Integrated Environmental Modelling Framework for Cumulative Effects Assessment

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Anil Gupta, Babak Farjad, George Wang,
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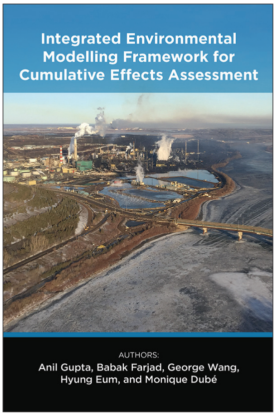

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Acronyms and Abbreviations

AD	Advection-dispersion
AET	Actual Evapotranspiration
AnnAGNPS	Annualized Agricultural Non-Point Source Pollution Model
AOGCM	Atmosphere–Ocean Global Climate Model
API	Application Programming Interface
ARO	US Army Research Office
BASINS	Better Assessment Science Integrating Point and Non-point Sources
BASS	Bioaccumulation and Aquatic System Simulator
BMPs	Best Management Practices
BSAF	Biota-Sediment Accumulation Factor
CA	Cellular Automata
CALPUFF	California Puff Model
CAMx	Comprehensive Air quality Model with extensions
CBOD	Carbonaceous Biological Oxygen Demand
CEA	Cumulative Effects Assessment
CEH	Center for Ecology and Hydrology
CEMA	Cumulative Environmental Management Association
CEQ	US Council on Environmental Quality

CESM	Community Earth System Model
CFSR	Climate Forecast System Reanalysis
CIT	California Institute of Technology-Carnegie Institute of Technology
CLUE	Conversion of Land Use and its Effects
CMAQ	Community Multiscale Air Quality Modeling System
CMB	Chemical Mass Balance
CMIP	Coupled Model Intercomparison Project
CO	Carbon Monoxide
COD	Chemical Oxygen Demand
CORDEX	Coordinated Regional Climate Downscaling Experiment
CSO	Combined Sewer Overflows
CUF	California Urban Futures Model
DEM	Digital Elevation Model
DO	Dissolved Oxygen
DOC	Dissolved Organic Carbon
DON	Dissolved Organic Nitrogen
DOP	Dissolved Organic Phosphrus
ECMWF	European Centre for Medium-Range Weather Forecasts
EFDC	Environmental Fluid Dynamics Code
ESP	Ecosystem Services Processor
ET	Evapotranspiration
FEFLOW	Finite Element subsurface FLOW system
FRAMES	Framework for Risk Analysis Multi-Media Environmental Systems

GCM	General Circulation Model
GIS	Geographic Information System
GLVHT	Generalized Longitudinal-Vertical Hydrodynamics and Transport Model
GUI	Graphical User Interface
HD	Hydrodynamic
HEC	United States Army Corps of Engineers Hydrologic Engineering Center
HEC-RAS	Hydrologic Engineering Center River Analysis System
HEC-HMS	Hydrological Modelling System
HGS	HydroGeoSphere
HRU	Hydrologic Response Unit
HSI	Habitat Suitability Index
HSPF	Hydrologic Simulation Program-Fortran
HSS	Hydrocarbon Spill-Source Package
IDW	Inverse distance weighted interpolation
IEM	Integrated environmental modelling
IMPLND	Impervious Land Module in HSPF
IPCC	Intergovernmental Panel on Climate Change
LAI	Leaf Area Index
LARM	Laterally Averaged Reservoir Model
LCCM	Land Cover Change Model
LID	Low Impact Development
LSPC	Loading Simulation Program in C++
LTM	Land Transformation Model
LUCK	Land Use Change Scenario Kit
LULC	Land Use/Land Cover

LUR	Land Use Regression
MBC	Multivariate Bias Correction
MHK	Marine and Hydro-kinetic
MLM	Mercury Loading Model
NARR	North American Regional Reanalysis
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction
NELP	NERC/ESRC Land Use Programme
NO_2	Nitrogen dioxide
NRBS	Northern River Basins Study
O_3	Ozone
OGS	OpenGeoSys
OpenMI	Open Modelling Interface
pH	Potential of Hydrogen
PERLND	Pervious Land Module in HSPF
PHABSIM	Physical Habitat Simulation System
PM	Particulate Matter
PMF	Positive Matrix Factorization
PRMS	Precipitation-Runoff Modelling System
QDM	Quantile Delta Mapping
RADM	Regional Acid Deposition Model
RCHRES	Free-flowing Reach or Mixed Reservoirs Module in HSPF
RCM	Regional Climate Model
RCPs	Representative Concentration Pathways
REMSAD	Regional Modelling System for Aerosols and Deposition
RPEM	Rooted Plant and Epiphyte Model

RUSLE	Revised Universal Soil Loss Equation
SNL-EFDC	Sandia National Laboratories modified Environmental Fluid Dynamics Code
SP	Streeter–Phelps
SRES	Special Report on Emissions Scenarios
SUTRA	Saturated-Unsaturated Transport
SWAT	Soil and Water Assessment Tool
SWMM	Storm Water Management Model
TKN	Total Kjeldahl Nitrogen
TMDL	Total Maximum Daily Load
TN	Total Nitrogen
TOC	Total Organic Carbon
TON	Total Organic Nitrogen
TOP	Total Organic Phosphorus
TP	Total Phosphorus
UGM	Urban Growth Model
UH	Unit Hydrograph
UrbanSim	Urban Development Simulation Model
VBA	Visual Basic for Applications
VOGG	Visual Orthogonal Grid Generator
WASP	Water Analysis Simulation Program
WES	United States Army Engineer Waterways Experiment Station
WLA	Waste Load Allocation

1.0 INTRODUCTION

Global warming and population growth have resulted in an increase in the intensity of natural (e.g., climate change) and anthropogenic stressors. Investigating the responses of environmental processes to the cumulative effects of stressors – now known as cumulative effects assessment (CEA) – was already being practiced (e.g., groundwater resources described in Schoff & Sayąn, 1969) when the concept of environmental impact assessment (EIA) was introduced in 1969. However, the theory and concept of CEA was defined by the US Council on Environmental Quality (CEQ) in 1978. The concept of CEA has then been gradually described in more detail by other scholars (e.g., Canter, 1999; Ross, 1998; Cooper, 2004), and many well-designed approaches have been proposed in the literature (e.g., Dubé & Munkittrick, 2001; Dubé et al., 2013; Løkke et al., 2010).

There are different definitions for CEA in the literature (Cooper & Sheate, 2002; Bérubé, 2007; Noble et al., 2014). However, it is defined here as *an assessment of cumulative environmental changes due to human and natural stressors over a period of time for the past, present, and future, relative to a baseline or standard*. CEA not only includes analyzing and modelling environmental changes, but it also supports planning alternatives that promote environmental monitoring and management. A variety of methods are used in literature (Table 1) for cumulative effects assessment, such as spatial analysis, network analysis, interactive matrices, and ecological modelling (Smit & Spaling, 1995). In addition to demanding the development of models to help answer policy questions (Castronova et al., 2013), CEA also requires observations (i.e., monitoring) of changes in natural phenomena.

Investigating the complex nature of environmental problems requires the integration of different environmental processes across major components of the environment, such as water, climate, ecology, air, and social aspects. The increasing dissatisfaction resulting from disjointed and narrowly focused environmental management approaches has recently encouraged the use of integrated environmental modelling approaches (Jakeman & Letcher, 2003). Integrated environmental modelling refers to coupling of thematic based numerical or conceptual models to solve complex real-world problems involving the environment and its relationship to human systems and activities.

The concept of developing integrated models first appeared decades ago (Mackay, 1991). However, there has recently been an increased interest in further developing integrated modelling frameworks in response to the emergence of problems related to regional scale land-use management, impacts of global climate change, evaluation of ecosystem services, fate and transport of nanomaterials, and life-cycle analysis. A variety of models have been developed to investigate the processes of each individual environmental component and the way they interact with each other. However, they have failed to consider environmental processes of other components of the environment and their complex interplay within the environment as a whole. Integrated modelling frameworks are often the only way to take into account the important environmental processes, interactions, relevant spatial and temporal scales, and feedback mechanisms of complex systems for CEA. The other obstacle is the uncertainty as to whether an applied modelling system meets its intended purposes and sufficiently represents reality, an issue which is reinforced by a lack of clear understanding of models' mechanisms. In this regard, this book looks at (i) understanding interactions and relationships between environmental components, such as climate, land, hydro, ecology, and resulting responses due to anthropogenic/natural stressors in CEA, (ii) reviewing modelling approaches for each component, (iii) reviewing existing integrated modelling systems for CEA, and (iv) proposing an integrated modelling framework and perspectives for future research avenues for CEA (Figure. 1).

Figure 1. Overview of the Components of this Report

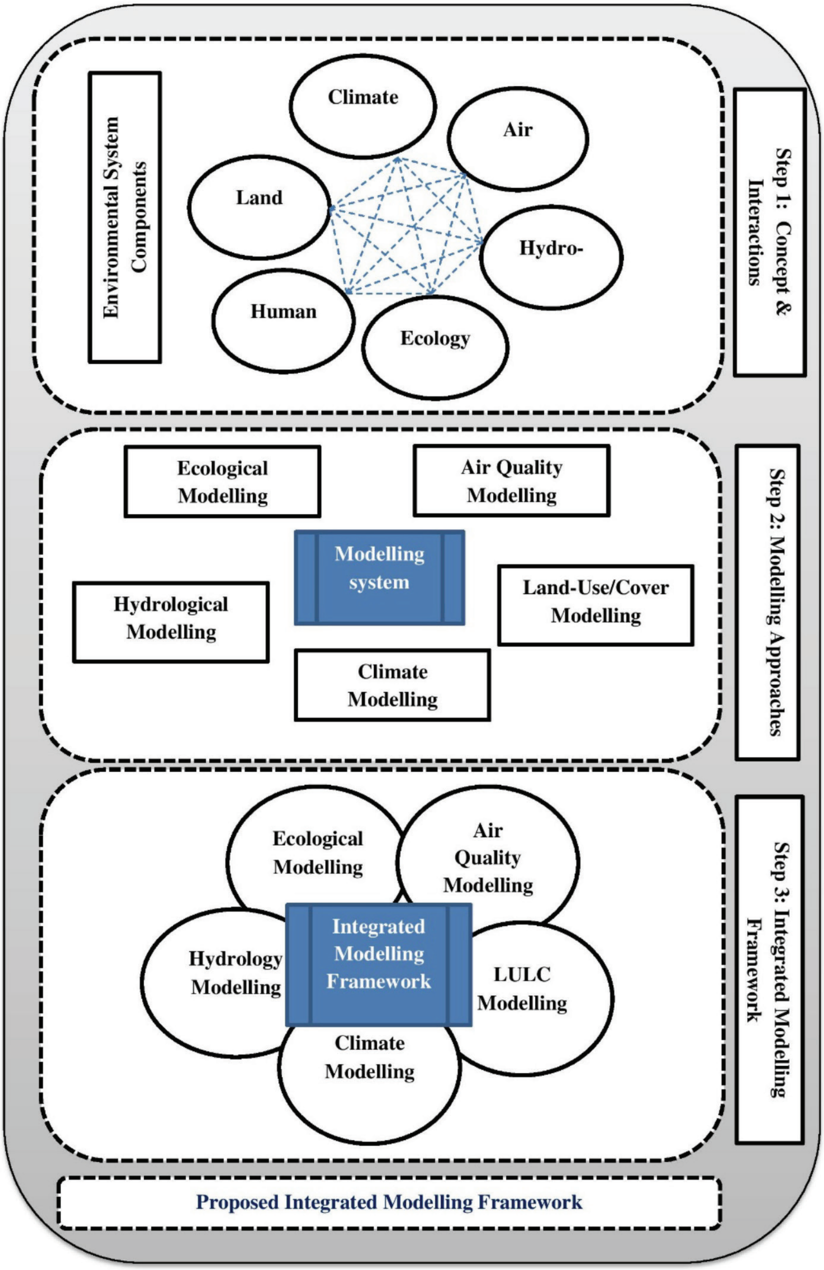


Table 1. Examples of Cumulative Effects Studies

Authors	Objective	Study area	Method	Indicators	Response
Shrestha et al., 2017	Quantify the impacts of climate change on monthly, seasonal, and annual water balances of blue and green water resources at sub-basin, regional, and basin-wide spatial scales.	Athabasca River Basin (ARB), Canada	Soil and Water Assessment Tool (SWAT), calibrated over 1990-2005 period	Blue (surface freshwater & groundwater) and green water (soil moisture)	Results projected the climate of the ARB to be wetter by 21–34% and warmer by 2.0–5.4 °C on an annual time scale. The annual average blue and green water flow (streamflow and evapotranspiration) was projected to increase by 16–54% and 11–34%, respectively.
Cho et al., 2017	Simulate dry, wet and total deposition of acidifying compounds using four different emission scenarios and provide guidance on possible priorities for oil sands emissions management for addressing acid deposition in the Alberta's oil sand region (AOSR).	Athabasca River Basin (ARB), Canada	Community Multi-Scale Air Quality (CMAQ) model	Annual dry, wet, and total depositions of acidifying sulphur and nitrogen compounds	Average nitrogen deposition increases from the historical to existing and future cases. Sulphur deposition decreases from the historical to existing cases but increases to future cases even though regional SO_2 emission continuously decreases.

