

Modeling Constructed Wetlands for Hot and Arid Regions: Model Development

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1 Modeling Constructed Wetlands for Hot and Arid Regions: Model Development

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7 **ABSTRACT**

8 A mechanistic model was developed to assist with design of constructed wetlands intended to treat
9 industrial wastewater in the Arabian Gulf region. The model is deterministic in nature and thus allows
10 explicit evaluation of the fate and transport of wastewater constituents throughout constructed
11 wetlands to assess their efficacy in treatment. Although the model was developed for the purpose of
12 evaluating treatment wetlands in the hot and arid climate of the Middle East, the model is generalized in
13 order to allow users to simulate a wide range of climates, any type of wetland, with any configuration,
14 and any selection of material and plants. The model simulates the majority of physical, chemical, and
15 biological processes that could occur in wetlands that are responsible for the removal of constituents.
16 The model is designed to be flexible enough to allow the simulation of any number pre-selected
17 constituents or other constituents of the user's choice made based on the quality of influent. The model
18 relies on a large body of existing literature to formulate each process. The model development discussed
19 in this report and the resulting model, CWM, is considered "in progress". During the present stage, the
20 model framework and algorithms have been developed and made functional. Subsequently, model
21 formulations will need to be validated, model limitations analyzed and addressed, and model
22 refinements made, before and during use in full-scale operations and design. As such, it is recognized

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23 that the present stage of model development is “experimental”, and future refinements of the model
24 are anticipated. Model results at this time consist of evaluation of key model features and how they
25 perform in Middle Eastern climates.

26 **Keywords:** Constructed wetland; Contaminant fate modeling; Hot arid climate; Produced water; Process
27 water; Water treatment and reuse

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59 **1 INTRODUCTION**

60 Water scarcity has long been a persistent challenge in the Arabian Peninsula. Due to the arid and often
61 hyper-arid conditions, the majority of countries in the region are classified as having extreme water
62 scarcity. This situation is worsening due to growing population, agriculture, urbanization and
63 industrialization (Stefanakis, 2020). Moreover, it is expected that climate change will further exacerbate
64 the situation with increased temperature and evaporation and reduced precipitation. Therefore, there is

65 a recent vision and initiative to recycle domestic and industrial wastewater and the green technology of
66 Constructed Wetlands (CWs) have been proposed as an appropriate technology to address the main
67 issues in the wastewater sector in this region (Stefanakis, 2020). As discussed in this paper, the use of
68 CWs is particularly suited to the region due to enhanced performance under the warm temperatures of
69 the region.

70 The value of natural wetlands in water quality improvement has long been recognized (Kadlec and
71 Wallace, 2009; Mitsch and Gosselink, 2007). After some of the earliest studies of the use of wetlands to
72 treat municipal wastewater (Odum, 1985; Marshall, 1971), civil engineers began the implementation of
73 constructed wetlands to further this practice (Spangler, et al, 1976; James and Bogart, 1989). Over the
74 years, considerable knowledge has been gained about how these complex systems work (Moshiri, 1993;
75 Kadlec and Wallace, 2009), and so has the knowledge needed to design these systems. Constructed
76 wetlands have been successfully used to treat a various types of wastewater (Vymazal, 2009) including
77 municipal wastewater (Sudarsan, et al, 2018), urban stormwater runoff (Scholz, 2006), industrial
78 wastewater (Knight, et al., 1999), agricultural runoff (Vymazal and Brezinova, 2015), and mine discharge
79 (Wieder, 1989; Eger and Wagner, 2002).

80 Wetlands are complex systems; the water quality benefits achieved by wetlands rely on natural
81 microbial, biological, physical, and chemical processes to treat wastewater. Constructed wetlands,
82 similar to natural wetlands, act as a watershed filter, a sink for sediments and precipitates, and a
83 biogeochemical engine that recycles and transforms nutrients. A constructed wetland can perform many
84 of the functions of conventional wastewater treatment systems such as sedimentation, filtration,
85 digestion, oxidation, reduction, adsorption, and precipitation (Kadlec and Wallace, 2009; USEPA, 2000;
86 Brix, 1993; Chu and Rediske, 2012; Tchobanoglous, 1993). Many of these individual mechanisms have
87 been well-studied, however few studies address the role each plays in an integrative fashion.

88 The overall aim of this study was to assist in design of treatment wetlands for industrial wastewater
89 reuse that is appropriate for the Arabian Gulf region. The Constructed Wetland Model (CWM) is
90 therefore designed to assist in selecting from a choice of designs such that effluent levels can be
91 achieved pursuant to applicable standards. The model was specifically developed to allow key effluent
92 water quality parameters, such as suspended solids, organic matter, pathogens, and in some instances,
93 nutrients, and heavy metals, to be directly evaluated against target levels for reuse.

94 There exist numerous guidelines for the design of constructed wetlands (ITRC, 2003; RREL, 1993; IDEM,
95 1997; UN-HABITAT, 2008). While there are simplified models that can be used to describe the
96 performance of existing operational wetlands (Kadlec, 2000), there are few mechanistic models
97 available. Mechanistic models are an important tool to understand the various wetland processes,
98 identify which processes drive treatment efficacy, and therefore be of great assistance to wastewater
99 managers in the design of these systems. The intent of this paper is to present the development of a
100 model of constructed wetlands to address this growing need. Although developed to address wetlands
101 in Middle Eastern climates, because the CWM is mechanistic in nature, it is generalized so as to be
102 capable of simulating a wide range of wetlands and climates. The model is based on a combination of
103 existing frameworks available for modeling of surface and sub-surface flows, and theoretical concepts of
104 various fate processes available in the literature.

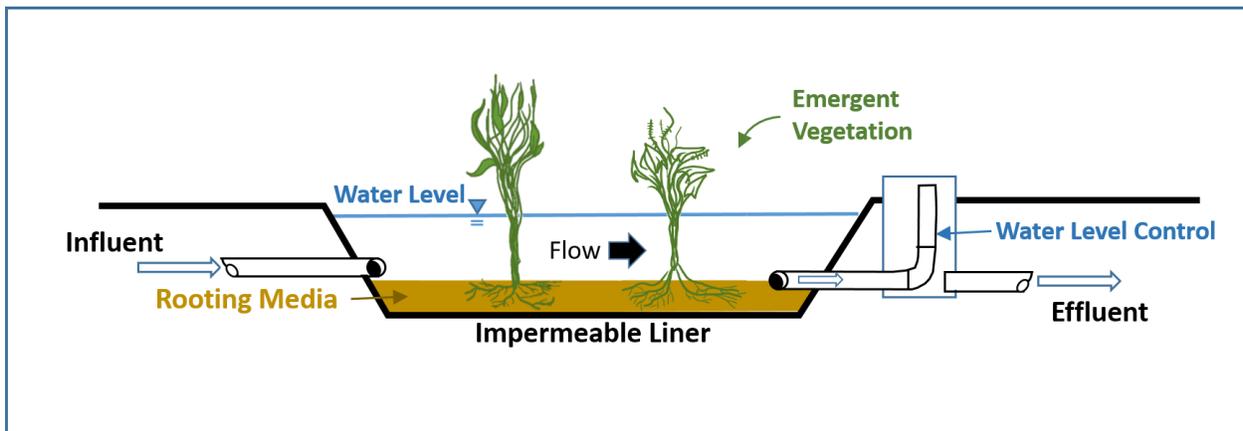
105 The model includes a graphical user interface that allows the user to input physical characteristics of the
106 wetland design (e.g., regions of substrate, length, depth, gradient, hydraulic head, porosity,
107 transmissivity, etc.), environmental parameters (air temperature, relative humidity, wind speed), input
108 water characteristics (e.g., flow rate, temperature, constituent concentrations), as well as values for all
109 key parameters associated with the algorithms used within the model to predict flow and the
110 fate/transport of target components (nutrient and non-nutrient); as well as output data and
111 visualization options.

