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1 MODELLING CONSTRUCTED WETLANDS: SCOPES AND AIMS – 2 A COMPARATIVE REVIEW

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46 Keywords

47 constructed wetlands, model, modelling, simulation, review, comparison

48

49 Abstract

50 During the last two decades a couple of models were developed for constructed wetlands with
51 differing purposes. Meanwhile the usage of this kind of tool is generally accepted, but the
52 misuse of the models still confirms the skepticism. Generally some groups of models can be
53 distinguished: On one hand mechanistic models try to display the complex and diffuse
54 interaction of occurring processes, on the other hand the same kind of models are used to
55 investigate single processes. New kinds of ‘simplified’ approaches – well appreciated by
56 engineers - try to display system performances without going to deep into details. All types of
57 models are valuable – some more for scientific usage, others more for engineering. The given
58 summary tries to support potential users in taking the right choice in model selection. Big
59 differences can be found in the model availabilities. Whereas some of the compared software
60 packages are purchasable without limitation, some others are only accessible on their platform
61 level, and some can be seen as exclusive property. From the experience of the authors it can

62 be summarized, that research groups starting modelling / simulation studies should be
63 encouraged to use the given knowledge before starting from scratch again.

64

65 1. Introduction

66 Over the last two decades, an abundant literature has been published to present the modelling
67 efforts performed to simulate the main bio-geo-chemical processes occurring in constructed
68 wetlands (CWs). CWs can be built according to numerous designs - mostly linked to the flow,
69 which can be saturated/unsaturated, vertical/horizontal, surface/subsurface, and all the
70 possible combinations (See the latest nomenclature in Fonder and Headley, 2013).

71 In CW systems, pollutants are treated by a combination of physical, chemical and biological
72 processes. The biological removal of each category of pollutant is typically associated with a
73 specific microbial functional group. Pioneering modelling research works have employed
74 circumstantial evidence (black box approach) to compute these basic assumptions into models
75 mostly for domestic wastewater. Then mechanistic models have been developed trying to
76 consider the hydrodynamic and the biodegradation processes occurring in CW systems at the
77 same time for a larger range of sources of wastewater (industrial, diffuse, surface runoffs...)

78 The need for CW models can be summarized as follow:

- 79 - describing the phenomena ongoing in a CW system (e.g. water flow, adsorption, O₂
80 transfer)
- 81 - using models as a tool to compare 2 similar systems and their behavior under different
82 conditions (e.g. effect of loading characteristics, effect of plant species, effect of
83 season, etc.)
- 84 - predicting the performances of a given system (e.g. developing design
85 recommendations)
- 86 - answering “what if?” questions (e.g. over or under loads, etc.)

87 - performing system control (especially in case of system intensification like the use of
88 artificial aeration, recycling etc.)

89 In this context an increasing number of publications dealing with CW modelling has been
90 observed over the last 3 years (2011-2013) as it represents more than 38% of the number of
91 papers ever published containing the words “constructed/treatment wetland” and
92 “model/modelling” in the title (Science Direct research engine).

93 Among the most cited review papers, most of the most common modelling approaches of
94 CWs treating domestic wastewater, including biokinetic models and process models, have
95 been reported in Rousseau et al. (2004), Marsili-Libelli et al. (2005); Langergraber (2008);
96 Langergraber et al. (2009) and more recently Kumar and Zhao (2011).

97 Although the previous review efforts were performed to establish a non-exhaustive list of all
98 the modelling approaches successfully developed (including their main results), this review
99 paper aims at describing a sort of guideline to help users to choose the most appropriated
100 modelling approach adapted to their needs at different levels: the level of knowledge of the
101 process considered, the complexity associated to the model and its spatial resolution, and the
102 resources necessary to the usage of the reviewed models.

103 In 2013, in the frame of the 5th International Symposium on Wetland Pollutant Dynamics and
104 Control, WETPOL 2013, a wide range of recent simulation and modelling studies were
105 presented. Most of the concepts initially applied to CWs for pre-treated domestic wastewater
106 have been developed, adapted and applied to more and more case studies including for (raw)
107 domestic wastewater, combined sewer overflows (CSOs) and intensified CWs. All
108 publications from the WETPOL conference dealing with modelling and simulation were
109 selected for this review, and all main authors contributed to this paper.