Table 1. (*continued*)

Authors	Objective	Study area	Method	Indicators	Response
Zhang et al., 2016	Provide a quantitative assess-ment on how forest disturbances affect the components of flow regimes at a large water-shed scale.	Baker Creek and Willow River watersheds, British Columbia, Canada	Time series cross-correlation analysis and paired-year approach	Flow regime	The magnitude, variability, and return period of high flows in the Baker Creek watershed were increased on average by 154.3%, 324.2%, and 11 years, respectively, and the timing of high flows was advanced by about 9 days during the disturbed periods.
Ahmed, 2013	Discern and quantify the hydrologic functions of wetlands within the context of the Rideau River watershed.	Rideau River watershed, Ontario, Canada	Numerical modelling techniques (Mike 11)	Low and peak discharge	It was demon-strated that the flood risk would increase if wetlands are removed. The low flow will likely increase if wetlands are removed.

Table 1. (*continued*)

Authors	**Objective**	**Study area**	**Method**	**Indicators**	**Response**
Deitch et al., 2013	Predict streamflow impairment caused by 438 small reservoirs in the study area	Sonoma County, California, USA	GIS-based hydrologic model	Streamflow	Results illustrate that impairment caused by reservoirs varies appreciably over space, but as reservoirs fill over time, impairment is lower through most of the drainage network.
Cormier et al., 2000	Assessing ecological risk in a watershed	Big Darby Creek watershed, central Ohio, USA	Conceptual models for exposure of fish and benthic macroinvertebrates, surveys of fish and molluscs, biological indices	Fish and molluscs, water quality, sedimentation, and hydrologic regimes	A decrease in the percentage of Tanytarsini midges along with an increase in the percent of toxic-tolerant invertebrate species found in fish is expected to be consistently associated with an increase in the concentrations of toxic chemicals in the water.

2.0 INTERACTIONS BETWEEN ENVIRONMENTAL COMPONENTS FOR CUMULATIVE EFFECTS ASSESSMENT

2.1 Climate and hydrology

The hydrological cycle is linked with the Earth's radiation balance (Figure 2). Changes in radiation balance due to increasing amounts of greenhouse gases tend to increase atmospheric and oceanic temperatures and alter the seasonal frequency, intensity, and location of precipitation. Changes in precipitation patterns can cause a change in runoff and consequently influence soil moisture and infiltration.

In addition, an increase in temperature can result in a change in air humidity and alter the evaporation and evapotranspiration processes. The melting of snow and glacier ice that results in rising global sea levels is also caused by the increased temperature that would lead to increased winter runoff and decreased late spring and summer runoff. An increase in the evapotranspiration rate will decrease soil water storage and will change the amount of water that infiltrates and percolates into the soil. Climate change can also alter the type of native vegetation cover, the leaf area index (LAI), and the soil moisture content at local and regional scales (Arnell, 1994).

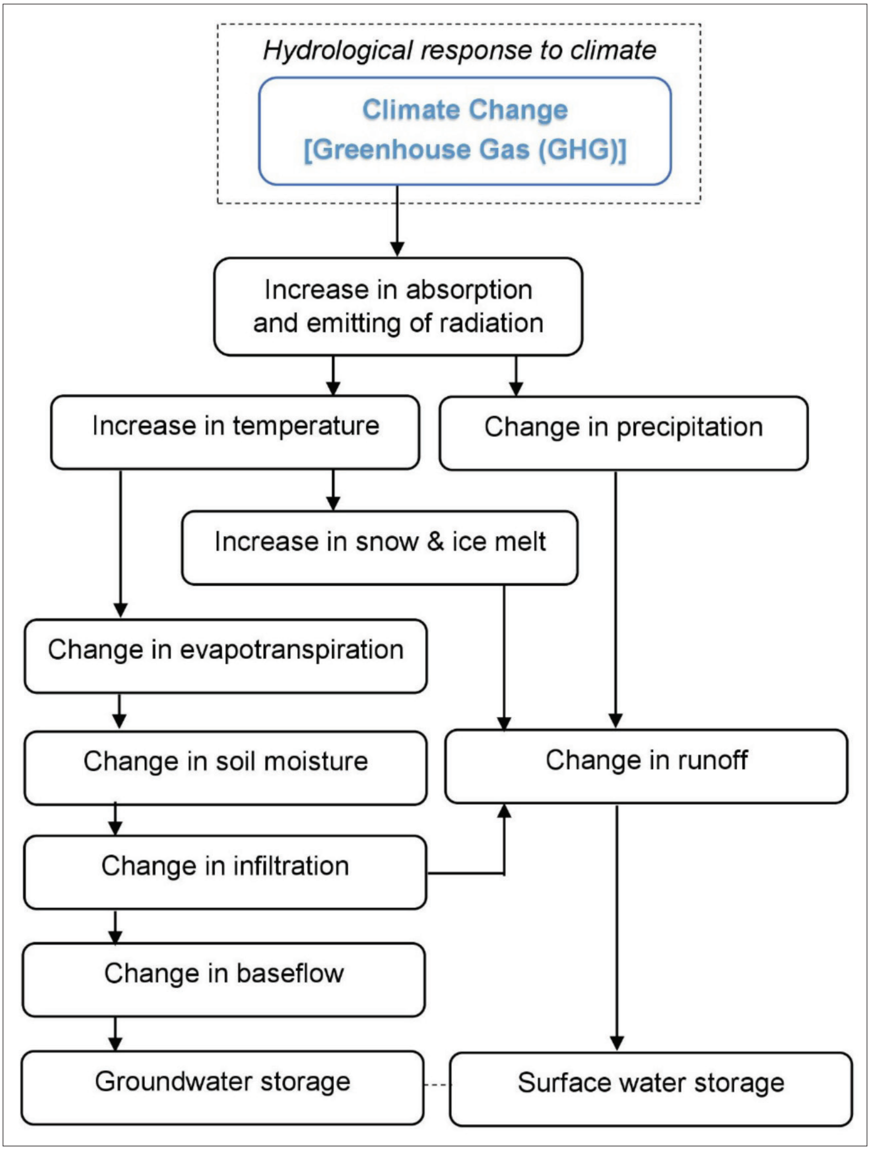
Temperature, precipitation, and evaporation are the main climate variables that impact water resources at local to global scales and are common climate inputs for hydrological models. Temperature is the most important variable compared to other meteorological components, since along with its effects on hydrological processes, it has a significant impact on precipitation and evaporation. An increase in temperature increases rain in proportion to snow in areas where precipitation is a combination of snow and rain in the winter season.

An increase in precipitation generally increases the amount of water stored in the soil and thus has an influence on recharge to groundwater, actual evapotranspiration, and surface runoff. Surface runoff supplies rivers and lakes; this water, along with rainfall, will then recharge groundwater. Spatial and temporal changes in precipitation will likely alter timing, duration, and magnitude of aquifer recharge, thus affecting groundwater in return. Changes in flood frequency are influenced by the timing and duration of rainfall (and/or snowmelt) events, and changes in drought frequency may occur as a result of a lack of rainfall.

Evaporation is directly influenced by temperature and precipitation. It increases with an increase in temperature, since evaporation occurs in response to the availability of thermal energy. A decrease in precipitation results in increased solar radiation (leading to more frequent occurrences of clear skies). Consequently, there is a decrease in humidity and therefore increased evaporation. Evaporation is thus considered a key link between the atmosphere and the soil water within the hydrological cycle.

Studies that examine the relationship between climate and hydrology began in the early 1940s (Veijalainen, 2012) but were limited due to availability of computing technology. In the 1980s, with drastic advances in the domain of climate science and hydrological modelling, a major step was taken in the study of climate systems and their interaction with hydrology. However, there was still considerable uncertainty in the calculations due to unreliable scenarios and low model resolution (Veijalainen, 2012). In the 1990s, many comprehensive and complex climate and hydrological models were developed, and as computers became more powerful, studies began to probe into different aspects of climate and hydrology.

Figure 2. Impacts of Climate Change on Hydrological Processes (modified from Arnell, 1994)



Recently, several studies have been conducted to evaluate climate change impacts on hydrology (Boyer et al., 2010; Cherkauer & Sinha, 2010; Grillakis et al., 2011; Forbes et al., 2011; Stefan et al., 2012; Barron et al., 2012; Farjad et al., 2016; Bajracharya et al., 2018). In general, most of these studies have considered the following approach (Di Baldassarre et al., 2011):

1. use of a scenario or set of global climate model (GCM) scenarios;
2. transfer the scale of projected GCMs variables into local scale (downscaling);
3. apply the downscaled GCMs data into hydrological models; and
4. simulate responses of hydrological processes to climate change.

Different studies have been carried out in each of the above steps of the framework using different climate and hydrological models (Matondo et al., 2004; Steele-Dunn et al., 2008; Kuhn et al., 2011; Tshimanga & Hughes, 2012; Dobler et al., 2012). Each study focused on different aspects such as hydrological processes of interest, required climate variables, geography of the study area, scale, and availability of models and data. These studies have illustrated changes in hydrological processes in response to climate and could be grouped in three broad categories:

1. *Changes in runoff/streamflow*: A number of studies have explored potential changes in mean annual runoff in response to climate change (Jones et al., 2006; Gardner, 2009). Chang and Jung (2010) assessed the effects of climate change on annual, seasonal, and high and low runoff in the 218 sub-basins of the Willamette River basin in Oregon. The study showed that snowmelt-dominated basins exhibit large reductions in summer flow in response to increased temperature, while rainfall-dominated basins show large increases in winter flow

in response to precipitation change. Thus, an increase in temperature and precipitation can affect the quantity and seasonal distribution of streamflow (Campbell et al., 2011). Jha et al. (2004) found that a unit increase in precipitation due to climate change will cause a larger increase in streamflow.