112 2 BACKGROUND

113 2.1 TYPES OF CONSTRUCTED WETLANDS

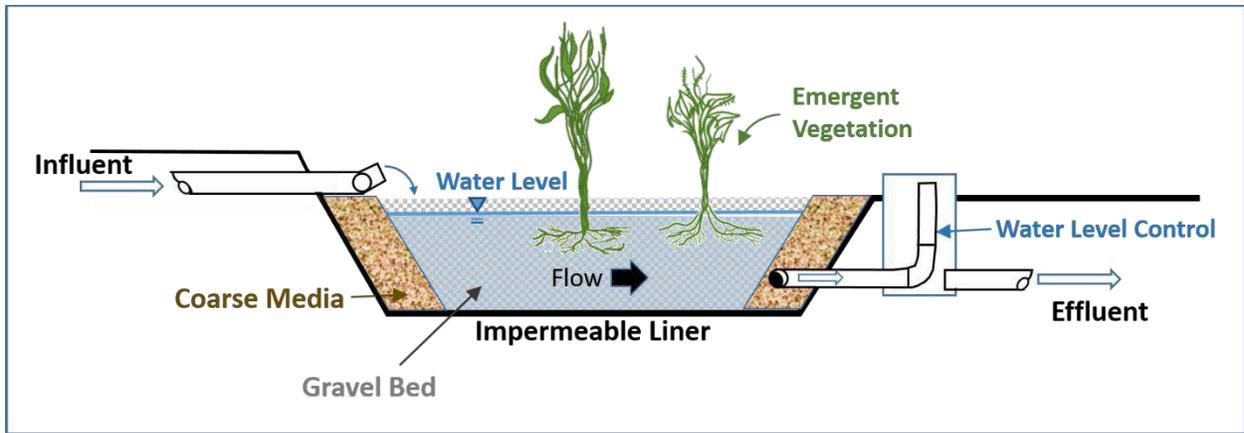
114 Constructed wetlands can typically be classified into two types of systems: free water surface (FWS)
115 wetlands or vegetated submerged bed (VSB) wetlands (USEPA, 2000). A surface flow (FWS) wetland, as
116 shown in Figure 1, consists of a shallow basin, soil or other medium to support the roots of vegetation,
117 and a water control structure that maintains a shallow depth of water. The water surface is above the
118 substrate. A VSB wetland consists of a sealed basin with a porous substrate of rock or gravel. The water
119 level is designed to remain below the top of the substrate. In most of such VSB systems, the flow path is
120 horizontal (VSB-H; Figure 2), although some systems use vertical flow paths (VSB-V; Figure 3). The bed of
121 VSB wetlands can be either saturated or unsaturated with water. Typically, VSB wetlands are best
122 suited for wastewaters with relatively low concentrations of solids given the hydraulic constraints
123 imposed by the substrate.

124



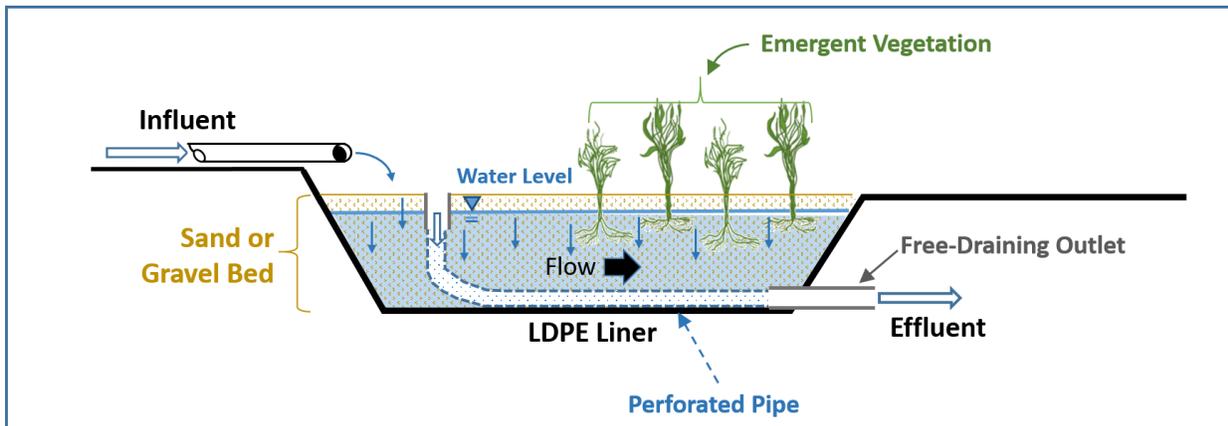
125

126 Figure 1 Schematic of a typical free water surface (FWS) constructed wetland



127

128 **Figure 2 Schematic of a typical horizontal vegetated submerged bed (VSB-H) constructed wetland**



129

130 **Figure 3 Schematic of a typical vertical vegetated submerged bed (VSB-V) constructed wetland**

131 **2.2 WETLAND FEATURES**

132 The wetland processes that can enhance water quality generally fall into two categories: solids
 133 separation and constituent transformation. Solids separation includes settling, filtration, and sorption.
 134 Chemical transformations include microbial degradation, vegetative uptake, oxidation/reduction, and
 135 precipitation (USEPA, 2000). The role of various processes and the overall efficacy of the constructed
 136 wetland is governed by the choices made during design (i.e. the type of wetland, hydraulic
 137 characteristics, porous media selection, and plant selection), and of course the composition of the
 138 influent. For example, settling of particulate constituents is largely dependent on the hydraulic

139 characteristics of the overlying water. Filtration (which is only of significance in VSB wetlands) will be
140 largely driven by the choice of porous material. The choice of plants (rooted and/or algal) will have a
141 large impact on the vegetative uptake of constituents, as different plants have differing uptake rates
142 (Kadlec and Wallace, 2009). Microbial degradation is closely connected to the oxygen levels in the
143 wetland (Bodelier and Dedysh, 2013), which in turn is affected by a wide variety of physical, chemical
144 and biological characteristics.

145 *2.3 WETLAND PERFORMANCE IN HOT AND ARID CLIMATES*

146 With respect to the performance of CWs in the hot and arid conditions of the Arabian Peninsula, the
147 primary defining characteristics affecting wetlands are:

- 148 • High Temperature
- 149 • High Evapotranspiration
- 150 • Low Precipitation

151 The average annual temperatures in the Middle East reach 25°C and summer temperatures exceed 30°C
152 (Stefanakis, 2020). Some regions of the Arabian Peninsula experience even more extreme conditions
153 with average annual temperatures at sea level of 27°C and up to 45°C during summer months (Burt,
154 2017). Many biological processes, both macro- and micro-biotic, are enhanced under these higher
155 temperatures compared to more temperate climates. Enhanced biological activity generally accelerate
156 the growth and other transformative processes that are the main drivers of CW constituent removal in
157 wastewater.

158 There can be challenges to CW operation in hot and arid climates due to the increased
159 evapotranspiration (evaporation and plant transpiration). Transpiration generally will dominate the
160 water loss (Kadlec, 2006). The combined water loss in these regions is often above 10%, and can exceed
161 40% of the inflow. These losses will result in increased constituent values, which will generally degrade

162 the quality of resulting CW effluent. The increased salinity values, if sufficiently high, may also have
163 inhibitive effects on biological activity. CWs intended for arid climates are typically designed to
164 minimize evapotranspirative losses, often by use of submerged (i.e. VSB) designs or minimizing the
165 water exposed surface area. Selection of proper plant species is also essential as different species will
166 have differing transpiration needs as well as differing salinity tolerances.

167 However, despite the challenges of increased transpiration, it can also have benefits. As plants absorb
168 more water to cover their needs, more water is pulled down into the substrate, promoting nutrient and
169 other constituent removal (Stefanakis, 2020).

170 Reduced precipitation in arid climates generally does not present much of a challenge for most CWs as
171 long as the CW is provided with a continuous source of wastewater.

172

173 **2.4 PREVIOUS MODELING**

174 The complexity associated with wetlands can make them difficult to understand. For this reason, most
175 of the available design guidelines are based on empirical observations or simple first-order decay
176 models (Langergraber et al, 2008). While first-order models are of common use, they are mainly based
177 on the influent characteristics, and the internal workings of the wetlands presume constancy of
178 parameters. The result is simple first-order, irreversible pollutant reduction removal models that
179 typically only work for particular wetlands under relatively steady conditions (Kadlec, 2000). Although
180 useful, these types of models face difficulties in predicting wetland treatment efficiencies through
181 different evolution stages of wetlands, over a long period of time, or when these wetlands may start to
182 lose treatment capacity due to substrate saturation or decaying vegetation.