110 The concepts selected in this paper mostly deal with three main approaches that can be ranked
111 as follows:

- 112 1) Biokinetic models: the most advanced models using saturated water flow are those
113 developed by Rousseau (2005) and Langergraber et al. (2009), both considering
114 bio-kinetic models that are based on the IWA Activated Sludge Models (ASMs)
115 (Henze et al., 2000). For modelling vertical flow CWs with intermittent loading,
116 transient variably-saturated flow models are required. These systems are highly
117 dynamic, adding requirements to the complexity of the overall system. The most
118 advanced reaction models are implemented in the Wetland Module of the
119 HYDRUS software package (Langergraber and Šimůnek, 2005), based again on
120 the mathematical formulation of the ASMs (Henze et al., 2000).
- 121 2) Process dedicated models, which rely on simple kinetics employed to model a
122 single process related to the degradation/transfer of one compound or one family
123 of compound (e.g. COD, NTK, O₂ etc.).
- 124 3) Design support models such as GPS-X, enabling to model the system according to
125 an initial Residence Time Distribution analysis; or RSF_Sim for the specific
126 context of combined sewer overflow treatment.

127 After a description on how the three main modelling approaches are implemented and
128 computed, this paper will describe the main reasons to choose one modelling strategy rather
129 than another, finally the paper will compare the pros and cons of each modelling strategy.

130

131 2. Material and methods

132 2.1. Description of models and simulation studies

133 Modelling begins with ideas and concepts for simplified descriptions of the real world.
134 Publications usually deal with new mathematical descriptions (models) and/or with model
135 applications (simulation). On conferences like Wetland Pollutant Dynamics and Control
136 (WETPOL) both are often put together in one session, but for a comparative review a

137 separation is required. In a first step of comparison, all participating publications were
 138 assorted in three differing groups: The first group contains applications of generally agreed
 139 biokinetic reaction models. The second group is dedicated to models focusing on single
 140 processes or phenomena within the diffuse and complex interactions of real processes in
 141 CWs. The third group was chosen for a new generation of modelling approaches aiming more
 142 at engineering than on science.

Table 1: Reviewed modelling and simulation studies overview

Contributing modelling / simulation study	Model used	Water Flow	Biochemical processes		Additional processes	Dimension
			Species considered	Reactions		
Pálffy and Langergraber, 2013	HYDRUS/CW2D	Saturated and unsaturated (Richards eq.)	12, incl. forms of COD, N and P	9		2D
Morvannou, 2012	HYDRUS/CW2D	Saturated and unsaturated (Richards eq.)	12, incl. forms of COD, N and P	9	Ammonium adsorption	2D
Pálffy and Langergraber, 2014	HYDRUS/CWM1	Saturated and unsaturated (Richards eq.)	16, incl. forms of COD, N and S	17	Heat transfer and root effects	2D
Rizzo et al., 2014	HYDRUS/CWM1	Saturated and unsaturated (Richards eq.)	16, incl. forms of COD, N and S	17	Ammonium adsorption	2D
Samsó and Garcia, 2013a,b	BIO_PORE (COMSOL Multiphysics™)	Saturated (Darcy + adapting water table level)	18, incl. forms of COD, N and S	17	Root effects	2D
Petitjean et al., 2012 Forquet et al., 2009a,b	Diph_M (MATLAB)	Unsaturated (two-phase flow)	forms of COD, NH ₄ -N, oxygen	5		1D
Morvannou et al., 2013	Dual-porosity model (DPM) in HYDRUS-1D	Saturated, unsaturated and preferential (Richards eq. + dual porosity)	0	0	Non-reactive tracer transport	1D
Claveau-Mallet et al., 2012, 2014	PHREEQC P-hydroslog	Saturated	post treatment, no biochemical model	0	4 inorganic reactions	1D
Sani et al., 2013	Wang-Scholz-Model (COMSOL)	Vertical-flow wetlands with uniform water flow	no biochemical model	0	Clogging processes (particle setting)	1D
Zeng et al., 2013a,b	RTD/GPS-X	Tanks in series with recycle and dead volumes under variable water content	12, incl. forms of COD, N (only soluble)	11	Interaction with biofilm growth	2D
Meyer and Dittmer, 2014	RSF_Sim	Tanks in series with variable water content	no biochemical model	0	transport, filtration, adsorption, degradation	1D, 1.5D in future?