2. *Changes in subsurface water (including soil water, deeper-vadose zone water, and confined and unconfined aquifer waters)*: Any impact of climate change on surface hydrology has a potential influence on the subsurface hydro-geology as both systems are coupled together and inseparable. However, feedback between soil water and unsaturated zones with climate change occurs over short periods of time compared to saturated zones, which might take decades (Green et al., 2011). Goderniaux et al. (2009) estimated the potential climate impacts on groundwater in the Geer Basin in eastern Belgium. They applied a physically based surface-subsurface flow model combined with six climate change scenarios. They found that the groundwater level is expected to decrease up to 8 m by 2080.
3. *Change in extreme events*: A change in climate will result in a change in the magnitude of events and their frequency of occurrence. The extreme hydrology-related events can be analyzed in two categories. The first is peak flow (flood) frequency, which refers to the peak discharges for recurrence intervals. Mareuil et al. (2007) assessed flood frequency and severity in the Châteauguay River Basin, in the province of Quebec, Canada, and they recognized that both traits are affected by spring snowmelt and summer/fall storms, since an increase in temperature will have considerable effect on earlier spring runoff in areas where snowmelt composes the major proportion of the streamflow. The second category is low flow (drought) frequency, which refers

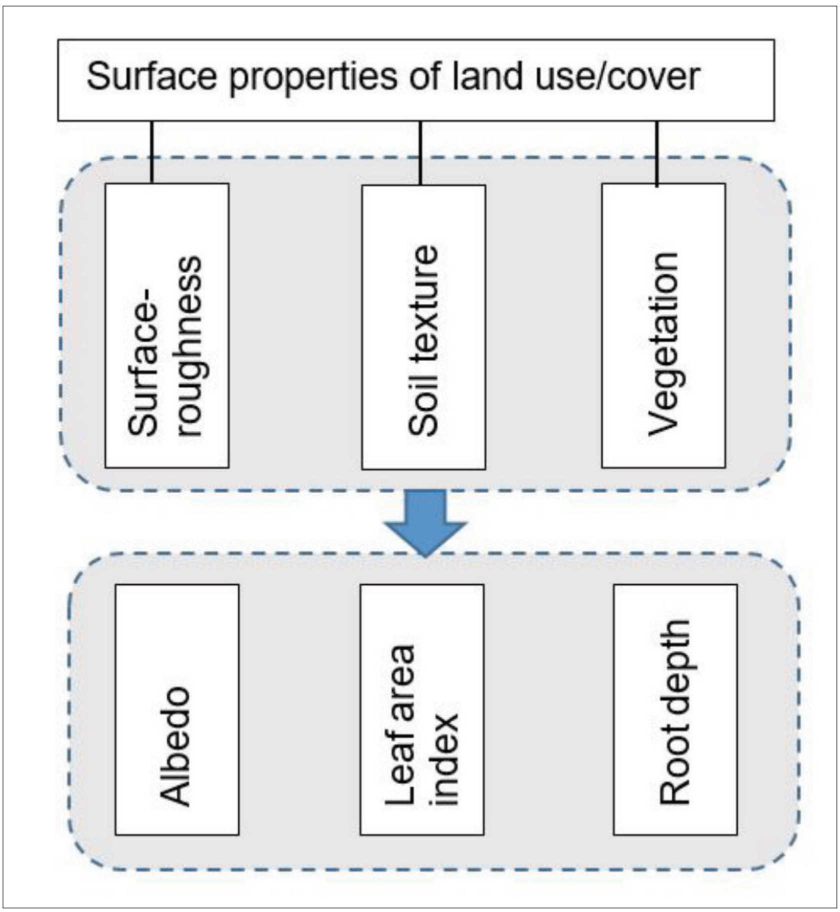
to the lowest streamflow during dry periods for a given recurrence interval. Yulianti and Burn (1998) investigated the influence of air temperature on low flow frequency due to climate change in the Prairies Region of Canada. They found that the frequency of low flow events has increased due to an increasing temperature trend over the past century, and that there is a significant relationship between regional air temperature and low flows in the Prairies.

2.2 Land, ecology, and climate

Changes in land surface/ecology could have effects on regional and global climate variables (Li & Molders, 2008; Steyaert & Knox, 2008; Findell et al., 2009). Many studies have shown that land practices such as deforestation (Meher-Homji, 1991; Werth & Avissar, 2002) and agriculture (Feddema et al., 2005) may affect regional climate to a similar or greater extent than would climate change driven by global changes in atmospheric chemistry alone. However, land-related variations in surface exchanges can have a more pronounced impact at a local scale than globally. In their study, Findell et al. (2007) concluded that observed changes in land surface properties have slight impact on globally averaged climatic variables, while such changes are highly significant locally in the annual mean and in most months of the year.

Changes in land surface cause changes in the surface energy and moisture balances (Findell et al., 2007) and consequently can impact climate variables such as air temperature, precipitation, and evapotranspiration. Also, Werth and Avissar (2002) found that deforestation can result in a significant reduction of summertime precipitation in the Amazon region as well as the surrounding area. Changes in the physical character of the land surface include surface roughness, soil texture, and vegetation. Changes in surface properties will result in changes in albedo (the proportion of the incident light or radiation that is reflected by a surface), leaf area index (LAI, leaf area per unit ground surface area), and root depth (Figure 3). Different surface properties have different influences on climate. For instance, forests have more net radiation (the balance between incoming and outgoing energy that can be exchanged between land surface and climate) than pastures. This is because pastures have a higher albedo with more longwave radiation but a lower aerodynamic roughness, as well as less evapotranspiration (shallow-rooted vegetation cannot extract water in deep soil) compared to forests not only during the dry season, but also in the wet season due to the reduced roughness and available energy. Therefore, forests can make the climate cooler and pastures can make it warmer.

Figure 3. Changes in the Physical Character of the Land Surface



Even though evapotranspiration in forests generally exceeds that of grassland based on an annual time scale, this might not be true in all climate conditions and temporal scales due to the complex behavior of guard cells around stomata. It is likely that the strong regulation of stomatal opening in response to radiation, temperature, vapour pressure deficit, and the larger rooting depth contributes to the conservative character and persistence of evapotranspiration in forests. Therefore, it is possible that evaporative cooling over grasslands exceeds that over forests when there is plenty of soil moisture; however, the opposite could happen when the soil moisture condition is low (Teuling et al., 2010).

The relative division of available energy between sensible and latent heat fluxes (types of energy released or absorbed in the atmosphere) is sensitive to land cover conditions, as is the division of precipitation between runoff and evaporation (Pitman, 2003; Findell et al., 2007). This is because less latent heat results in less water vapour to the atmosphere and tends towards decreasing cloudiness and precipitation. Decreases in sensible heat flux tend to cool the planetary boundary layer (Figure 4) and lessen convection (Betts et al., 1996; Pitman, 2003).

Variations in the vegetation cover change the surface area of vegetation that is in contact with the atmosphere and the balance between fluxes from the soil and vegetation (Pitman, 2003). Changes in the leaf area index (LAI) can result in variations in the exchange of both sensible heat flux and latent heat flux (Figure 5). LAI can also affect the interactions between the biosphere and the atmosphere through various processes such as respiration, transpiration, photosynthesis, and rain interception.

The root zone has the ability to return soil water to the atmosphere through evapotranspiration. Root depth (RD) can affect the extent of the exchange between soil and the atmosphere. A change in climate can result in changes in vegetation and consequently the root depth, which can ultimately affect the global water cycle. RD is adversely affected by the removal of natural vegetation, which reduces moisture availability leading to increased sensible heat flux and warmer and deeper boundary layers. Conversely, reforestation usually increases the latent heat flux via transpiration and interception loss (Betts et al., 1996; Pitman, 2003; Findell et al., 2008). The amount of soil moisture available to plants for transpiration can undergo dramatic variations if the distribution of roots changes.

Furthermore, one may also find positive feedback between reduced root water uptake, rainfall, and further reductions in root depth (Figure 6).

Changes in climate variables can influence the vegetation species and vegetation phenology. As mentioned, extremely cold or hot soil temperatures can damage plant growth. Warmer climates can cause earlier flowering and accelerate the growth of plants. Extremely cold climates can damage cell walls of growing plants in spring or fall. On the other hand, drier climates and lack of precipitation can damage plant cells and roots, which could lead to leaf scorch, wilting, and eventually leaf drop. Wetter climates with too much water can reduce the amount of oxygen in the soil, which can result in root loss as well as vulnerability to fungal diseases. Climate change and variability can also influence animal species; for example, an increase in sea temperature can result in a loss of oxygen, which can negatively affect certain fish species.

Figure 4. Responses of Vegetation and Climate Components to a Change in Albedo (modified from Pitman, 2003)

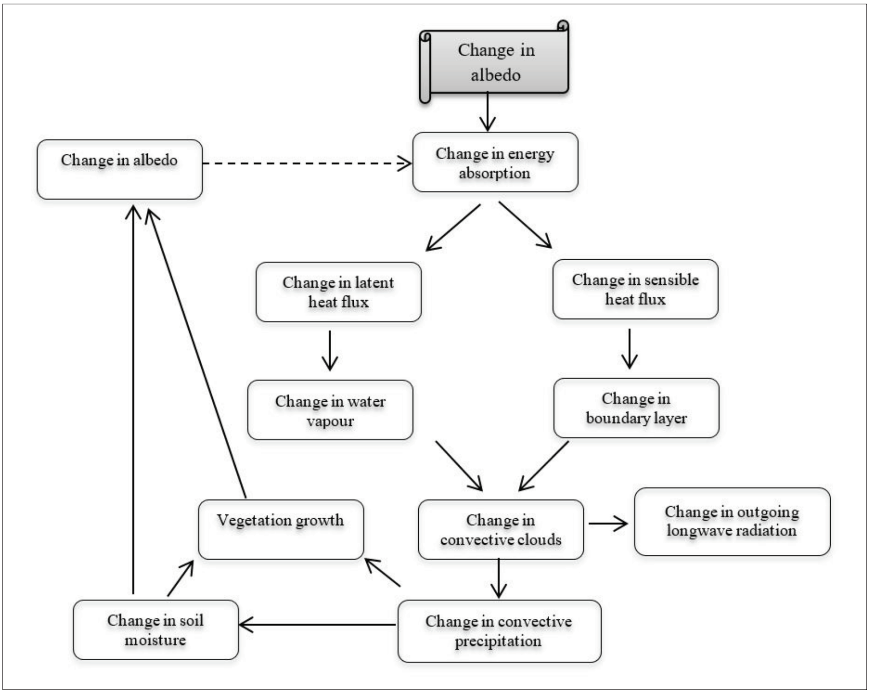


Figure 5. Responses of the Hydrological Cycle to a Change in LAI (modified from Pitman, 2003)

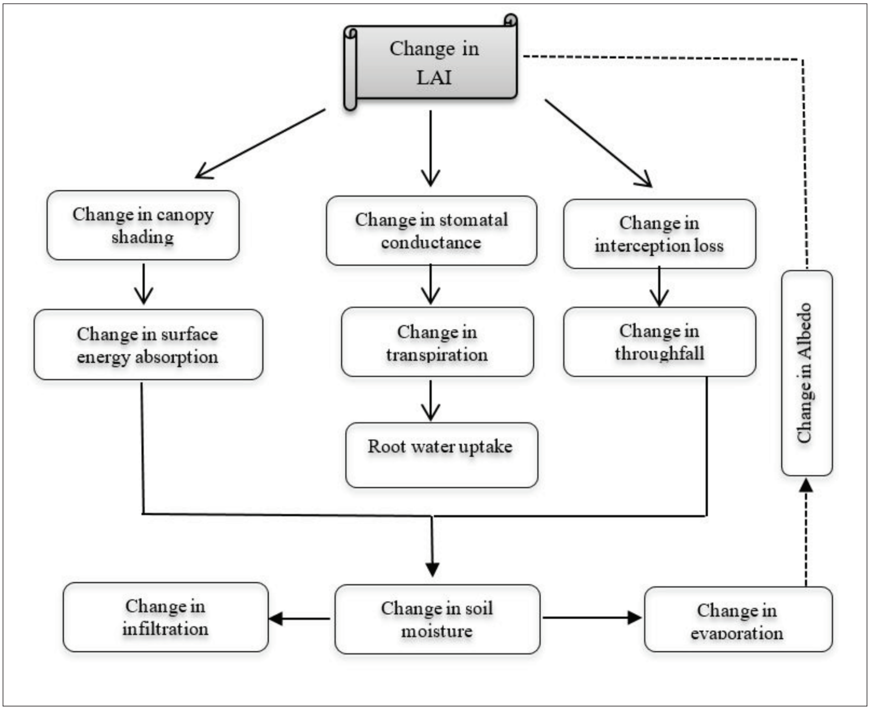
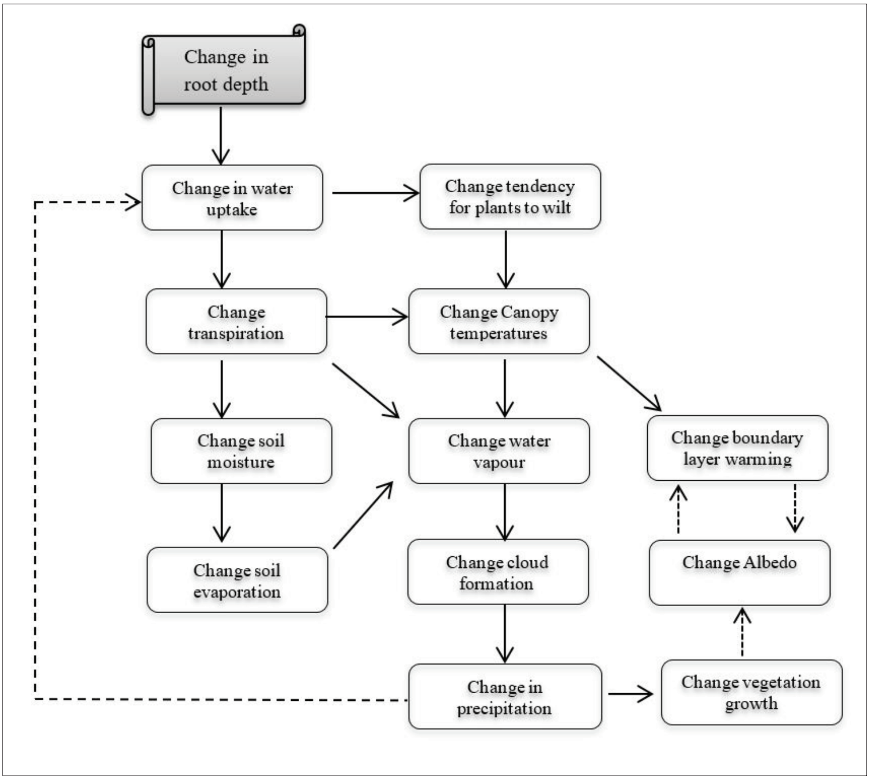