183 Mechanistic models are generally built bottom-up based on first principles. They are robust and general;
184 however they require extensive data collection. Consequently, there have been few studies of

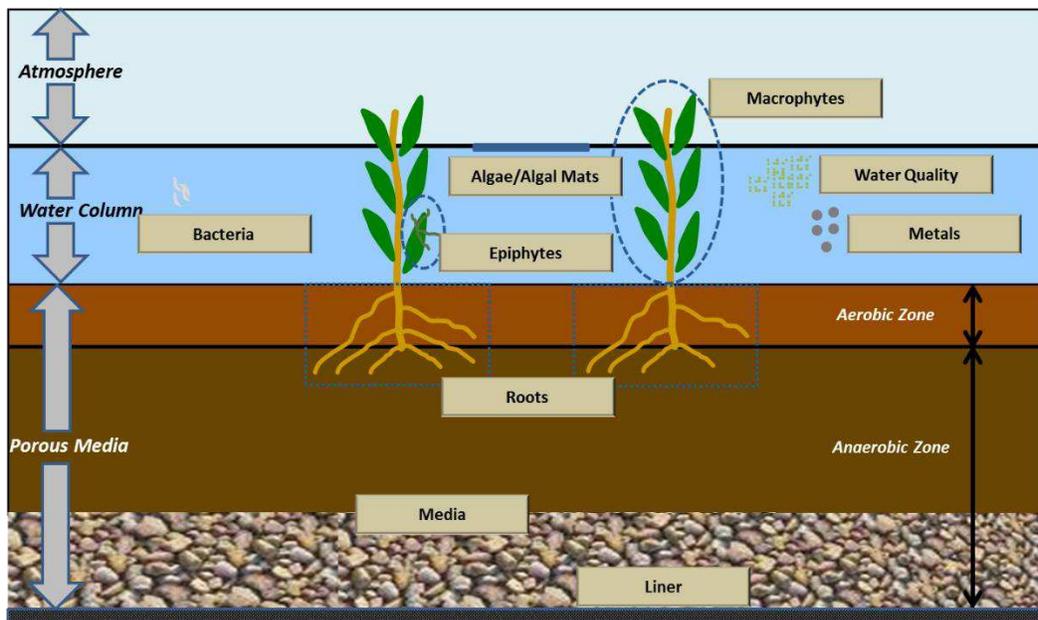
185 constructed wetlands with sufficient data available to support the theory and to calibrate the models
186 (USEPA, 2000). There has been recent advances in developing mechanistic wetland models, however
187 the relatively few that have been developed in recent years have been somewhat limited by modeling
188 only certain types of wetlands (Langergraber et al, 2008), certain types of constituents (Cancelli et al,
189 2019; Chu and Rediske, 2012), and/or certain processes (Mayo and Bigambo, 2005).

190 **2.5 SCOPE OF WORK**

191 The CWM is an expansion of the fate and transport models that were already available in Environmental
192 Resource Management's (ERM's) Generalized Environmental Modeling System for Surfacewaters
193 (GEMSS®). These models have been expanded based on information available from United States'
194 Environmental Protection Agency (EPA) guidance document (USEPA, 2000) in addition to various other
195 resources, as cited in relevant sections below. ERM and ExxonMobil Research Qatar (EMRQ) have
196 developed several fate and transport models collaboratively (Kolluru et al., 2005; Adenekan et al., 2009;
197 Febbo et al., 2012; Kolluru et al., 2003a; Kolluru et al. 2012,)for the region offshore of Ras Laffan
198 Industrial City in the Arabian Gulf. These models, based on GEMSS, consists of several modules that
199 compute the fate of various water quality and nutrient constituents. GEMSS® is an integrated system of
200 three-dimensional hydrodynamic and transport modules embedded in a geographic information and
201 environmental data system. Due to its vast capabilities, flexible design and previous use in Qatar, GEMSS
202 was identified as the primary framework to be used to develop CWM.

203 GEMSS is designed in a modular fashion where hydrodynamic platform ("kernel") provides three-
204 dimensional surface (open water) flow fields from which the distribution of various constituents can be
205 computed. The constituent transport and fate computations are grouped into modules. Prior to the
206 development of the CWM, GEMSS® modules included those used for thermal analysis, water quality,
207 sediment transport, particle tracking, oil and chemical spills, entrainment, and toxics. Therefore, the
208 design of CWM required two enhancements: inclusion of sub-surface flows and inclusion of an

209 additional module specifically designed for fate and transport of relevant industrial wastewater
210 constituents. These two enhancements, when combined with several existing modules (e.g.
211 macrophytes, nutrients, etc.) provides the entire spectrum of constituents and features necessary to
212 mechanistically model industrial wastewater treatment through constructed wetlands. A simplified
213 representation of a constructed wetland and its features, as implemented in CWM, is shown in Figure 4.
214 The theoretical basis and implementation of each process and capability is described below in each
215 subsection.



216

217 **Figure 4 Simplified schematic showing various features within a constructed wetland**

218

219 **3 METHODOLOGY**

220 The present section provides a brief theoretical background on the various concepts implemented
221 during this model development.

222 **3.1 MODEL DESIGN**

223 Throughout this paper terms are used to define these features and, therefore, it is important to
224 establish a consistent terminology. Certain distinctions are being made to denote what is included as
225 pre-defined (general properties set as default) versus what is user-defined (properties specifically
226 defined by the user to represent engineered materials). These terms include:

- 227 • Zones: defined as process based
 - 228 ○ Water
 - 229 ○ Aerobic sediments
 - 230 ○ Anaerobic sediments
- 231 • Media: defined as physical state
 - 232 ○ Water
 - 233 ○ Sediments
- 234 • Materials: defined as sediment (porous media) types
 - 235 ○ Pre-defined (sand, gravel, clay, silt, etc.)
 - 236 ○ User-defined (engineered material, etc.)
- 237 • Regions: defined as materials/constituent specific
 - 238 ○ Materials
 - 239 ■ Water – lack of any porous material
 - 240 ■ Sediment – presence of various porous materials
 - 241 ■ Vertically constant
 - 242 ○ Constituents
 - 243 ■ Water – presence of various plants, algae, bacteria, concentrations, etc.
 - 244 ■ Sediment – presence of various roots, concentrations, etc.
 - 245 ■ Vertically variable

246 **3.2 THEORY**

247 Several basic assumptions regarding the zones, media, materials, and regions were made in the
248 development of the CWM. These assumptions include:

249 • Two Media:

250 ○ Water

251 ○ Sediments

252 • Three Zones:

253 ○ Water

254 ○ Aerobic zone: dynamic location of aerobic/anaerobic interface

255 ○ Anaerobic zone

256 ○ Root “zone”: part of the sediment zone

257 • Unlimited Materials

258 ○ Pre-defined or user-defined

259 • Unlimited Regions

260 ○ User-defined

261 **3.2.1 Transport**

262 A constructed wetland may have surfacewater overlying and flowing above porous or impermeable
263 media. The porous media could be submergent (surfacewater above porous media) or emergent (no
264 surfacewater above porous media). Accordingly, the wetland may also have subsurface flow through
265 porous media. The CWM simulates the transport of water in both of these mediums under a combined
266 interactive system.

267 **3.2.1.1 Surface Flows**

268 The movement of surface flows is modeled using the GEMSS hydrodynamic kernel. The theoretical basis
269 of the kernel is the three-dimensional Generalized, Longitudinal-Lateral-Vertical Hydrodynamic and

270 Transport (GLLVHT) model which was first presented in Edinger and Buchak (1980) and subsequently in
271 Edinger and Buchak (1985). The GLLVHT computation has been peer reviewed and published (Edinger
272 and Buchak, 1995; Edinger, et al., 1994 and 1997; Edinger and Kolluru, 1999). The hydrodynamic kernel
273 is an extension of the well-known longitudinal-vertical transport model originally developed by Buchak
274 and Edinger (1984) that forms the hydrodynamic and transport basis of the Corps of Engineers' water
275 quality model CE-QUAL-W2 (U. S. Army Engineer Waterways Experiment Station, 1986). Improvements
276 to the transport scheme, construction of the constituent modules, incorporation of supporting software
277 tools, GIS interoperability, visualization tools, graphical user interface (GUI), and post-processors have
278 been developed by Kolluru et al. (1998; 1999; 2003a; 2003b) and by Prakash and Kolluru (2006).