143
 144 Table 1 gives an overview of the studies contributing to the given review, including
 145 abbreviations. Short descriptions of the used models and the according studies presented
 146 during WETPOL 2013 (or published in journals previously) can be found thereafter.

147 **2.1.1. Group 1: CWM1 and CW2D in HYDRUS and BIO_PORE**

148 The HYDRUS Wetland Module and BIO_PORE are general mechanistic models and both use
 149 biokinetic models inspired by the Activated Sludge Models (ASMs) for simulating biological
 150 transformation and degradation processes and microbial dynamics in subsurface flow
 151 constructed wetlands: the Constructed Wetland Model 2D (CW2D) (Langergraber and
 152 Šimůnek, 2005) and the Constructed Wetland Model N°1 (CWM1) (Langergraber et al.,

153 2009). Both CWM1 and CW2D are implemented in the HYDRUS software (Langergraber
154 and Šimůnek, 2012) while a modified version of CWM1 is implemented in the COMSOL
155 MultiphysicsTM platform for the BIO_PORE model (Samsó and Garcia, 2013a). CWM1 and
156 CW2D include the biochemical degradation and transformation processes for organic matter
157 and nitrogen and additionally for phosphorus in CW2D and sulfur in CWM1 with the main
158 objective to predict effluent concentrations. CW2D is suitable to the VFCWs modelling as it
159 considers aerobic and anoxic biokinetic processes. In addition, CWM1 considers the
160 anaerobic biokinetic processes and therefore it is appropriate for both HF and VF CWs.

161 The CW2D requires a total of 46 parameters to solve the equations describing 9 different
162 processes. For each element of the model, 12 variables are calculated: 9 for the liquid phase
163 and 3 for the biomass which is immobile and therefore exclusively associated with the solid
164 phase (heterotrophic and two autotrophic bacteria groups).

165 The CWM1 is more complex as it also takes anaerobic reactions into account. It considers 17
166 processes and 16 components (8 soluble and 8 particulate out of which 6 represent bacteria
167 groups). It requires a total of 65 parameters.

168 As a distinctive feature from the original CWM1's formulation, slowly biodegradable and
169 inert particulate COD are divided into aqueous and solid phases in BIO_PORE which allows
170 describing their retention and re-suspension. Moreover, the unlimited and unrealistic
171 exponential growth of biomass affecting most of the available CW models based on the ASM
172 formulation is avoided in BIO_PORE model by including two logistic functions in the growth
173 expressions of all functional bacterial groups. These two functions take into account the
174 carrying capacity of the system and the presence of accumulated inert solids on the growth
175 rate of bacteria (Samsó and García, 2014a).

176 The biokinetic equation set has to be coupled with water flow, solute and heat transport
177 models to simulate the operation of CWs. This is done in HYDRUS by solving the Richards
178 equation describing capillary-driven flow in variably-saturated porous media and equations

179 describing convective-dispersive transport of solute and heat and diffusion in the gaseous
180 phase. Another sub-model of HYDRUS is the root model describing water and solute uptake
181 and oxygen release (Šimůnek et al. 2012).

182 Regarding BIO_PORE, the flux of water is described by combining the Darcy's equation with
183 a mass-balance equation to determine the exact location of the water table at each time. This
184 strategy was adopted to avoid the growth of bacteria in the unsaturated areas of the bed. All
185 these models were spatially discretized in a two-dimensional domain.

186 Among the five studies carried out using the two described mechanistic models, Morvannou
187 (2012) as well as Pálffy and Langergraber (2013) employed CW2D in HYDRUS, Rizzo et al.
188 (2014) as well as Pálffy and Langergraber (2014) employed CWM1 in HYDRUS, and Samsó
189 and Garcia (2013a,b) presented CWM1 in BIO_PORE.

190 Pálffy and Langergraber (2013) aimed at designing a HFCW for polishing treatment of the
191 outlet of a sequencing batch reactor (SBR). Despite it was used to simulate a HFCW, CW2D
192 was preferred over CWM1 as it includes phosphorus removal processes. Furthermore if the
193 organic load is low, the filter will remain in anoxic conditions justifying the choice to be put
194 on CW2D.