Figure 6. Responses of the Hydrological Cycle to a Change in RD (modified from Pitman, 2003)



2.3 Land use/land cover (LULC) and hydrology

In addition to climate variables, changes in land use/land cover (LULC) can also impact hydrological processes. LULC changes alter water balance, causing changes in infiltration, evapotranspiration, and interception. LULC changes result from anthropogenic activities such as urbanization, agriculture, deforestation, and afforestation. These activities modify the physical properties of the surface such as vegetation and soil, which in turn alter impervious surfaces, soil moisture, and runoff. This ultimately leads to changes in surface and groundwater balance and may cause floods and/or a change in drought frequency (Arnell, 1994). For example, the conversion of natural vegetation into agricultural land decreases evapotranspiration and hence increases fresh water availability (Gordon et al., 2003), while the conversion of land and natural vegetation into impervious surfaces decreases infiltration, evapotranspiration, and groundwater recharge and increases the rate of surface runoff (Arnold & Gibbons, 1996). Arnold and Gibbons (1996) reported that the conversion of forest into 10–20%, 35–50%, and 75–100% impervious surfaces increases runoff two times, three times, and five times, respectively. Consequently, urbanization changes many of the processes that affect streamflow by replacing vegetation and soil with impervious surfaces (McGrane, 2016). Rose and Peters (2001) identified five major impacts of urbanization on hydrology: (i) a higher proportion of precipitation converts to surface runoff while impervious surfaces increase; (ii) the catchment response to precipitation is accelerated and the lag time between precipitation and runoff is decreased; (iii) peak flow magnitudes are increased for all but the largest storm events; (iv) low flow is decreased due to reduced contributions from groundwater storage; and (v) water quality is degraded by effluent discharges.

The impacts of LULC changes on hydrological processes can be summarized as follows:

> *Runoff and infiltration*: Many studies have demonstrated the relationships between LULC properties and runoff and infiltration. Different results have been obtained in different studies, but most of them demonstrated an inverse relation

between forest cover and runoff for many types of forested landscapes (S. Wang et al., 2008). Bosch and Hewlett (1982) concluded that changing annual and perennial herbaceous vegetated land by establishing forest cover decreases water yield. In this order, coniferous hardwood, brush, and grass cover have the highest consumptive use of water with the implication that conversions from these respective cover types to annual crops will increase water yield accordingly. Bruijnzeel (1990) concluded that vegetation type, plant maturation stage, and management practices affect the change in water yield. Calder (1998) reported that vegetation after clear-cutting, depending on the species, may consume more water than very old forests. Other studies indicate deforestation increases runoff (Coe et al., 2011), water yield (Bosch & Hewlett, 1982), and flood peaks (Hornbeck et al., 1970; Harr et al., 1975; Harr, 1981, 1986).

Baseflow: LULC changes are one of the main human-induced activities affecting the groundwater system. LULC changes that lead to increased infiltration, such as terracing, contour farming, and organic matter build-up, may offset the adverse effects caused by deforestation. For example, agricultural practices can offset the adverse effects of deforestation by increasing infiltration resulting in increased baseflow (Bruijnzeel, 1990). Conversion of land for agricultural purposes alters key vegetation parameters that affect recharge, including fractional vegetation coverage, wilting point, and rooting depth. Reducing fractional vegetation coverage to zero during fallow periods between crop rotations can increase recharge as shown in the Northern Great Plains of the United States (Scanlon et al., 2005).

Streamflow/Peak flows: Peak flow is significantly inversely related to the infiltration and water storage capacity of soil. Verry et al. (1983) and Bruijnzeel (1990) found increase in peak flows after cutting trees in a watershed. Also, Bruijnzeel (1990) reported the diminishing role of soil and plants in modulating peak flows resulting from larger magnitude of storm precipitation. In large watersheds, the effects of land-use changes on peak flows may not be that pronounced at the watershed outlet mainly due to the time lag between different tributaries and spatial variation in rainfall (Bruijnzeel, 1990); however, it is more significant in smaller sub-watersheds (Brooks et al., 2003). According to Calder (1998), increasing transpiration in dry periods will increase soil moisture deficits and reduce dry season flows. It is widely reported that an increase of urban lands is usually associated with an increase in high streamflow, decrease in low streamflow, and an increased variability in streamflow. This is a result of the increase in impervious surface caused by urbanization, which decreases infiltration of precipitation and increases runoff (White & Greer, 2006; Tu, 2009).

2.4 Air quality, climate, water, and ecology

Air pollutants are emitted from a range of both natural (e.g., wind-blown dust, wildfires, volcanos) and manmade sources including mobile sources (e.g., transportation vehicles), stationary sources (e.g., power plants, industrial facilities, and factories), and aerial sources (e.g., cities, agricultural area, and wood burning fireplaces). The six common air pollutants, known as the criteria pollutants, are particulate matter (PM), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), carbon monoxide (CO), ozone (O_3), and lead (Pb). Air pollutants can either be released directly into the atmosphere as primary emissions or formed as a result of chemical interactions between precursor substances. CO, Pb, NO_2, and SO_2 are directly emitted from different air pollution sources. PM can be formed when emissions of SO_x, NO_x, ammonia, organic compounds, and other gases react in the atmosphere, or it can be emitted. Ozone is not directly emitted but is formed when oxides of nitrogen (NO_x) and volatile organic compounds (VOCs) react in the presence of sunlight.

Gases and particulates from the atmosphere can fall into water, soil, and on vegetation in dry or wet forms by a process known as air deposition or atmospheric deposition. Dry deposition is a slow and continuous process, whereas wet deposition can occur at a faster rate when precipitation intercepts gases and particulates and falls on the landscape. However, both processes depend on several other environmental factors and are influenced by the properties of the gases or particles (Table 2).

Air pollution, especially that caused by emissions of sulphur and nitrogen and ground-level ozone, can influence ecosystems. Sulphur dioxide and nitrogen oxides can deposit as acid rain on the landscape (e.g., on water bodies, soil, and vegetation). This can result in increasing water and soil acidity with adverse effects on the ecosystem. For example, soil acidity can alter the soil chemistry, which can consequently influence water quality and plant growth. Atmospheric deposition of nitrogen can be lethal for aquatic organisms such as fish. It is a risk for the eutrophication (the process of accumulation of nutrients) of water systems. Nutrient overload in aquatic ecosystems can cause algae blooms (a rapid accumulation in the population of algae in marine water bodies or freshwater) and consequently a loss of oxygen. An increase in ground-level ozone can result in the loss of plant cover by damaging plant cell membranes, inhibiting key processes.

Table 2. Factors Affecting Dry and Wet Deposition of Gases and Particles

Components	**Wet deposition**	**Dry deposition**
Aerosol particles	Cloud parameters Precipitation Particle properties	Particle properties Near-surface concentration Weather condition
Gases	Gas-specific parameters Cloud parameters Precipitation	Soil, surface, vegetation properties Physical and chemical properties of tracer Near-surface concentration Chemical reactions Weather condition

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, evapotranspi-ration	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
HydroGeo-Sphere	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 Processes	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 nonlinear 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 propri-ety)	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 ground-water flow with energy transport or chemically-reactive (sorption, first-order decay) single-species solute transport.	Reactive and non-reactive, single species	Yes (par-tially publicly avail-able, partially propri-ety)	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 man-made 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).

4.0 INTEGRATED ENVIRONMENTAL MODELLING

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

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

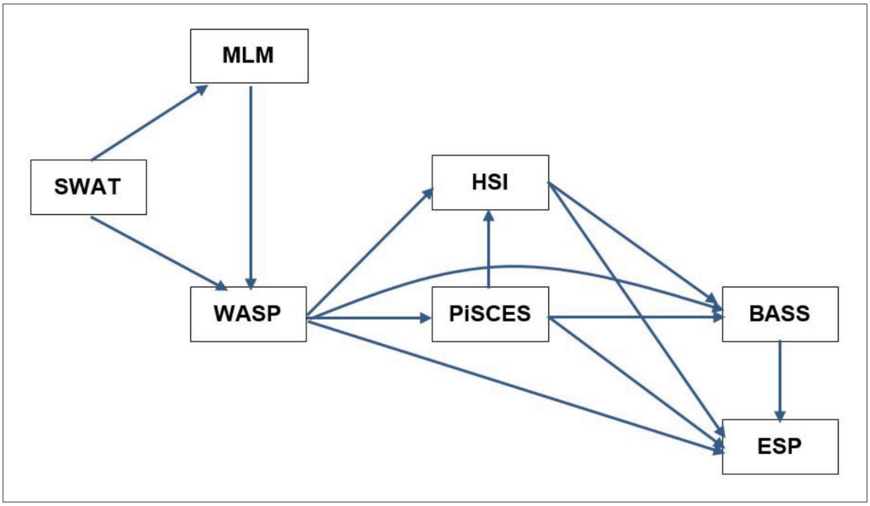
- *Fully coupling*: Equations governing all model components are solved simultaneously within a single monolithic code.
- *Dynamic coupling*: Two or more individual models are tightly coupled via the exchange of data dynamically during simulation at each timestep/predefined frequency.

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

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

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

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



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

4.1 Integrated surface water–groundwater quantity modelling

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

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

GSFLOW

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

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

MIKE SHE

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

HydroGeoSphere

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

MODHMS

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

ParFlow

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

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

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

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

4.2 Integrated watershed and receiving water quality modelling

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

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

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

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

Table 10. (*continued*)