279 3.2.1.2 Vegetative Resistance

280 The vegetation in CWM is implemented through the use of two different existing modules within
281 GEMSS: macrophytes and epiphytes. Macrophytes are the rooted vegetation and epiphytes are plants
282 attached to the macrophytes. In heavily vegetated waterbodies such as wetlands, vegetation can restrict
283 flow through the surfacewater through both friction and the reduction of cross-sectional area. These
284 flow restrictions were implemented through the use of free surfacewater frictional forces, and are
285 based on the total plant area normal to the direction of flow $\sum A_i$ which is estimated using biomass to
286 surface area ratios from Sher-Kaul et al. (1995) and surface area to volume ratios from Sand-Jensen and
287 Borum (1991). The drag coefficient C_d is a calibration parameter that is of the order of 1.0 for
288 vegetation. Vegetative drag results in an effective Manning's friction factor n , as calculated by Petryk
289 and Bosmajian (1975) and shown in:

$$290 \quad n = n_b \sqrt{1 + \frac{C_d \sum A_i}{2gV} \frac{1}{n_b^2} R^{4/3}}$$

291 where:

n	=	Effective Manning's friction factor	[]
n _b	=	Manning's friction factor due to bed friction only	[]
C _d	=	Drag coefficient	[]
R	=	Hydraulic radius	[L]
A _i	=	Area of i th plant in the direction of flow	[L] ²
V	=	Cell volume	[L] ³
L	=	Cell length in direction of flow	[L]
g	=	Gravitational acceleration	[L][T] ⁻²

292

293 The reduced cross-sectional area is simply achieved by applying an effective porosity of the
 294 surfacewater:

295
$$\phi = \frac{V - V_m}{V}$$

296 where:

φ	=	Water porosity due to vegetation (macrophytes only)	[]
V _m	=	Cell volume occupied by macrophytes	[L] ³

297 *3.2.1.3 Sub-Surface Flows*

298 As noted earlier, the main kernel of GEMSS includes the surface flows. A separate module was
 299 developed and integrated with the main surface flow kernel to provide flow connectivity between
 300 surface and sub-surface flows. The sub-surface flow module is called GEMSS-GWM (GroundWater
 301 Module). This linkage is dynamic, with real time information shared between the free surfacewater
 302 elevation and piezometric head within the porous media.

303 In a groundwater (or porous media) system, the mass balance for the three-dimensional movement of
 304 constant density ground water through a porous material can be shown to be represented by the
 305 Richards Equation (written in term of local pressure head):

306
$$S_s \frac{\partial h}{\partial t} = \vec{\nabla} \circ (k \vec{\nabla} h) + W$$

307 where:

S_s	=	Specific storage, the change in saturation per unit head	$[L]^{-1}$
h	=	Local pressure head	$[L]$
k	=	Hydraulic conductivity	$[L] [T]^{-1}$
W	=	Volumetric flux of sources and/or sinks per unit volume	$[T]^{-1}$
t	=	Time	$[T]$

308

309 The specific storage can be rewritten as shown:

$$S_s = \frac{\phi}{V_v} \frac{\partial V_w}{\partial h}$$

310 where:

V_w	=	Water volume	$[L]^3$
V_v	=	Void volume, volume potentially filled by water or air	$[L]^3$
ϕ	=	Porosity (V_w/V_v)	$[-]$

311

312 The sub-surface transport is completely specified by the Richards Equation, transport and/or head at the
 313 boundaries of the modeled region, and initial head throughout the region. For finite-difference models
 314 such as GEMSS, these equations need to be discretized into a solvable system of equations. The method
 315 used for discretization is based on a scheme adopted in MODFLOW (Harbaugh, 2005).

316 GEMSS-GWM performs the temporal calculations using a combined implicit and explicit formulation. An
 317 implicit formulation is more numerically stable; however, it requires longer computational times. Due to
 318 the complexity of calculations in the CWM, the hybrid system is utilized. The explicit formulation is used
 319 in the horizontal direction and the implicit formulation is used in the vertical direction.

320 The GEMSS-GWM module of CWM includes conditions possible within the porous media such as partial
 321 saturation and wetting/drying (water level moving up and down leaving parts of the porous media
 322 completely dry). For the sake of brevity, details on the approach used for partially saturated flow is not
 323 described here, but can be obtained from MODFLOW-2005 documentation (Harbaugh, 2005). The

324 approach taken for wetting/drying is to have a dry cell convert to wet when the computed head in the
325 cell directly below exceeds a bottom elevation of the dry cell.

326 *Evapotranspiration*

327 An important mechanism for water loss is the evapotranspiration. This mechanism was included to
328 simulate water losses through plant transpiration and direct evaporation by removing appropriate water
329 from the groundwater zone. The approach is based on a few assumptions as follows:

- 330 • When the water table is at or above a specified elevation, termed the "ET surface",
331 evapotranspiration loss from the water table occurs at a maximum rate specified by the user;
- 332 • When the depth of the water table below the ET surface elevation exceeds a specified interval,
333 termed the "extinction depth" or "cutoff depth", evapotranspiration from the water table
334 ceases; and
- 335 • Between these limits, evapotranspiration from the water table varies linearly with water-table
336 elevation.

337 **3.2.2** *Constituent Fate*

338 In consultation with the various industries in Qatar, ERM and EMRQ identified a list of constituents that
339 would be typically present in the wastewater, including those that have been generally been found in
340 produced water resulting from natural gas extraction. These constituents were designated for inclusion
341 in the CWM. These constituents were further evaluated from the perspective of their role in
342 nutrient/vegetative interaction and their role in eutrophication/water quality (Cercio and Cole, 1995;
343 Cole and Wells, 2013; Pelletier and Chapra, 2008; Thomas and Scott, 2004; USEPA, 2006; USEPA, 2013).

344 The CWM utilizes the existing GEMSS water quality module (GEMSS-WQM) that includes the various
345 nutrient cycles and associated water quality parameters such as dissolved oxygen and algae. The fate
346 processes applicable to the nutrients (carbon, nitrogen and phosphorus) have been well-studied (Cole
347 and Wells, 2013; Chapra, 1997; Thomann and Mueller, 1987; USEPA, 2006). GEMSS-WQM (and CWM) is
348 based on the concepts discussed and published by USEPA (USEPA, 2000) for these nutrients. The

349 GEMSS-WQM module addresses most of the constituents related to the dissolved and particulate forms
350 in the water column.

351 The fate processes of constituents that were not originally included in GEMSS were then added as part
352 of the CWM development. In addition to the expansion of the existing modules and implementation of
353 additional nutrient cycle processes, various fate processes for the non-nutrient constituents (metals, pH,
354 sulfide, calcium, oil and grease) were implemented. The fate processes related to these constituents are
355 specific to the choice of plants and media. Therefore, the assumptions and basis for the formulas used
356 for model calculations are based on generic but user-definable concepts. Processes such as ionization,
357 dissolution, adsorption, settlement and speciation are also calculated in the model. All processes
358 governed by formulas with theoretical or experimentally derived parameters, are initially set to default
359 values based on valid assumptions, but are also available as user inputs through the model GUI.

360 The table below contains the complete list of constituents and associated processes included in the
361 CWM.

362 **Table 1 List of constituents and associated fate processes**

Constituent	Processes
Algae	Excretion, respiration, photosynthesis, mortality
Macrophytes	Respiration, photosynthesis, mortality
Epiphytes	Excretion, respiration, photosynthesis, mortality
Organic Matter: Dissolved	Excretion, decay
Organic Matter: Particulate	Decay, mortality, sorption, settlings, burial