195 Morvannou et al. (2014) applied CW2D to a French-type VFCW (Molle et al., 2005).
196 Particular emphasis was given to the modelling of ammonium removal. Therefore linear
197 adsorption was taken into account with a value changing according to the organic matter
198 content. Furthermore one biokinetic parameter was estimated based on a solid respirometric
199 method (Morvannou et al., 2011). The model was calibrated over a two-week dataset
200 including continuous measurements of inlet and outlet pollutant concentrations.

201 Pálffy and Langergraber (2014) presented simulations of water-saturated batch operated
202 mesocosms. The aim was to verify the biokinetic sub-model only, the CWM1 implementation
203 in HYDRUS. Using data from controlled greenhouse column experiments, the effects linked
204 to water flow, heat transport and other processes occurring in an uncontrolled environment

205 were excluded. The numerical results were calibrated on experimental data by iteratively
206 adjusting the biokinetic parameters. The results were evaluated by a new goodness of fit
207 analysis method, the deflection analysis.

208 Based on HFCW experimental results (Galvão and Matos, 2012), Rizzo et al. (2014) explored
209 the capability of the HYDRUS Wetland Module to model the response of HFCW to unsteady
210 load. In addition to the biokinetic processes in CWM1, Rizzo et al. (2014) included
211 ammonium adsorption using a Langmuir isotherm. Qualitative comparisons were carried out
212 between simulated and measured effluent concentrations of COD and NH₄-N by calculating
213 the mean percentage error.

214 The BIO_PORE model was calibrated using data from the first operation year of a pilot-scale
215 HFCW (Samsó and Garcia, 2013a). Then the simulation was extended over a 3-years period
216 in order to qualitatively describe the bacteria communities distribution and dynamics (Samsó
217 and Garcia, 2013b). In Samsó and García (2014a), the necessity of limiting the growth of
218 bacterial communities when using ASM-based models is justified and a theory to describe the
219 most basic functioning patterns of HFCWs, namely The Cartridge Theory, is presented.

220

221 **2.1.2. Group 2: Process-dedicated models**

222 Besides displaying process interactions, mechanistic models can also be used to gain in-depth
223 understanding of a particular phenomenon. Some researchers carried out specific simulations
224 for this purpose: Petitjean et al. (2011, 2012) and Forquet et al. (2009a,b) investigated the
225 influence of the air phase on hydrodynamics (Diph_M), Morvannou et al. (2013) focused on
226 non-equilibrium flow in French-type VFCW with the dual-porosity model (DPM), Claveau-
227 Mallet et al. (2012, 2014) studied the phosphorus removal by precipitation in steel slag filters
228 (P-hydroslag) and Sani et al. (2013) investigated particulate transport (Wang-Scholz-Model).

229 The new model called Diph_M was used to describe the interplay between gaseous oxygen
230 and bacteria during the feeding of a second-stage vertical-flow sand filter. Under partly-
231 saturated conditions, feeding involving ponding leads to water flow disturbance by the air
232 phase. In order to overcome this issue, Forquet et al. (2009a,b) implemented a 1D numerical
233 model in MATLAB which solves simultaneously the Richard's equation for both the air and
234 the water phases. Aside from improving the hydrodynamic description of the filter, this model
235 permits an accurate estimation of the gaseous fluxes within the filter. Petitjean et al. (2011,
236 2012) coupled a hydrodynamic set of equations solving reactive transport according to the
237 ASM1 model.

238 The dual-porosity model DPM was developed to simulate the preferential flows occurring in
239 gravel filters. A dual-porosity hydraulic model (Šimůnek and van Genuchten, 2008) was
240 chosen in Hydrus-1D (Šimůnek et al., 2013) with a mass-exchange coefficient proportional to
241 the water content. The model assumes that the water phase is divided between a mobile part
242 (in our case the macroscopic pores) and an immobile part (water contained in the organic
243 matter matrix and also some capillary water). The flow only occurs in the mobile part but
244 exchanges are possible between the two water parts. The model was fitted versus a tracer test
245 experiment carried out on a French first-stage VFCW.