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

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

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

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

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

4.3 Integrated watershed and groundwater quality modelling

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

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

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

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

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

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

4.4 Integrated groundwater and receiving water quality modelling

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

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

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

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

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

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

4.5 Integrated atmospheric deposition and water quality modelling

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

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

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

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

4.6 Integrated load allocation and water quality modelling

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

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

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

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

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

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

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

4.7 Integrated water allocation and water quality modelling

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

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

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

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

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

5.0 MODELLING IN THE ATHABASCA RIVER BASIN – CASE STUDY

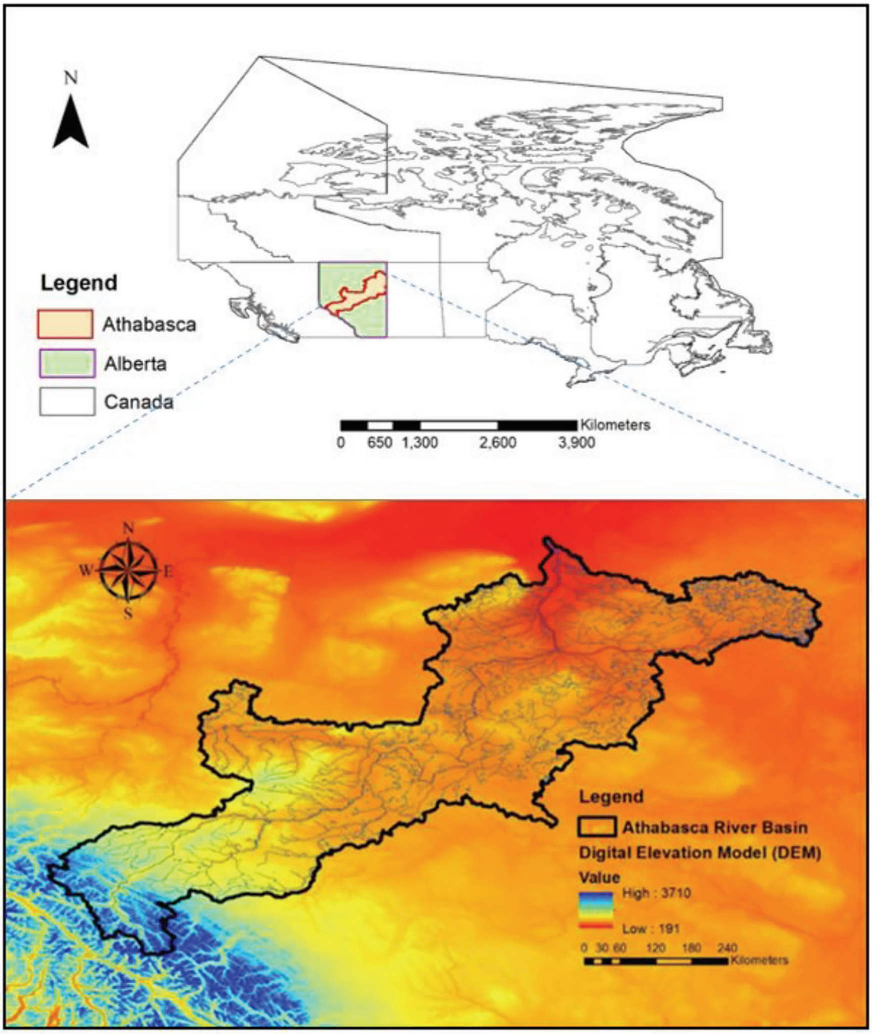
The Athabasca River, located in Alberta, Canada, originates at the Columbia Ice Fields near the Alberta–British Columbia border and flows approximately 1300 km northeast before entering Lake Athabasca at the northeastern corner of Alberta (Figure 8). Water from Lake Athabasca flows into the Slave River and joins the Mackenzie River, which eventually enters the Arctic Ocean. The elevation of the watershed varies from more than 3000 m a.s.l. in headwaters in the Columbia Icefield to about 205 m a.s.l. at its outlet in Lake Athabasca. The Athabasca River basin is physically and ecologically diverse and covers an area of approximately 159,000 square kilometers. The region is endowed with many natural resources such as forests, coal, minerals, agriculture, and oil and gas. The Athabasca oil sands are large deposits of bitumen or extremely heavy crude oil and are the largest reservoir of crude bitumen in the world and the largest of three major oil sands deposits in Alberta (along with the nearby Peace River and Cold Lake deposits).

Interest in bitumen from the oil sands dates back to the 1930s, when intensive industrial development of the region began, and reached a peak in the late 1960s. In the mid 1990s, new project applications and the expansion of existing oil sands operations were underway. As a result, the lower Athabasca watershed was getting more attention for CEA in response to the large-scale oil sands operations that can disturb environmental conditions in the watershed. In-situ and open pit mining developments can directly affect subsurface and surface hydrological processes such as runoff, soil moisture, and infiltration. For instance, the utilized steam-assisted gravity drainage (SAGD) has a potential to modify the hydrogeological regime of the basin. A part of the surface water used in SAGD operations (i.e., steam production and then injection) is lost to the bitumen recovery. (It occupies the space previously occupied by oil in formations.) In response to the changes in environmental conditions, the Alberta government took steps to initiate several strategies and plans. In the late 1990s, the Alberta government designed its Regional Sustainable Development Strategy (RSDS) to address potential cumulative environmental effects in the Athabasca oil sands area. The aim of the RSDS was to provide a framework for managing cumulative environmental effects and to ensure sustainable development in the Athabasca oil sands area. The strategy prioritized 72 environmental issues which had been divided into a list of 14 themes and 3 priority categories that should be assessed in response to the oil sands development.

In 2008, the Government of Alberta commenced a comprehensive initiative to develop a new approach for managing cumulative effects by releasing a land-use framework, known as the Lower Athabasca Regional Plan (LARP). The LARP is a comprehensive, forward-thinking, and legally binding roadmap that enhances environmental management, addresses growth pressures, and supports both human and ecosystem needs, while balancing social, environmental, and economic outcomes. The regional plan considers the cumulative effects of all activities on air, water, and biodiversity. Five environmental management frameworks were developed under the Lower Athabasca Regional Plan, including the Air Quality, Surface Water Quality, Groundwater, Surface Water Quantity, and Tailings Management frameworks. A biodiversity management framework is being developed.

In 2012, the Governments of Alberta and Canada embarked on a new plan, known as the Joint Oil Sands Monitoring Program (JOSM), to ensure a comprehensive and systematic monitoring and reporting of environmental conditions in the lower Athabasca River basin to support sustainable resource development.

Figure 8. Athabasca River Basin (ARB)



The above-mentioned programs, plans, and strategies were composed of different themes and sub-themes to build an understanding of the environment as a whole and to ensure that any major environmental impacts are considered. As a result, many individual studies were conducted with a focus being on either theme or environmental processes. Some of the environmental modelling studies in the region (especially in the oil sands areas) are described in the following sections.

5.1 Hydrodynamic and water quality modelling in the Athabasca River

Water quality modelling of the Athabasca River began in 1984 when the first model was implemented using Water Quality for River and Reservoir Systems (WQRRS) for the main stem from Hinton to Lake Athabasca (Charles Howard and Associates Ltd., 1984). The calibration process was challenging due to limited monitoring data (e.g., hydraulic, non-point and point source loadings, and in-stream water quality data). Flows under ice cover could not be simulated. A dissolved oxygen simulation model named DOSTOC (Dissolved Oxygen STOChastic model) had been widely used since its development in 1987, originally for the Planning Division of Alberta Environment (HydroQual Consultants Inc. & Gore and Storrie Ltd., 1989). In 1988, trial runs of the DOSTOC model were undertaken for the Athabasca River using data collected during the 1987 and 1988 winters (Culp & Chambers, 1994). The model was used to simulate the water quality in the Athabasca River under various levels of development in the basin and low flow conditions during ice-coved periods. The calibration of the DOSTOC model was updated with data collected during winter synoptic surveys in 1988, 1989 (Macdonald & Hamilton, 1989), and 1990 (Macdonald & Radermacher, 1992), and then further evaluated and validated by the Northern River Basins Study (NRBS) using winter survey data obtained in 1991 and 1992 (Macdonald & Radermacher, 1993) as well as 1993 and 1994 (Chambers et al., 1996; Pietroniro, Chambers, & Ferguson, 1998). The DOSTOC model is a component of the Stochastic River Quality Model (SRQM) that consists of three modules: DOSTOC for dissolved oxygen, NUSTOC for nutrients, and UNSTOC for user-specified substances.

The model was formulated as a one-dimensional steady state model and based on the analytical solution to the stochastic version of the Streeter-Phelps equation, assuming that random parameters follow normal distributions. The model can be run in either deterministic or stochastic mode. Hydraulic characteristics of the river were represented by the Leopold-Maddock equations, which are exponential functions relating mean depth, top width, and mean velocity to river discharge. Ice cover processes were not simulated, and effects were implemented by assuming zero volatilization and reduced photolysis and biodegradation rates. Water quality processes represented in the model include atmospheric reaeration, decay of BOD, and nitrogenous oxygen demand (NOD) in the water column, photosynthesis and respiration, and benthic SOD (McCauley, 1997).The calibrated model was used to evaluate the impacts of pulp and paper industry development in the region. It was determined that although the treated pulp effluents from two mills (Wildwood at Hinton and Millar Western at Whitecourt) would increase BOD and ammonia concentrations directly downstream of the mills, the impact is negligible further downstream on the river. As the DOSTOC model is a steady state model over a short period, it could not capture the cumulative effects over time from spatially distributed sources.

During the NRBS, one-dimensional dynamic models with separate and interacting water column and bed sediment compartments were also developed to simulate the fate and transport of organic chemicals for the Athabasca (Hinton to Old Fort) and Wapiti/Smoky Rivers, using the USEPA's Water Quality Analysis Simulation Program version 4 (WASP4) (Golder Associates Ltd., 1997a, 1997b). The Leopold-Maddox method was added to WASP4 code so that water column velocities, cell volumes, and mass exchange areas would be updated at each timestep for the water column segments. This approximate approach is suitable for gradually varied flows. A sediment transport algorithm for the Athabasca River, developed by Krishnappan et al. (1995) was incorporated in WASP4 to predict resuspension and deposition rates within the Athabasca River contaminant fate model. Out of the seven selected organic chemicals, the best calibration over the two-year period of 1992-1993 was achieved for 2,3,7,8-TCDF. For other substances, especially phenanthrene, observed data were so sparse, or conflicting, that it was not possible to evaluate the calibration. By incorporating the sediment transport algorithm into WASP4, the model predicted a very dynamic exchange of sediment between the water column and bed, with an accumulation of fine bed sediment over the late fall and winter, removal by resuspension during the spring freshet, and very little net accumulation during the summer.

Subsequently, a one-dimensional model, WASP7 (water quality analysis simulation program), was set up using a kinematic wave routing scheme and was hydrodynamically calibrated and validated for the Lower Athabasca River with 1999–2008 data (Kannel & Gan, 2013). The model represented the field data quite well except during winter seasons (mid-November to April). The model was applied to investigate the potential impact of oil sands processed water (OSPW) in the event that OSPW, which contained naphthenic acids (NAs), was accidentally discharged to a stretch of the Athabasca River, simulating NAs as a lumped state variable and assuming it is degraded by natural dilution, biodegradation, sorption, photodegradation, or combinations of these processes. NAs in the Lower Athabasca River were predicted to be sensitive to changes in the discharge rate and concentrations of OSPW, as well as the rates of photodegradation and biodegradation.

Numeric modelling of flow and transport processes in the Athabasca Oil Sands Region is challenging due to the complex morphology, cold climate, and highly variable flows in the river. Being located in northern Alberta, the Lower Athabasca River has some special hydrodynamic and water quality characteristics, especially the ice formation, jams, melting and break-up processes, and the relatively long ice-cover period for the river. Early attempts to model flow in the Lower Athabasca River used one-dimensional models that were implemented based on approximate and simplified rectangular cross-sections to represent channel geometry. Khanna and Herrera (Khanna & Herrera, 2002) applied the cdg1-D model in the Lower Athabasca River basin to estimate high flows during open-water season. The cdg1-D model, originally developed at the University of Alberta, solves the St. Venant equations by the finite element method using the characteristic dissipative Galerkin (cdg) scheme. Trillium Engineering and Hydrographics Inc. (Trillium Engineering and Hydrographics Inc., 2003) conducted field surveys to measure transverse mixing coefficients and travel time in the Lower Athabasca River during ice-covered winter low flow periods at five key locations (short reaches) downstream of the Firebag River, Ells River, Muskeg River, Steepbank River, and Fort McMurray. A HEC-RAS model for each reach was constructed to evaluate the hydraulic roughness and to predict water levels and mean velocities for a range of discharges. Two-dimensional flow characteristics required for the mixing analysis were evaluated using a lateral discharge distribution approach. Two methods of evaluating transverse mixing coefficients were employed: (i) an analytical model with reach-average hydraulic characteristics and (ii) a numerical model, TRSMIX, which employed local hydraulic characteristics. These dimensionless coefficients may be applied over the range of typical winter discharges that occur as long as the river is ice-covered.