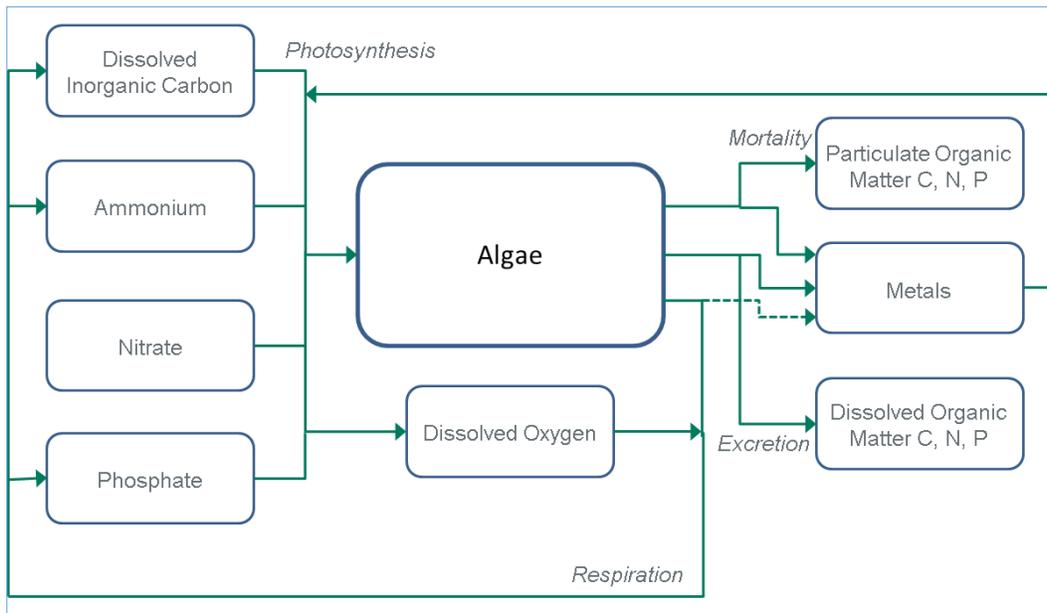
Constituent	Processes
Dissolved Oxygen	Respiration, photosynthesis, reaeration, decay
Dissolved Inorganic Carbon	Respiration, photosynthesis, reaeration, decay
Organic Nitrogen: Dissolved	Excretion, decay
Organic Nitrogen: Particulate	Decay, mortality, settlings, burial
Organic Phosphorus: Dissolved	Excretion, decay
Organic Phosphorus: Particulate	Decay, mortality, settlings, burial
Ammonium	Respiration, photosynthesis, decay, nitrification
Nitrate/Nitrite	Photosynthesis, denitrification, nitrification
Phosphate	Respiration, photosynthesis, decay
Bacteria/Pathogens	Mortality, settling, burial
Cyanide	Volatilization, decay, sorption, settling, burial
Phenol	Volatilization, decay, sorption, settling, burial
Oil & Grease	Volatilization, decay
Sulfide	Uptake, oxidation, reduction, sorption, settlings, burial
Sulfate	Uptake, oxidation, reduction, sorption, settlings, burial
pH	Various reactions, see section Error! Reference source not found.

Constituent	Processes
Alkalinity	Various reactions, see section Error! Reference source not found.
Inorganic Solids	Settling, burial
Metals: Aluminum	Respiration, excretion, mortality, vegetative uptake, sorption, precipitation, settling, burial, volatilization (Mercury only)
Metals: Arsenic	
Metals: Barium	
Metals: Cadmium	
Metals: Chromium	
Metals: Cobalt	
Metals: Copper	
Metals: Iron	
Metals: Lead	
Metals: Manganese	
Metals: Mercury	
Metals: Nickel	
Metals: Zinc	

364 For the sake of brevity, detailed formulations of the various fate and processes are shown only for
 365 selected and representative constituents are discussed below. Formulations related to other
 366 constituents follow similar approach and are process based, as shown below:

367 *3.2.2.1 Algae*

368 The overall fate processes related to algal groups (algae and algal mats) are shown in Figure 5. CWM
 369 allows any number of algal groups that can be defined by modifying the various rates related to the
 370 individual processes. Each of these processes serves as either a source for increase in algal
 371 concentration or sink for decrease in algal concentration.



372

373 **Figure 5 Fate processes associated with various algal groups**

374 The overall source/sink mass balance equation based on Figure 5 is shown as:

375 $S_a = K_{ag} ALG - K_{ar} ALG - K_{ae} ALG - K_{am} ALG$

376 where

S_a = Algal source/sink in Carbon (C) $[M][L]^{-3} [T]^{-1}$

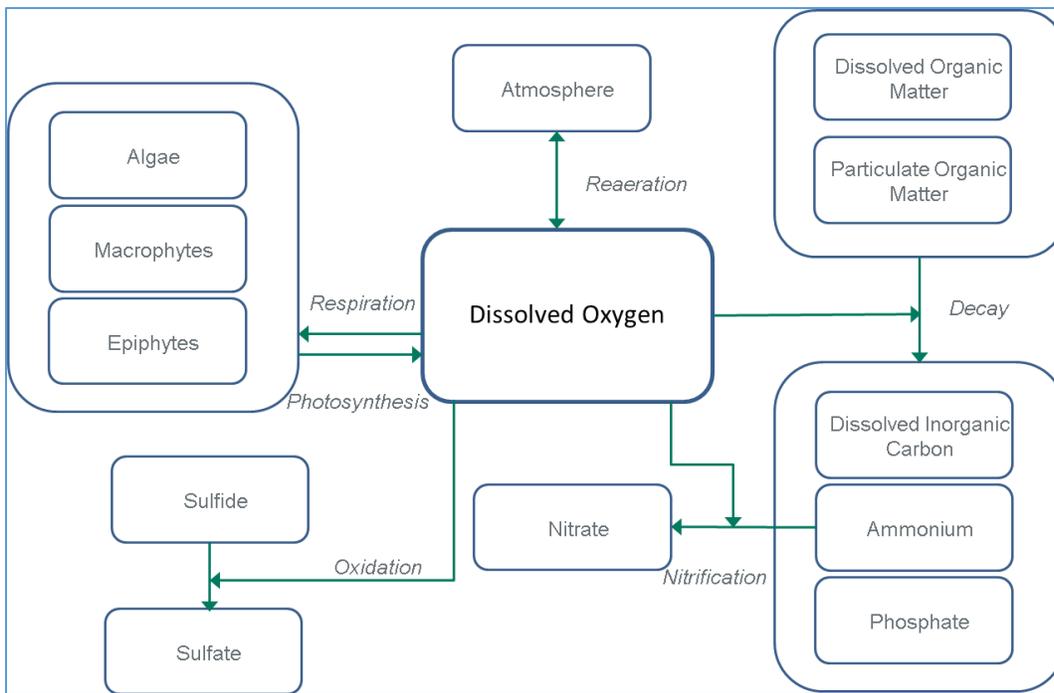
ALG	=	Algal Concentration in C	[M][L] ⁻³
K _{ag}	=	Algal Growth Rate	[T] ⁻¹
K _{ar}	=	Algal Respiration Rate	[T] ⁻¹
K _{ae}	=	Algal Excretion Rate	[T] ⁻¹
K _{am}	=	Algal Mortality Rate	[T] ⁻¹

377

378 3.2.2.2 Dissolved Oxygen

379 The overall fate processes related to dissolved oxygen (DO) are shown in Figure 6. Each of these

380 processes serves as either a source for DO concentrations or sink for DO concentrations.



381

382 **Figure 6 Fate processes for dissolved oxygen**

383 The overall source/sink equation based on Figure 6 is shown as:

$$\begin{aligned}
 S_{DO} = & \left(\frac{MW_{O_2}}{MW_C} \right) \{ K_{ag}ALG + K_{eg}EPI + K_{mg}MAC - K_{ar}ALG - K_{er}EPI - K_{mr}MAC - K_{DOM}DOC \\
 & - K_{POM}POC \} + \frac{Kl_{O_2}}{h} (DO_s - DO) - \frac{3MW_{O_2}}{2MW_N} K_{nit}NH_4 - 2MW_{O_2}O^{S^{2-}} \cdot SO_4^{2-}
 \end{aligned}$$

385

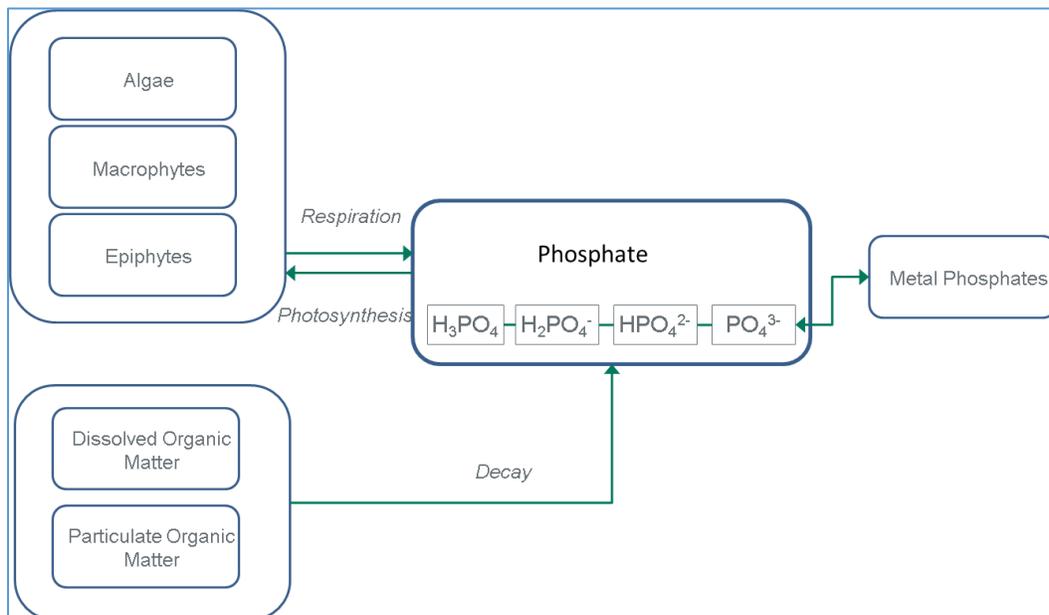
386 where:

S_{DO}	=	Dissolved Oxygen source/sink	$[M][L]^{-3} [T]^{-1}$
DOC	=	Dissolved Organic Carbon Concentration in C	$[M][L]^{-3}$
POC	=	Particulate Organic Carbon Concentration in C	$[M][L]^{-3}$
EPI	=	Epiphyte Concentration in C	$[M][L]^{-3}$
MAC	=	Macrophyte Concentration in C	$[M][L]^{-3}$
DO	=	Dissolved Oxygen Concentration	$[M][L]^{-3}$
NH ₄	=	Ammonium Concentration in Nitrogen (N)	$[M][L]^{-3}$
K_{DOM}	=	Dissolved Organic Matter Decay Rate	$[T]^{-1}$
K_{POM}	=	Particulate Organic Matter Decay Rate	$[T]^{-1}$
K_{eg}	=	Epiphyte Growth Rate	$[T]^{-1}$
K_{mg}	=	Macrophyte Growth Rate	$[T]^{-1}$
K_{er}	=	Epiphyte Respiration Rate	$[T]^{-1}$
K_{mr}	=	Macrophyte Respiration Rate	$[T]^{-1}$
K_{lO_2}	=	DO Reaeration Rate	$[L][T]^{-1}$
h	=	Depth	[L]
DO_s	=	Saturation DO Concentration	$[M][L]^{-3}$
K_{nit}	=	Nitrification Rate	$[T]^{-1}$
O^{S-SO_4}	=	Oxidation Rate of Sulfide to Sulfate	$[L][T]^{-1}$
MW_{O_2}	=	Molecular Weight of Oxygen (O ₂)	[g/mol]
MW_C	=	Molecular Weight of Carbon	[g/mol]
MW_N	=	Molecular Weight of Nitrogen	[g/mol]

387 3.2.2.3 Phosphate

388 The overall fate processes related to phosphate (PO₄) are shown in Figure 7. Each of these processes

389 serves as either a source for phosphate concentrations or sink for phosphate concentrations.



390

391 **Figure 7 Fate processes for phosphate**

392 The overall source/sink equation based on Figure 7 is shown as:

393

$$394 \quad S_{PO_4} = K_{DOM}DOP + K_{POM}POP - \alpha_{apc}K_{ag}ALG - \alpha_{epc}K_{eg}EPI - \alpha_{mpc}K_{mg}MAC + \alpha_{apc}K_{ar}ALG$$
$$395 \quad + \alpha_{epc}K_{er}EPI + \alpha_{mpc}K_{mr}MAC - R_{M \cdot PO_4}$$

396 where:

S_{PO_4}	=	Phosphate source/sink in Phosphorus (P)	$[M][L]^{-3} [T]^{-1}$
DOP	=	Dissolved Organic Phosphorus Concentration in P	$[M][L]^{-3}$
POP	=	Dissolved Organic Phosphorus Concentration in P	$[M][L]^{-3}$
PO ₄	=	Phosphate Concentration in P	$[M][L]^{-3}$
α_{apc}	=	Algal Phosphorus to Carbon Ratio	[g-P/g-C]
α_{epc}	=	Epiphyte Phosphorus to Carbon Ratio	[g-P/g-C]
α_{mpc}	=	Macrophyte Phosphorus to Carbon Ratio	[g-P/g-C]
$R_{M \cdot PO_4}$	=	Metal Phosphate Precipitation/Dissolution Rate	[g-P/m ³ -s]

397 3.2.2.4 Metals

398 The CWM models the fate of thirteen (13) metals. These metals experience a varied range of fate

399 processes including vegetative (algae, macrophytes and epiphytes) uptake and sorption to organic

400 matter. Additionally, the precipitates of these metals settle or dissolve. These three fate processes are

401 common to all metals and are discussed in the following sub-sections separately. For full details of each

402 metal, including additional processes specific to individual metals, the reader is directed to the complete

403 CWM documentation available by request to the authors.

404 *Vegetative Metal Uptake/Release*

405 The net vegetative metal uptake rate [mol/L-s] (sink) for each metal is given by:

$$406 \quad U_{VEG}^M = \frac{r_a^M K_{ag}ALG + r_e^M K_{eg}EPI + r_m^M K_{mg}MAC}{MW^M}$$

407 where:

U_{VEG}^M	=	Metal Vegetative Uptake Rate	$[mol][L]^{-3} [T]^{-1}$
-------------	---	------------------------------	--------------------------

M	=	Metal Constituent	
r_a^M	=	Algae Uptake Constant for Metal M	$[L][L]^{-1}$
r_e^M	=	Epiphyte Uptake Constant for Metal M	$[L][L]^{-1}$
r_m^M	=	Macrophyte Uptake Constant for Metal M	$[L][L]^{-1}$
MW^M	=	Molecular Weight of Metal M	$[g/mol]$

408

409 For each metal, the vegetative metal release rate [mol/L-s] due to respiration, excretion, and mortality is
 410 given by:

$$411 \quad R_{VEG}^M = (K_{ar} + K_{ae} + K_{am})C_a^M + (K_{er} + K_{ee} + K_{em})C_e^M + (K_{mr} + K_{mm})C_m^M$$

412 where:

R_{VEG}^M	=	Metal Vegetative Release Rate	$[mol][L]^{-3} [T]^{-1}$
C_a^M	=	Concentration of Metal Constituent in Algae	$[mol/L]$
C_e^M	=	Concentration of Metal Constituent in Epiphytes	$[mol/L]$
C_m^M	=	Concentration of Metal Constituent in Macrophytes	$[mol/L]$
K_{ee}	=	Epiphyte Excretion Rate	$[T]^{-1}$
K_{em}	=	Epiphyte Mortality Rate	$[T]^{-1}$
K_{mm}	=	Macrophyte Mortality Rate	$[T]^{-1}$

413

414 *Sorption to Organic Matter*

415 For each metal, the freely dissolved metal is assumed to be in equilibrium with the metal sorbed to
 416 organic matter. The dissolved and particulate fractions, respectively, are given by:

$$417 \quad f_d^M = \frac{\phi}{\phi + Kd^M POC}$$

$$418 \quad f_p^M = \frac{Kd^M POC}{\phi + Kd^M POC}$$

419 where:

f_d^M	=	Metal Dissolved Fraction	$[\]$
f_p^M	=	Metal POC Particulate Fraction	$[\]$
K_d^M	=	Organic Carbon Partition Coefficient for M	$[L]^3[M]^{-1}$
Φ	=	Porosity	$[\]$

420

421 *Precipitate Reactions*

422 The rate of precipitation/dissolution [mol/L-s] of each of the metal precipitate can be given by:

423
$$P^{M \cdot p} = K^{M \cdot p} (C_d^M - C^{M*})$$

424 where:

$P^{M \cdot p}$	=	Rate of Precipitation/Dissolution of Metal Precipitate	[mol][L] ⁻³ [T] ⁻¹
$M \cdot p$	=	Metal Precipitate Constituent	
$K^{M \cdot p}$	=	Rate Constant for Constituent, M·p	[T] ⁻¹
C_d^M	=	Freely Dissolved Concentration of Constituent, M	[mol/L]
C^{M*}	=	Solubility of Constituent, M	[mol/L]

425

426 The solubility of the constituent, M is based on the solubility product as shown:

427
$$K_{sp}^{M \cdot p} = \prod_i C_i^*$$

428 where:

$K_{sp}^{M \cdot p}$	=	Metal Precipitate Solubility	[mol/L]
i	=	Precipitate Ions	
C_i^*	=	Solubility of Ion i	[mol/L]

429

430 **3.2.3 Constituent Transport**

431 The fate processes discussed in the previous section provide the sink and source for each individual

432 constituent modeled within CWM. The transport equations referenced and discussed earlier provide the

433 flow velocities for each discretized model cell. These two combine to form the generalized constituent

434 transport equation shown below.