246 The conceptual model used in P-hydroslag focuses on tertiary treatment with enhanced
247 requirements of phosphorus removal. It is based on slag dissolution and hydroxyapatite
248 ($\text{Ca}_5(\text{PO}_4)_3\text{OH}$) crystallization rates. It included three steps: (i) dissolution of slag as Calcium
249 oxide (CaO), (ii) phosphorus precipitation and crystal growth in alkaline conditions, (iii)
250 evolution of slag filter properties (slag dissolution rate, porosity and hydraulic conductivity)
251 related to slag exhaustion and to the presence of crystals (Claveau-Mallet et al.; 2012). The
252 conceptual model was mathematically expressed in a 1D geochemical model including
253 equilibrium and rates (Claveau-Mallet et al., 2014). The software PHREEQC was used for
254 numerical simulations. The slag dissolution equations were determined from a simple

255 experimental batch test. Numerical simulations of a 1D filter were run and the evolution of
256 phosphorus concentration at the outlet of the system was computed.

257 The Civil Engineering Research Group at The University of Salford used a 1-D model for
258 particulate transport in a VFCW implemented in COMSOL MultiphysicsTM. It has initially
259 been introduced by Sani et al. (2013). Wastewater contains waste particles of different size
260 and composition. As these particles build up within the filters, the efficiency of subsequent
261 removal is reduced due to the decrease in pore space. Some particles are electro-statically
262 attracted and stack onto each other, often forming dendrites. These dendrites block the pore
263 space, thus increasing particle interception. The proposed Wang-Scholz Model assumes a
264 uniform water velocity throughout a saturated column, which was experimentally estimated
265 using Darcy's law. The model aims at estimating particle settling in the porous media. Three
266 major mechanisms that affect the particle transport in the filter were taken into consideration,
267 namely, dispersion, sedimentation and adsorption of particles. Sedimentation process can be
268 divided into three major mechanisms: settling and deposition, aggregation of SS via
269 coagulation, and mass exchange between SS and the dissolved phase. Because of its relatively
270 slow rate the latter can be treated separately and is not taken into account in the current
271 model.

272

273 **2.1.3. Group 3: Design support models**

274 RTD/GPS-X employs a two-step model coupling hydraulic and kinetic modelling on fixed
275 bed aerated biofilm reactors. Despite it relies on the ASM1 model for biokinetic reactions
276 which clearly is a mechanistic model, we choose to classify it among design support models
277 because of the chosen hydraulic model. It is based on Residence Time Distribution analysis
278 (tracer injection and detection) carried out on different steps of biofilm development in the
279 reactor. Based on the shape of the breakthrough curves, a hydraulic model is chosen (among

280 models like Plug Flow, Tank in Series, Tank in Series with exchange) regarding saturation
281 conditions and biofilm development (Zeng et al, 2013a). This first step aims at determining
282 hydraulic parameters like number of tanks in series, type of tanks (plug flow or perfectly
283 mixed), average retention time, dead volume, recycle ratio and actual volume of the reactor.
284 These parameters are then implemented in GPS-X software to simulate biodegradation
285 processes (Zeng et al, 2013b). The biokinetic model chosen in GPS-X is a 2-step nitrogen
286 model based on ASM in a biofilm reactor with biofilm diffusion fraction for substrates (Vigne
287 et al, 2010). It is then calibrated with experimental kinetic parameters from different heights
288 of the fixed bed biofilm reactor. Finally this model simulates TOC removal and several NH₄-
289 N conversion processes taking into account biofilm development, oxygen concentration,
290 water saturation level and height of the biofilter.

291 Meyer and Dittmer (2014) presented the model RSF_Sim, which was created in order to
292 estimate long-term treatment performance of constructed wetlands for combined sewer
293 overflow treatment (CSO-CWs), also known as Retention Soil Filters (RSFs). The
294 development of RSF_Sim (Meyer and Dittmer, 2014) was based on a fundamental research
295 study (Dittmer and Schmitt, 2011), but also on experiences in the application of HYDRUS-
296 2D/CW2D (Dittmer et al., 2005; Henrichs et al., 2007, 2009; Meyer et al., 2006; Pálffy et al.,
297 2014). CW2D was generally applicable to simulate laboratory RSF column operation, but
298 extended dry periods exceeded the ability of reasonable nutrient/biomass balances due to the
299 missing description of particulate organic matter degradation.