Hydrodynamic and fish habitat modelling have been performed for reaches of the Lower Athabasca River and Peace-Athabasca Delta using the River2D model calibrated with synoptic bathymetry and hydrometric survey data obtained during summer and winter (ice-covered) periods as part of a multi-year program led by the Surface Water Technical Group of the Cumulative Environmental Management Association (CEMA) (AMEC-nhc, 2009). The program aimed to assess in-stream flow needs and evaluate fish habitats for open water and winter conditions for the Lower Athabasca River, in which five study segments along the Lower Athabasca River were investigated, including: Reach #1 – Athabasca Delta below Embarras, Reach #2 – Embarras, Reach #3 – Poplar Point, Reach #4 – Bitumount, and Reach #5 – Northlands. River2D is a two-dimensional finite element-based numerical hydrodynamic model that was developed at the University of Alberta to simulate the depth-averaged flow characteristics in a river segment (Steffler & Blackburn, 2001). To match measured velocities and water levels, a range of roughness heights was adopted for the calibration of flows: 3.0 mm for sand, 500 mm for the cobble regions, and 10 mm for ice at Reach #4 (Trillium Engineering and Hydrographics Inc., 2004, 2005); 10 mm for sand and 150 mm for ice at Reach # 2 (Northwest Hydraulics Consultants Ltd., 2007a), and 1 mm for sand and 150 mm for ice at Reach #3 (Northwest Hydraulics Consultants Ltd., 2007b). Katopodis and Ghamry (2005) conducted similar ice-covered hydrodynamic model calibrations and comparisons for three reaches of the Lower Athabasca River (Fort McKay below Peter Lougheed Bridge, Bitumount, and Northlands). It was found that the applied bed and total roughness along the thalweg profiles for Bitumount and Northlands Reaches were comparable for similar substrate sizes. The Northlands Reach has the coarsest bed materials over most of the thalweg profile, the Peter Lougheed Reach has the finest ones, and the Bitumount Reach is in-between. Although the applied ice roughness differed between the three reaches, its low values had a small effect on the composite roughness.

In the Peace-Athabasca Delta, 2D-River models were developed and calibrated for the two divergence areas under each of the open water and under-ice conditions. The ice thickness data obtained in the winter survey was processed to produce River2D ice input files (AMEC-nhc, 2009). A River1D model for the Peace-Athabasca Delta was also developed at the University of Alberta (Andrishak & Hicks, 2009, 2011), for the primary purpose of simulating river discharges across the Lower Athabasca Region to provide boundary conditions for more detailed (e.g., River2D) hydraulic and habitat modelling at flow divergence sites. Both 1D- and 2D-River models for the Peace-Athabasca Delta were updated in 2014 with new survey data (Hatfield Consultants, 2014). Note that the 1D- and 2D-River models for the Lower Athabasca River and Peace-Athabasca Delta were all calibrated with steady-state runs under steady-state conditions and specified temporally constant ice thickness inputs interpolated from data collected from synoptic surveys. Steady-state runs were performed for fish habitat modelling and assessment due to their limited functionality for unsteady modelling. Efforts were made and preliminary results were obtained by updating the 1D-River (Andrishak et al., 2008) and 2D-River model (Wojtowicz et al., 2009) to include thermal ice processes to simulate the freeze/thawing of the Athabasca River.

Integrated hydrodynamic and water quality modelling over a continuous period covering open-water and under-ice conditions in the Athabasca Oil Sands Region started in the late 2000s. A two-dimensional vertically-averaged Environmental Fluid Dynamics Code (EFDC) model with hydrodynamic and eutrophication water quality models for the Lower Athabasca River from Fort McMurray to Old Fort was developed by TetraTech in 2009. The model was used to simulate an eight-year period from 2000 to 2007 with a partial calibration due to limited monitoring data. The model was enhanced by Dynamic Solutions International LLC

(DSI) in a scoping study by updating model bathymetry to the best available data and adding preliminary setup of sediment and toxics modules without calibration. The model did not simulated the ice formation and melting processes but required external inputs for ice cover thickness (Dynamic Solutions International LLC., 2012). A two-dimensional laterally averaged model for the Upper Athabasca River (Hinton to Grand Rapids) was developed using CE-QUAL-W2 to simulate the hydrodynamics, and DO including the ice formation and melting processes over the period from 2000 to 2006 (Martin et al., 2013). The modelling results indicated that the DO concentration in the Upper Athabasca River was very sensitive to the sediment oxygen demand (SOD), which represented about 50% of the DO sink in winter. The model was applied under steady-state winter low-flow scenarios to predict assimilation capacity for the BOD load. The CE-QUAL-W2 model has also been utilized to develop for CEMA a general two-dimensional laterally averaged integrated hydrodynamic and water quality model, simulating oil sand pit lakes. Named CEMA Oil Sands Pit Lake Model (OSPLM), it can simulate potential water quality implications of mature fine tailings placement in pit lakes (Berger & Wells, 2014; Golder Associates Ltd. & ERM, 2012; Prakash et al., 2015; Vandenberg et al., 2014).

Modelling the fate and transport of fine sediments and associated chemical constituents in the Lower Athabasca River originating from natural and potential anthropogenic sources is recognized as a subject of increasing importance, as studies have shown that the concentrations of sediment-associated chemicals such as PAHs and heavy metals in the Lower Athabasca River are affected by development activities (Droppo et al., 2018). To quantify and model the sources, transport, and fate of chemicals, a reliable integrated hydrodynamic, sediment transport and water quality model of the Lower Athabasca River is needed. Experimental and field assessment of sediment dynamics and associated chemicals in the Lower Athabasca River and tributaries have been investigated in several previous studies under the JOSM program. Droppo and Krishnappan (Droppo & Krishnappan, 2016) applied a modelling approach combining two existing models (RIVFLOC and MOBED) to simulate the hydrophobic, cohesive sediment transport in the Ells River. Using fine sediment transport parameters derived from laboratory flume experiments (e.g., settling velocity of sediment as a function of floc size and the critical shear stresses for deposition) and the calculated flow field from the MOBED model (using field survey data such as cross-sectional geometry, river slope, grain size of bed material, and discharge), the RIVFLOC model was used to predict the transport characteristics of the hydrophobic Ells River sediments. Although flocculation was shown to occur with increasing floc size downstream, there was a breakpoint at approximately 50 μm where the settling velocity decreased with increasing floc size due to a decreasing floc density. The high bed shear stresses in the Ells River also negated the influence of flocculation on settling. The entrapment process was thus concluded as an important aspect of sediment dynamics within high-energy cobble/gravel bed rivers, particularly where sediments are hydrophobic like those from the McMurray Formation in Northern Alberta.

It is well known that integrated watershed and water body modelling systems or tools are needed to support the assessment of cumulative effects from climate change, land use changes, developments, and operational activities in the oil sands region. Nevertheless, there is no existing modelling system or tool that possesses the capability to simulate dynamic interactions among environmental and human sub-systems and their impacts on water quality and the aquatic habitat health of the Lower Athabasca River, accumulated over both spatial and temporal scales. A unique, comprehensive, and practical system for integrated watershed and water quality modelling in the Athabasca Oil Sands Region was developed by Golder Associates, which has been applied to support a series of environmental impact assessment (EIA) studies of oil sands development projects (Golder Associates Ltd., 2003a, 2003b, 2004a, 2004b; Teck Resources, 2011). The component models include, CALMET/CALPUFF air quality dispersion model, regional 3D MODFLOW groundwater model, MT3D solute-transport model, regional HSPF hydrologic model, CE-QUAL-W2 Pit lake hydrodynamic model, Golder Pit Lake Water Quality Model, quasi-dynamic 2D ARM (Athabasca River Model) water quality model, steady-state sediment quality model, and habitat suitability models. Component models were calibrated for historical periods. Future scenarios and non-point source loadings were estimated based on the watershed modelling of LULC changes and development scenarios, with the consideration of operational releases from oil sands development as well as withdrawals from the Lower Athabasca River. As HSPF is a semi-distributed watershed model, the system does not simulate fully distributed interactions between surface and subsurface water. Being a tool supporting project EIAs, the system predicts impacts under certain future snapshot scenarios and does not simulate the cumulative effects over time. Some general impacts predicted by the integrated modelling system (Teck Resources, 2011) include:

i. Drawdown propagation due to basal water depressurization will largely be constrained to the mining project area. Groundwater levels will begin to recover following shutdown of depressurization pumping, and the groundwater flow model predicts that far future groundwater levels would be similar to those of predevelopment.

ii. Activities such as muskeg drainage and overburden dewatering during mine construction and operation will result in increased flows to receiving watercourses. Reductions in drainage area because of closed-circuit operation and the creation of pit lakes at closure will reduce flood flows to receiving waters.

iii. Oil sands developments were predicted to have negligible effects on acute and chronic toxicity and tainting potential in all receiving waters in the local and regional study areas. The proposed mitigation measures will ensure that acute and chronic toxicity and tainting potential will be at levels appreciably lower than the corresponding guideline or threshold values, and that additional adaptive management options exist in the event that they are required. The concentrations of several substances are predicted to increase above base case snapshots but remain below guidelines or chronic effects benchmarks (CEBs).

iv. Fish habitat in the local study area (LSA) is primarily of low value and composed of forage fish typical of the Athabasca Oil Sands Region. Construction of oil sands projects will result in the alteration or destruction of fish habitat and an associated loss of fish relative to abundance, but it will have no effect on fish or fish habitat diversity. The loss of fish habitat will be compensated for by the construction of the lake, which will offset the potential loss of fish habitat.

The ARM model, originally developed by Golder Associates and applied to EIAs of oil sands projects, is a two-dimensional vertically-averaged model based on an analytical solution to river dispersion equations under steady-state conditions, and implemented using VBA (*Visual Basic for Applications*) and the Microsoft Excel application. It has been updated by Four Elements Consulting Ltd. to include a new functionality for optimal regional substance load allocation in the Lower Athabasca River. Dynamic-link library (DLL) techniques were adopted to speed up computing time (Four Elements Consulting Ltd., 2014a, 2014b). A range of water quality parameters (including 11 general indicators such as chloride, TN and TP, 28 metals, 19 PAHs, total phenolics, and toxicity-chronic) can be simulated by the model. However, flow in the river was calculated using Leopold-Maddock equations rather than a hydrodynamic model. Similar to the DOSTOC model for the Lower Athabasca River, dynamic ice processes and river bed sediment transport processes cannot be simulated with the ARM configuration.

More recently, an integrated hydrodynamic and water quality modelling framework for the Lower Athabasca River was proposed by Environment Canada and Climate Change (ECCC), consisting of MIKE 11 for long-term one-dimensional simulations and EFDC for short-term detailed two-dimensional simulations, each externally coupled with a one-dimensional MIKE-ICE or CRISSP-1D model (Dibike et al., 2018; Kashyap et al., 2017; Shakibaeinia, Dibike et al., 2017; Shakibaeinia, Kashyap et al., 2016). A demonstrative rather than a full range of water quality parameters required for assessing impacts of oil sands development are configured in the models, including TSS, BOD, DO, phosphorus, and nitrogen components, three PAHs (pyrene, phenanthrene, and C1-benz[a] anthracenes/chrysenes) and three metals (lead, arsenic, and vanadium). The MIKE 11 model was developed for a 10-year historical period (2001-2010) and the EFDC model was calibrated over short periods under steady flow conditions. Both models were applied to hypothetical future scenarios. Non-point source loadings were estimated from limited measurements, rather than from watershed modelling of land use changes and development scenarios. The modelling framework is under further development to enhance the configuration and functionalities by restructuring the model grid for EFDC and cross-section profiles for MIKE 11, based on derived high-resolution DEM (Chowdhury, 2017). A two-dimensional hydrodynamic, sediment transport and water quality model for the Lower Athabasca River has been developed and calibrated using EFDC+ with a number of enhancements, including: extended model domain to cover the main channel and 10-year floodplain from the Athabasca River upstream of Fort McMurray to the Athabasca River near Old Fort; optimized model grid to improve computational burden to allow longer period (2000-2016) simulations in reasonable run-time; improved hydrodynamic model simulating dynamic ice cover formation and melting processes; cohesive and noncohesive sediment transport with the best available TSS and riverbed sediment data; and improved water quality (eutrophication and DO) and toxic (three representative toxics) modules by including all major tributaries, withdrawals and returns on the Lower Athabasca River, and point source effluents in the oil sands region (DSI, 2019). The river models are expected to be coupled with a distributed watershed model to achieve integrated watershed and river water quality modelling, as part of a multi-year mission to develop a comprehensive and integrated environmental modelling system for the cumulative effects assessment in oil sands region.

