disadvantages of interpolation models are that they depend on the availability of monitoring data and require a dense network of sampling data.

3.7.4.3 Land Use Regression (LUR) models:

Land Use Regression (LUR) models are multivariate regression models that are used for estimating individual exposure to air pollution at a fine spatial scale. They can estimate the pollution concentration at any given location by using surrounding attributes such as LULC classes, traffic, and topography within the area as independent variables (x). Therefore, the measured levels of pollutants in LUR models are considered as dependent variables (y).