435

436
$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + S$$

437 where:

C = Concentration of a constituent
 u, v, w = Velocities in x, y and z directions
 D_x, D_y, D_z = Diffusivities in x, y and z directions
 S = Net source/sink term

438

439 This constituent transport equation can be solved within CWM using a variety of schemes (Upwind,
440 QUICKEST and QUICKEST+ULTIMATE), and explicitly or implicitly (Prakash and Kolluru, 2006).

441 **4 RESULTS AND DISCUSSION**

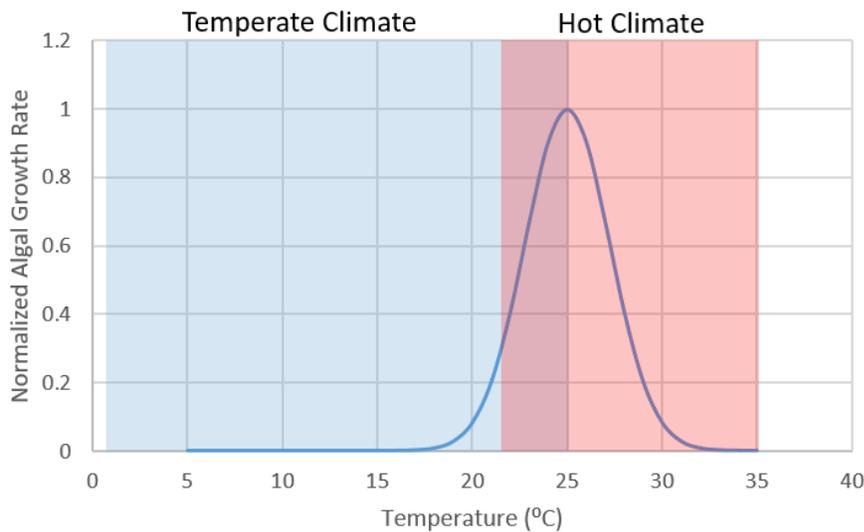
442 There are currently insufficient data to conduct an actual model performance evaluation as a result we
443 applied the model in an illustrative fashion. This application aims to demonstrate some key model
444 features. There are extensive efforts underway to calibrate the model using data from the biggest CW in
445 the Middle East, Nimr Project. In 2011, Petroleum Development Oman in collaboration with Bauer Nimr
446 LLC commissioned the construction of a constructed wetland, one of the largest industrial constructed
447 wetland systems in the world, to manage produced water from the Nimr oilfields in Oman. This wetland
448 has been operating since as part of the Nimr Water Treatment Plant (Nimr WTP) and has demonstrated
449 the utility of natural treatment process to achieve multiple significant environmental benefits as well as
450 substantial savings in operating costs compared to conventional methods of disposal (Stefanakis et al,
451 2018).

452 **4.1 EFFECTS OF HOT AND ARID CONDITIONS ON MODEL PERFORMANCE**

453 **4.1.1 Temperature**

454 Generally higher temperatures are conducive to wetland performance. Higher temperatures typically
455 result in higher biologic activity (vegetative and microbial), and these are reflected in the rate

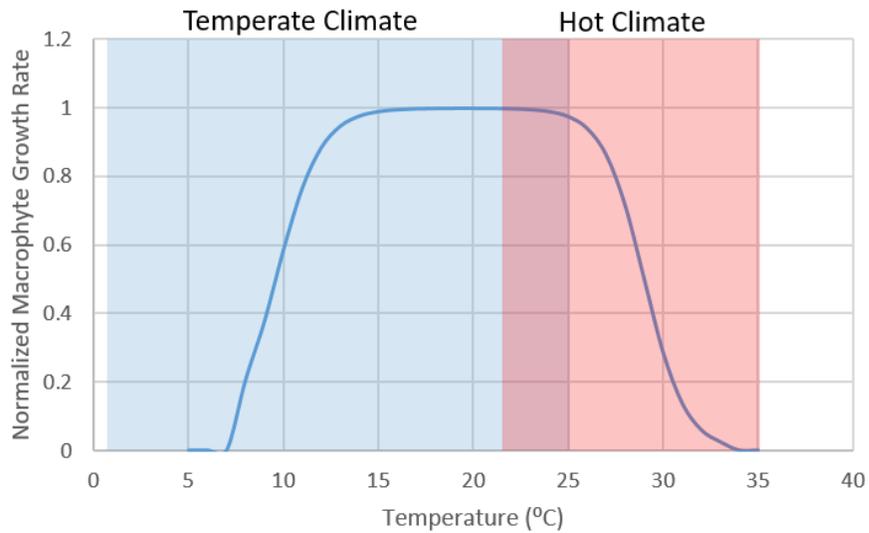
456 temperature dependencies in the model. Figure 8 and Figure 9 below show example algal and
457 macrophyte growth rates as a function of temperature. The shaded regions represent approximate
458 seasonal ranges in average temperature for temperate and hot climates. Algal growth rates usually
459 have an optimum temperature for growth, then sharply decline at both warmer and cooler
460 temperatures (Figure 8). Hot climates tend to capture more of the temperature window for algal
461 growth. Macrophytes, on the other hand, are much more tolerant of temperature changes, and
462 experience optimal growth at a broader range of temperatures (Figure 9). The optimal range of
463 temperature for macrophyte growth is highly dependent on the plant species. For the example shown,
464 the optimal temperatures are more in the range of temperate climates, but the selection of a more
465 heat-loving species would show the optimal temperatures in the hot climate range. This reinforces the
466 need for proper selection of plant species conducive to local climates.



467

468 **Figure 8 Example Algal Growth Temperature Response**

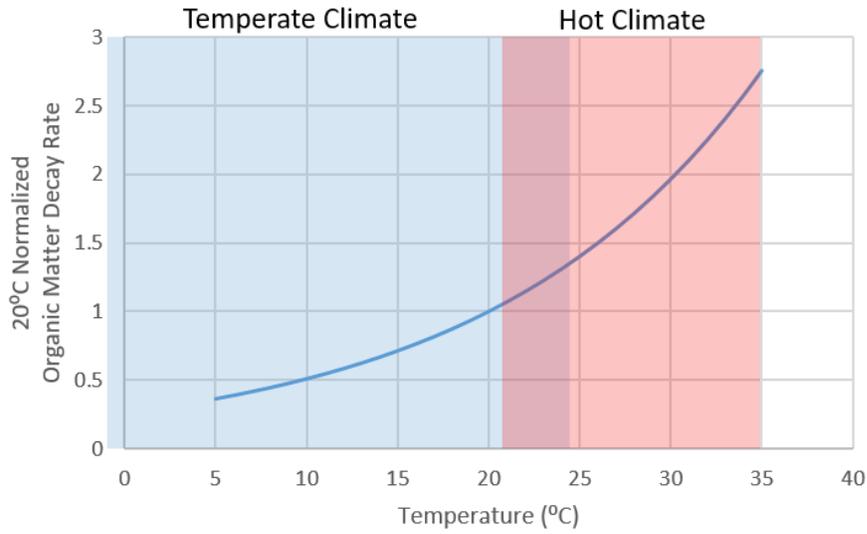
469



470

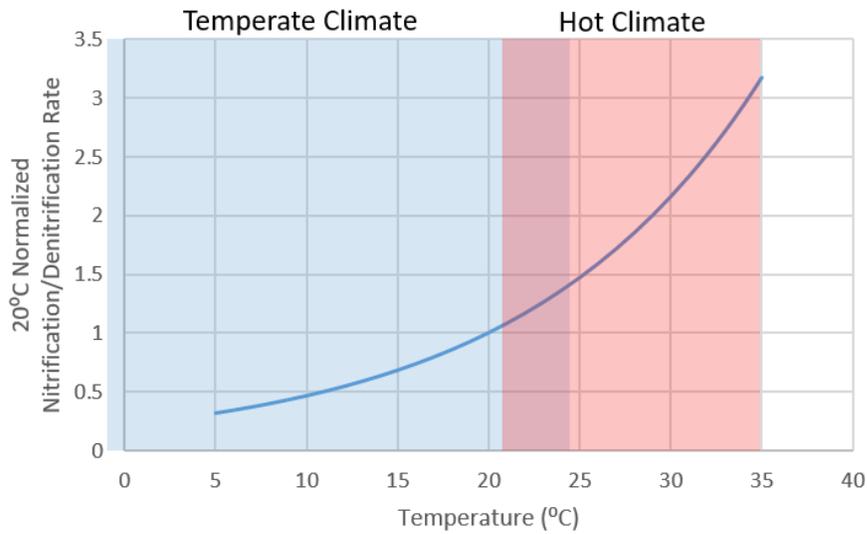
471 **Figure 9 Example Macrophyte Growth Temperature Response**

472 Microbial activity is also strongly dependent on temperature. However unlike algal and macrophyte
 473 activity, higher temperature nearly always favors higher activity. Some of the processes mediated by
 474 bacteria, such as organic matter degradation, nitrification, and denitrification, are shown in example
 475 Figure 10 and Figure 11. As can be seen from these figures, these wetland processes are significantly
 476 enhanced in hot climates, by factors of 2-3x.