5.2 Atmospheric deposition and acidification modelling in the Athabasca Region

In 2003, RWDI West Inc. (2003) conducted a CALMET/CALPUFF modelling study for CEMA. The model was run for a one-year period to predict ambient concentrations and annual deposition rates for 39 priority substances in the Athabasca Oil Sands Region, that can then be used to screen potential human health risks using multimedia risk assessment techniques. The 39 priority substances, including SO_2, NO_x, and VOCs, were identified in the emission inventory of the oil sands region. Based on comparisons with available monitoring data, the highest level-of-confidence in model predictions is associated with the priority substances the emissions of which are well-defined, whereas a lower level-of-confidence is associated with emissions of priority substances from fugitive sources. For some contaminant-receptor combinations, the predicted ambient levels are so sufficiently low that a background term is required to allow for a representative comparison.

CEMA considered applying one or both of two widely used air quality modelling systems, CALPUFF and/or CMAQ, for sulphur and nitrogen deposition modelling to assess historical, current, and future environmental exposures due to emissions from the oil sands industry and other sources in and around the Regional Municipality of Wood Buffalo (RMWB). ENVIRON International Corporation and Stantec Consulting Ltd. (2012) conducted a detailed evaluation and comparison of the performances of the CALPUFF and CMAQ modelling systems to understand the relative strengths and weaknesses of the two models for implementation of the Acid Deposition Management Framework (ADMF). It was determined that the differences between the two model outputs are strongly related to differences in the model inputs in spite of sharing the same data sources. There is no basis for choosing one model (CALPUFF vs. CMAQ) over the other. Both may be used, each with different advantages. The CALPUFF model has the advantage of consistency with previous ADMF studies and other EIA studies, predicts the peak one-hour SO_2 and NO_2 concentrations better than CMAQ, and requires a lower level of effort to apply. The CMAQ model has the advantage of improved chemistry algorithms and appears to perform better in simulating lower SO_2

and NO_2 concentrations and the wet deposition of sulphur and nitrogen compounds.

CALPUFF modelling (Exponent Inc., 2014) was also conducted to estimate acid deposition to provide input to the Model of Acidification of Groundwater in Catchments (MAGIC) to determine whether acid deposition-related changes to lakes and soils will or will not exceed defined thresholds. The CALPUFF model was calibrated with 2010 meteorology and observation data and then applied with 1980 representative year meteorology data, as well as with historical, base, and two future emission scenarios. The model was run for a one-year period to predict the annual dry, wet, and total depositions of acidifying sulphur and nitrogen compounds. The deposition measurement data was considered insufficient for a reliable comparison between measurements and predictions. In general, the predicted total Potential Acid Input (PAI) in 1980 is slightly lower than that in 2010 for the existing emission inventory. The area of peak total PAI is located in the Fort McKay area, which is the area with the largest emissions. The second highest peak area is located in the Bridge View area along the southern boundary of the domain.

A CMAQ modelling study was completed with the same source of data and procedures as Exponent's CALPUFF modelling (S. Cho et al., 2017). Similar findings were obtained that include (i) a predicted area of high sulphur and nitrogen deposition near the largest oil sands operations in Alberta's oil sands region, and predicted higher dry deposition than wet deposition in the study area; (ii) the predicted gross PAI (wet & dry) deposition increases from the historical to an existing case with further increases for the two future scenarios; and (iii) the nitrogen deposition predicted by the model, which comprises, on average, approximately 60% of the total PAI acidic deposition in the region.

ECCC calculated estimates of potential effects on ecosystems in the Canadian provinces of Alberta and Saskatchewan due to acidifying deposition (Makar et al., 2018). Based on a one-year simulation of a high-resolution implementation of the Global Environmental Multiscale-Modelling Air-quality and Chemistry (GEM-MACH) model, the critical loads of sulphur and nitrogen deposition (dry, wet, and total) for aquatic and terrestrial ecosystems were derived. The spatial extent of the regions exceeding critical loads varied between 1E+4 and 3.3E+5 km^2, for the more conservative observation-corrected estimates of deposition, with the variation dependent on the ecosystem and the critical load calculation methodology. Other findings of the study were outlined and include (i) the evaluation of the model simulation against two different sources of deposition data – total deposition in precipitation and total deposition to snowpack in the vicinity of the Athabasca oil sands, (ii) the variability of observed ions in wet deposition in precipitation (observed versus model sulphur, nitrogen, and base cation R^2 values of 0.90, 0.76 and 0.72, respectively), while being biased high for sulphur deposition, and low for nitrogen and base cations (slopes 2.2, 0.89 and 0.40, respectively), and (iii) the predicted potential ecosystem effects within each of the regions, represented by the ecosystem critical load datasets using a combination of 2011 and 2013 emissions inventories.

The Model of Acidification of Groundwater in Catchments (MAGIC) has been applied to soils and lake catchments in the oil sands region to determine sensitivity to acid deposition under two deposition scenarios (base case and double acid) (Whitfield et al. 2009, 2010, 2011; Whitfield and Watmough, 2010). The model simulated average monthly or annual soil solution and surface water concentrations for sulfate (SO_4^{2-}), calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^+), potassium (K^+) and pH, as well as exchangeable soil fractions of Ca^{2+}, Mg^{2+}, Na^+, and K^+. Lumped indicators include base cation (BC) and acid neutralizing capacity (ANC) for lakes, base saturation (%) and critical threshold, and molar base cation to aluminum ratio (BC:Al) for soil physicochemical characterization. The research demonstrated that lakes in the region would not be at risk of acidification under either deposition scenario. In contrast, forest soil weathering rates range from very low to moderate, and soil chemistry was predicted to change under both deposition scenarios.

With the annual atmospheric deposition rates generated by CALPUFF modelling, a modelling approach was implemented within Golder's comprehensive oil sands environmental modelling system for predicting the contributions and potential effects of aerially deposited PAHs and metals, as well as the impacts of snowpack and snowmelt on water quality from proposed oil sands developments (Dayyani, Daly, & Vandenberg, 2016). The contribution (loading) of snowmelt to surface water concentrations was estimated using two methods: a conservative mass balance approach adopted for metals, and an unsteady-state, mass balance, and multi-compartment fate model, or Coastal Zone Model for Persistent Organic Pollutants (CoZMo-POP). Simulations were run with a timestep of one hour. The model predicted that: i) under base case conditions, cadmium and chromium concentrations were both predicted to exceed guideline values in the Muskeg River; ii) All PAHs were predicted to remain below guidelines in surface water for both projects and under all assessment cases.

The model was thought to over-predict the concentration of metals in receiving water pathways because it did not account for retention of metals during snowmelt in the soil matrix. Refinements to the mass balance approach for modelling metals should focus on retention of metals on the landscape during the melt period. Refinements to CoZMo-POP might include application of the water-sediment partitioning module to predict sediment PAH concentrations.

5.3 Watershed modelling in the Athabasca Region

A variety of watershed models have been used in the region such as HSPF, SWAT, VIC, WATFOOD, and MISBA. Pietroniro et al. (2006) investigated the potential effects of climate change on the hydrological regimes of three large lakes and two inflow sources (from the Peace and Athabasca rivers) on the Peace-Athabasca Delta. They indicated that changes in climate can result in an earlier melt season, higher winter flows, an increase of flows (more at headwater), and a reduction of peak flow. Kerkhoven and Gan (2006, 2011) assessed the impact of climate change using the MISBA model. They reported a large decline in spring snowpack, annual runoff (-21%), mean maximum annual flow (-4.4%), and mean minimum flow (-41%) by the end of century for ARB. The decline in the average annual flows has been also reported by Golder Associates (2009) when they evaluated the climate impacts using the HSPF model. An increase in winter flows and a decrease in summer flows have been found in Eum et al. (2014) and in Leong and Donner (2015), through assessing the impacts of climate change on the hydrology of the region using VIC and Integrated

Biosphere Simulator – Terrestrial Hydrology Model with Biogeochemistry (IBIS-THMB), respectively.

5.4 Groundwater modelling in the Athabasca Region

CEA for groundwater requires a groundwater model with a mesh/grid that can conform to complex geology and hydrogeology and with the capability of simulating density-dependent flow and transport, as well as surface water-groundwater interactions. A group of 10 in situ oil sand operators (the SAOS Group) initiated a process in 2007 to develop a regional surface water-groundwater model for the oil sands in situ area south of Fort McMurray. They conducted a review of surface water-groundwater numerical modelling to select the most suitable model. MODFLOW and FEFLOW were selected with the capability of being coupled with surface water models – as MODHMS and FEFLOW/MIKE 11, respectively (WorleyParsons, 2010). Major groundwater modelling studies have been undertaken in the Lower Athabasca River watershed. For instance, in 2009, WorleyParsons Canada Services Ltd. developed a 3D MODFLOW groundwater model (2 km grid resolution) for the entire Lower Athabasca Regional Plan (LARP) region to assess the potential impacts from oil sands development. They indicated that the current drawdown for the various major aquifers was substantial and that the trend of drawdown was anticipated to decrease. Subsequently, modelling studies have been more regionally focused and based on operational purposes whereas the Athabasca Oil Sands (AOS) area has been split into the following three regions:

1. Northern Athabasca Oil Sands (NAOS) region, which mainly contains the surface mineable deposits. The boundaries of the NAOS study area are
    - North: starting in the northwest, the boundary follows the Sand River, Athabasca River, Firebag River, and Marguerite River sub-basin;
    - East: Alberta/Saskatchewan border;

- South: Athabasca and Clearwater Rivers; and
- West: northwest boundary follows the western extents of the Gardiner Lake and Snipe Creek sub-basins, then follows the Dunkirk River south to the western boundary of the MacKay River sub-basin, south to the Athabasca River.

2. Southern (SAOS) area where in situ extraction occurs in the region. The boundaries of the SAOS region are:
   - North: Athabasca and Clearwater Rivers;
   - East: Alberta/Saskatchewan border and Christina River Sub-basin;
   - South: Centre of Township (T) 69 from Range (R) 1 to 9 West of the Fourth Meridian (W4M) continuing along the Beaver River Basin; and
   - West: Southwest boundary follows the La Biche sub-basin to the confluence of the Athabasca and La Biche River. The boundary continues north along the Athabasca River.

3. Cold Lake region which has been given the name Cold Lake-Beaver River (CLBR) based on its location within the Beaver River Basin.

For the NAOS region, WorleyParsons Canada Services Ltd. developed a 3D FEFLOW model in 2012, which allows for a flexible mesh refinement, simulates density-dependent and fractured flow, and includes river flow interactions by linking the model to MIKE 11. The first phase of the model development was mainly focused on the configuration of the model and understanding the hydrology/hydrogeology of the region. They reported that the recharge rate ranges from 247 to 1,150 million m^3/year for the NAOS study area. The total annual discharge from groundwater to the Athabasca River (including its tributaries) ranges from 236 million m^3/year to 590 million m^3/year. In addition, as of October 2011, it was estimated that the rate of groundwater withdrawal was roughly 41.5 million m^3/year within the NAOS region. A FEFLOW model has been also used by WorleyParsons to model groundwater of the SAOS region in 2010. They reported that the recharge in the SAOS ranges from 290 million m^3/year to 1,500 million m^3/year. The total discharge from groundwater to the river ranges from 540 million to 1,350 million m^3/year. As of February 2009, it was estimated that the total annual non-saline allocation volume is more than 15 million m^3 within the SAOS region. In 2016, the FEFLOW model developed by WorleyParsons for the SAOS was further modified by MATRIX Solutions Inc., to improve the calibration of the model.

For the CLBR region, a MODFLOW groundwater model was developed by the Alberta Geological Survey in 2005 to better understand the regional water balances and groundwater flow regimes. It was reported that recharge rates estimated by the model were highest in the northeast and southeast of the domain area (13.2 mm/year and 7.6 mm/year, respectively) and were lower than 5 mm/year in the western portion.

5.5 Surface water and groundwater interactions in the Athabasca Region

Few attempts have been made to model surface water-groundwater (SW-GW) interactions. In a study conducted by WorleyParsons (Integrated Sustainability Consultants Ltd., 2013), the MODFLOW model was used for the lower Athabasca regional planning region and they found 50% exceedance of available drawdown in the basal McMurray Formation, especially in the mineable area. They also indicated that a more comprehensive modelling tool is required for CEA under multiple-stressors. A review of modelling studies for assessing the potential cumulative impacts to groundwater and surface water in the MacKay River watershed was conducted by the Cumulative Environmental Management Association (CEMA, 2014). It was predicted that groundwater discharge can reduce to -0.001 to 0.043 m^3/s when various oil sands projects are developed compared to the current condition 0.01-0.055 m^3/s. They indicated that many project EIAs used different models with different data sets and assumptions, which makes comparison of projects and impacts difficult. Kassenaar (2016) assessed the potential cumulative impacts to SW-GW from in-situ oil sands operations using GSFLOW in the MacKay River watershed. They indicated that drawdowns do not (on a watershed-scale) appear to grow over time. However, cumulative groundwater diversions appeared to create unsustainable local impacts under extreme and defined scenarios. Furthermore, the simulations showed that that groundwater diversions may significantly affect small to intermediate sized tributaries.

5.6 Land use/land cover modelling in the Athabasca Region

A State-and-Transition Model (STM) model was developed for CEMA and validated by Apex Resource Management Solutions Ltd. to simulate reclamation dynamics for the mineable oil sands region of Alberta, such that it supports the development of a Reclamation Classification System (RCS) (Daniel, 2011; Frid & Daniel, 2012). The model utilized landscape vegetation state and the probability of transition between states to find potential probabilities of changes. STMs can help managers establish a land classification system by describing the land units and phases in the system, including the relationships between the various units and phases. STMs explicitly recognize the relationship between management alternatives and land classification, ensuring that the classification system is management-oriented. A quantitative STM was developed which can be used to both conceptually and quantitatively model landscape level changes over time because of alternative reclamation scenarios. The model was parameterized with existing data from the Long-Term Plot Network and other CEMA projects.

The Alberta Biodiversity Monitoring Institute (ABMI) is one of the main sources of land use and land cover data which also provides new analytical methods and visualization approaches to deliver geospatial products, such as the ABMI province-wide wall-to-wall Human Footprint Inventory (HFI). The ABMI has also developed a predictive product, called Predictive Landcover (PLC), which classifies land cover into seven classes (open water, bog, marsh, swamp, fen, upland, and wetland general).

Another important product to support land use and land cover decision-making in Athabasca is ALCES, a landscape and mapping software.

ALCES has been applied to inform planners and stakeholders about possible future outcomes associated with land use and development.

5.7 Climate change in the Athabasca Region

Climate change can be considered as a natural stressor which needs to be taken into account along with other stressors for CEA. Climate change studies in the Athabasca watershed can be divided into two main categories: the assessment of climate change and variability, and the impact of climate change on environmental processes. Regarding climate change and variability in the Athabasca watershed, Bonsal and Cuell (2017) indicated that periodic extreme droughts and excessive moisture conditions are expected mainly due to persistent and mid-tropospheric circulation patterns that disrupt expected temperature and precipitation in the region (Bonsal & Cuell, 2017). Furthermore, substantial inter-annual variability with more drought-like summer and slightly wetter annual conditions, as well as decadal-scale variability are predicted over the entire region. On the other hand, according to the climate change impact studies, a comparison between current and future climate conditions in the watershed has indicated a significant shift towards an earlier melt season and also an increase in winter flows (Toth et al., 2006). The shortened snowfall season along with an increase in sublimation can result in a decline in the spring snowpack as well as an expected decline in average annual flows (Kerkhoven & Gan, 2011).

5.8 Limitation of modelling for cumulative effects assessment in the Athabasca Region

In order to build an understanding of changes in the environment and to ensure that the cumulative effects of the stressor/s are captured, CEA often requires to take into account: (i) the related theme and sub-theme areas and their environmental processes, (ii) interactions and feedback mechanisms between environmental processes (in different related theme and sub-theme areas), and (iii) both local and regional response scales.

However, the majority of modelling studies in Athabasca have the following limitations:

1. They often take into account either limited theme areas or environmental processes.
2. They often lack the capacity to capture the interactions between major system components.
3. They only consider either regional-scale response (which lacks the necessary detail on local-scale pathways) or local response (which might not be suitable for guiding a regional-scale decision-making process).

6.0 INTEGRATED MODELLING FRAMEWORK FOR CEA

This book has presented a comprehensive review of literature on environmental components, how they are connected and interact with each other, and the application of numerous modelling tools to understand the complex behaviors of environmental factors. Where possible, shortcomings of model applications have been highlighted to better understand the limitations and critical gaps in modelling the environment in a holistic way. The integrated environmental modelling framework proposed here addresses the gaps and limitations identified through this comprehensive literature review and could be applied at various temporal and spatial scales. The developed framework consists of a core and three supported layers, described as follows (Figure 9).

Core: The core consists of a comprehensive integrated watershed modelling system with the following characteristics:

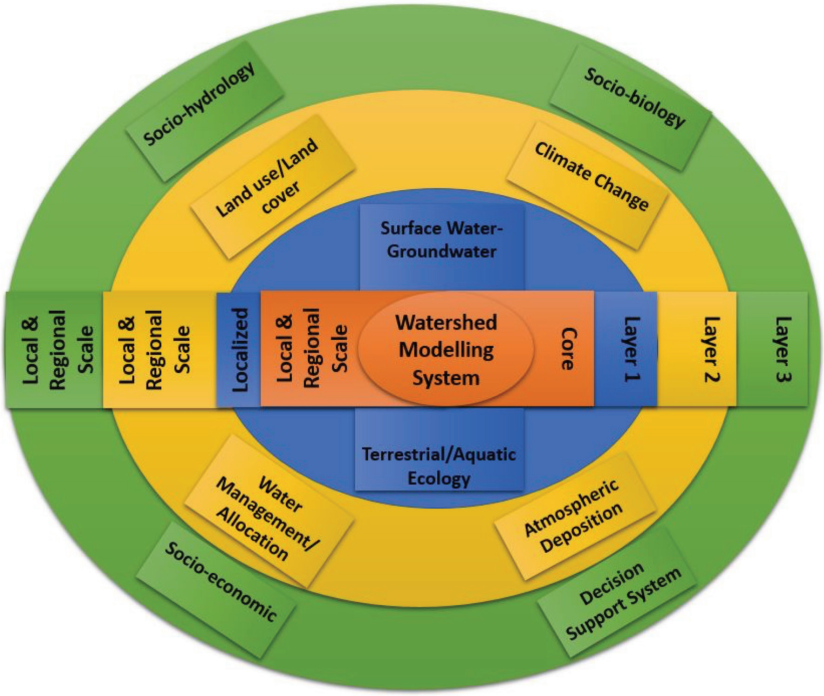
1. a physically based model which provides a detailed description of the processes that occur in the watershed;
2. a fully distributed model which considers the watershed as finite geo-referenced computational units with different responses to forced inputs;
3. a dynamic model that can employ both a short- and long-timestep along with either a detailed or coarse drainage network schematization of the watershed;

4. a dynamic model that can incorporate land surface changes at different time intervals during the simulation of environmental processes;
5. a model that can simulate environmental processes for both local and regional scales;
6. a model which either includes all the required processes to assess water (surface and subsurface) quantity, quality, land, climate, ecology, and air deposition components, or can be linked to other models to further evaluate the required mentioned processes; and
7. a model that can be linked to a socio-hydrology, -ecology, -economic model, as well as a decision support system.

Layer 1: Although, the core modelling system is capable of simulating surface water-groundwater at local to regional scale, this layer is considered when further assessment – with a higher resolution – is required for either surface water-groundwater or ecological components. This can support the modelling system for specific applications such as when strong inhomogeneities are present in the modelling domain or when a detailed cumulative effects assessment is required which is also linked to a regional CEA assessment.

Layer 2: this layer of the proposed integrated environmental modelling framework supports predictive modelling through scenario building for various system drivers, such as climate change, land use, atmospheric depositions, management practices, or policy changes. Scenarios developed under this layer are simulated using the modelling core and/or layer 1 to develop future or what-if projections.

Figure 9. Integrated Mechanistic Based Modelling Framework for CEA



Layer 3: this layer incorporates the interrelations between the social and economic factors with the environment to fill the gaps between policy development (public policy, economic policy, environmental policy, etc), decision-making, and science. This layer supports the modelling system to capture the interactions between three sustainability pillars (i.e. economic, environmental, and social) essential for existence of humankind on planet earth. The interactions could ideally be through a web-based interface which offers the flexibility of investigating a wide range of scenarios relating people and economy to environment.

6.1 Coupling strategy

A fully dynamic coupling is desired for the core of the modelling system which would dynamically capture the interactions and exchanges occurring with sub-systems of environment (i.e., land, surface water, ground water, air). Models on different layers (1, 2, and 3) could be linked using appropriate coupling strategy e.g., dynamic coupling (e.g., receiving waterbody hydrodynamic model and water quality model), iterative coupling (e.g., optimal water and load allocation model and receiving water quality model), or interactive coupling (e.g., land use model for changing time periods and watershed model). The linkages between core and other layers of the proposed framework could be achieved through hybrid coupling strategy where most models in different domains or disciplines are integrated through a sequential coupling.

6.2 Selection of models

The models should be selected based on their ability to capture the cumulative effects of identified stresses on defined environmental processes. Their strengths in respective disciplines should be considered as well as their acceptability as the state-of-the-art model with demonstrated applications worldwide. Furthermore, factors other than model capabilities should also be considered, such as the desired degree of complexity for cumulative effects assessment, watershed characteristics, and temporal and spatial scale.

The capability of the integrated modelling system is highly reliant on the selected core system and its characteristics (see section 6.1). Based on our literature review, the five most popular models, which might be able to meet the core requirements, are: *GSFLOW, MIKE SHE/MIKE 11, HydroGeoSphere, MODHMS, and ParFlow.* An appropriate model or models should be selected based on their capabilities and the objectives of CEA projects.

6.3 Novelty of the proposed integrated environmental modelling framework

Despite the conventional cumulative effects modelling approach which simplifies representation of environmental processes within a single environmental media, the proposed integrated environmental modelling framework brings together a set of interdependent components by characterizing the stress–response relationships based on modelling of interactions of a variety of components and cross-pathways. In other words, the proposed framework introduces a holistic systems-based approach that integrates multidisciplinary environmental components that can facilitate cumulative effects management strategies. The framework has the following main charactristics:

- It can explore dynamic, nonlinear, and complex interactions and feedbacks among environmental processes.
- It can tease out impacts of multiple stressors on environmental processes.
- It is capable of simulating environmental processes at different spatial and temporal scales.
- It serves the cumulative effects management needs to understand the complexity of the system by involving stakeholders and scenarios development, and consequently analyzing trade-offs among alternatives.

6.4 The challenges

CEA integrates various meteorological, hydrological, hydro-geological, biological, and chemical processes that occur at a broad range of spatial and temporal scales that characterize environmental processes. For instance, infiltration and soil hydraulic conductivity are pore scale and field scale processes, respectively, while transpiration occurs at a leaf area scale. On the other hand, overland flow is a watershed (local/regional) scale process, while climate change processes occur at the global scale. In terms of temporal scale, turbulent fluxes (e.g., moisture, sensible heat) and the land-atmosphere exchanges occur at the scale of seconds to minutes, while changes in land surfaces occur on the order of years to decades. Although interactions between these processes at different scales are well-established observationally and theoretically in integrated physical modelling systems, computational limitations have restricted the use of integrated cumulative effects predictive models for local and regional studies. For example, there are still many challenges, such as adaptation of water resources to climate and anthropogenic stressors that need to be addressed across large domain scales with a fine resolution, but integrated cumulative effects predictive modeling for a large domain scale is an intractable computational problem.

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Investigating the complex nature of environmental problems requires the integration of different environmental processes across major components of the environment. Cumulative effects assessment (CEA) not only includes analyzing and modelling environmental changes, but also supports planning alternatives that promote environmental monitoring and management.

The adoption of integrated modelling approaches requires the development of frameworks which may be used to investigate individual environmental processes and their interactions with each other. Integrated modelling frameworks are often the only way to examine important environmental processes and interactions, relevant spatial and temporal scales, and feedback mechanisms of complex systems for CEA.

This book examines the ways in which interactions and relationships between environmental components are understood, paying special attention to climate, land, water quantity and quality, and both anthropogenic and natural stressors. It reviews modelling approaches for each component and existing integrated modelling systems for CEA. Finally, it proposes an integrated modelling framework and provides perspectives on future research avenues for cumulative effects assessment.

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