477

478 **Figure 10 Example Organic Decay Temperature Response**

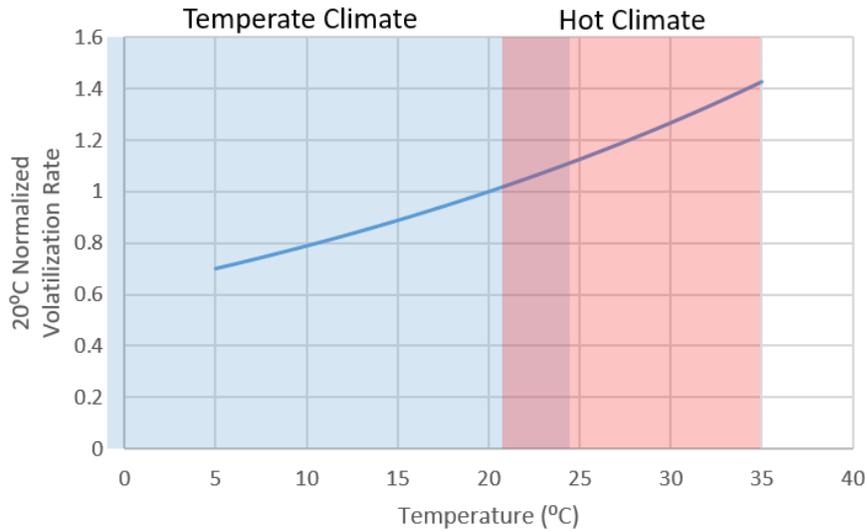


479

480 **Figure 11 Example Nitrification and Denitrification Temperature Response**

481 Another process significantly enhanced at higher temperatures is volatilization. While not an important
 482 process for nutrient or metals removal, volatilization can be important for the removal of volatile
 483 organic compounds, such as phenol, in FWS wetlands. An example of this the temperature effect on

484 volatilization is shown in Figure 12, which shows 20-30% increases in this wetland process in hot
485 climates.

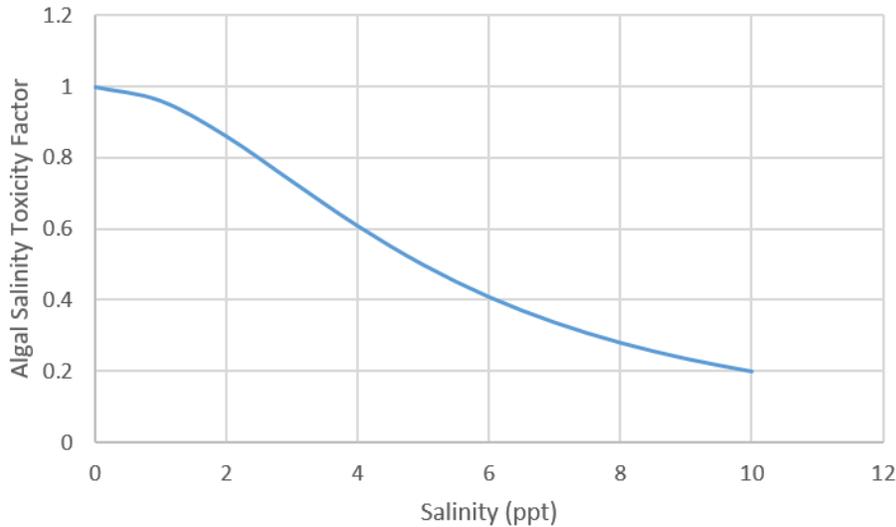


486

487 **Figure 12 Example Volatilization Temperature Response**

488 **4.1.2 Evapotranspiration**

489 Water loss through evapotranspiration in hot and arid climates will generally hinder CW performance as
490 the constituents in the water become more concentrated, making it more difficult to meet water reuse
491 standards. Another effect of this concentration of constituents is the increase in salinity, which can
492 retard algal growth. Figure 13 shows an example of the inhibitive effect of salinity on algal growth. To
493 put the effect into perspective, for a FWS in an arid region that experiences 20% water loss (and a
494 resulting salinity increase of 20%), algal growth may be inhibited by 5-25%.



495

496 **Figure 13 Example Algal Growth Salinity Response**

497

498 **5 MODEL LIMITATIONS**

499 The model development discussed in this report and the resulting model, CWM, is to be considered “in
 500 progress”. Development of the CWM is a stepwise, research-based modeling exercise. During the
 501 present stage, the model framework and algorithms have been developed and made functional.
 502 Subsequently, model formulations will need to be validated, model limitations analyzed and addressed,
 503 and model refinements made, before and during use in full-scale operations and design. As such, it is
 504 recognized that the present stage of model development is “experimental”, and future refinements of
 505 the model are anticipated. ERM and EMRQ are currently in the process of validating the CWM through
 506 its application to an existing wetland, as discussed later.

507 **6 CONCLUSIONS AND FUTURE WORK**

508 In 2020, a field data program was designed for the Nimr WTP with the purpose of providing data to
 509 allow simulation of the associated wetland through CWM. After collection and analysis of this data has
 510 been conducted, this data will be used to parameterize CWM inputs and begin calibration of the water

511 quality and vegetative components of the CWM to reproduce the observable data trends. The objective
512 of the application of CWM to Nimr WTP is to demonstrate the utility of the model to simulate
513 constructed wetlands at other locations to assist managers in the design of similar systems to achieve
514 suitable treatment of produced water for beneficial reuse. The results of these simulations will consist
515 of a follow-up paper documenting the application to the Nimr WTP and the utility of the CWM to further
516 the goal of constructed wetland design.

517 A mechanistic model was developed to evaluate the fate and transport of constituents throughout a
518 constructed wetland. The model is completely generalized in order to allow the user to simulate any
519 type of wetland, with any configuration, and any selection of material and plants. The model simulates
520 the majority of physical, chemical, and biological processes that occur in wetlands and are responsible
521 for the removal of constituents. The model was initially configured to simulate nutrients, metals, and a
522 wide variety of other water quality parameters, but is also flexible enough to allow the simulation of any
523 number of other constituents such as hydrophobic contaminants. The model relies on a large body of
524 existing literature to formulate each process.

525 At this time, the model has not been validated with a complete simulation of an actual wetland, however
526 a data collection program has been designed for the Nimr WTP constructed wetland in order to provide
527 a robust dataset to allow model testing, calibration, and validation. It is anticipated that the results of
528 this study and the corresponding model application will be published in subsequent paper(s) once
529 complete.

530 Upon evaluation of the accuracy and challenges of the model to reproduce an actual existing functional
531 wetland, the expectation is that the model can be used during the design phase of future constructed
532 wetlands as a tool to allow water treatment engineers to test various sizes, modes, configurations and
533 materials to arrive at optimal designs for their particular treatment needs.

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536 known competing financial interests or personal relationships that could have appeared to influence the
537 work reported in this paper.

538 **8** *CONFLICTS OF INTEREST*

539 There is no conflict of interest.

540 **9** *DATA AVAILABILITY*

541 Not applicable.

542 **10** *CODE AVAILABILITY*

543 The model will be part of the GEMSS model that is shared in limited capacity to universities, research
544 agencies, regulators and clients. Limited source code can be shared under separate sharing agreement.

545 **11** *AUTHOR CONTRIBUTIONS*

546 Prakash, Kolluru, Zahakos, and Saeed designed the study. Kolluru, Prakash, and Zahakos developed the
547 model. Zahakos wrote the article. Saeed, Prakash, and Prigent commented on draft versions of the
548 article. Varghese and Prigent assisted with data and logistics. All authors have approved the final article.

549 **12** *DISCLAIMER*

550 The authors alone are responsible for the views expressed in this publication and they do not necessarily
551 represent the views, decisions or policies of the ERM, EMRQ, or Bauer Resources.

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