300 RSF_Sim works with three complete stirred tanks in vertical series: [1] the retention layer
301 provides the water storage on top of the process layer (ponding), [2] the process layer
302 describes the sand/gravel layer (saturated during feeding, drained afterwards) in which
303 treatment occurs, [3] the drainage layer improves the volume balances (German model
304 version), but can also be used as a water reservoir under permanent saturation (French model
305 version) (Meyer et al., 2013).

306 Up to date, descriptions of treatment performances for COD and NH₄-N are kept basically
307 simple. The total COD needs to be separated into two fractions: particulate COD becomes
308 reduced by filtration (down to a background concentration), dissolved COD is reduced by a
309 treatment efficiency factor, which can vary due to influencing factors like temperature,
310 outflow limitation rates or the duration of previous dry periods (most important). The
311 retention of NH₄-N during the filter passage is calculated with a steady-state two-stage linear
312 isotherm, nitrification is considered only after re-aeration by 1st order kinetics (Meyer et al.,
313 2014).

314

315 2.2. Model comparison

316 In this section, the aim was not to provide performance comparison based on benchmark tests
317 but rather to provide guidance so that a new user may choose the appropriate model for
318 simulating constructed wetland behavior. We proposed a three-step method based on (i) the
319 type of constructed wetland the user is interested in, (ii) the objectives of the study, and (iii)
320 the resources dedicated to modelling.

321 In the first step, we associated the models with different types of constructed wetlands,
322 themselves classified in two categories: saturated or variably-saturated, similarly to what was
323 suggested by Fonder and Headley (2013).

324 The second step allows classifying the models based on the user goals. The first criterion is
325 whether the study aims at understanding the processes or at designing new systems. It also
326 gives an idea about the complexity associated with the model and its spatial resolution. The
327 second criterion is whether short or long-term simulation will be performed.

328 Finally, the user must take into account the resources necessary to the usage of the reviewed
329 models. They are expressed in terms of the user training level, the price of the model software
330 or of the modelling platform, and the level of development of the model and its associated

331 documentation (since it requires additional efforts to work with an uncompleted or poorly
 332 documented model).

333

334 3. Results of model comparison

335 3.1. Classification

336 Models and simulation studies participating to this review show a broad bandwidth of aims
 337 and scopes. In order to summarize the findings of comparisons it seems to be important to
 338 classify the tools and their applications. Modelling approaches range from a simple regression
 339 to a partial differential equations model (PDE). Description of these has already been
 340 discussed in previous papers (Kumar and Zhao, 2011, Langergraber et al., 2009). Models
 341 presented at the 2013 WETPOL symposium can be mainly found in the category of PDE
 342 models at the exception of RSF_Sim which is basically tank-in-series description.

343

344 3.2. Fields and limits of application

Table 2: Model comparison overview

Model used	Field of application	Required input data	Model availability
HYDRUS-2D CW2D/CWM1	Developed for HFCWs and VFCWs treating domestic wastewater, but was also applied for e.g. CSO-CWs, CWs treating artificial wastewater, hillslopes	a) Filter material parameters for proper water flow characterization (VFCWs: unsaturated most important) b) Characterization of the inflow in terms of i) diurnal variations and ii) fractionation of COD, N, P, S, species based on the selected biokinetic model	The HYDRUS Wetland Module is commercially available as part of the HYDRUS software.
BIO_PORE (COMSOL Multiphysics™)	HSSFCWs treating domestic wastewater	Inflow pollutant concentrations (fractionated COD), water temperature, flow rates, granular media properties	Open access, on demand
Diph_M (MATLAB)	VFCW: 2nd stage of 'French design' CWs 1st stage VFCW after septic tank	Soil and air parameters, dynamic hydraulic and pollutant loads	Open access, on demand
HYDRUS-1D – Dual-porosity	Modelling of preferential flows in first-stage of French VFCW	Inflow and outflow, water contents and pressure head at different filter depths, tracer test	The HYDRUS software is commercially available
PHREEQC P-hydroslag	Post treatment steel slag filters	a) Dissolution kinetic parameters of slag based on a short-term batch test b) Characterization of inorganic inflow compounds	Currently not commercially available
Wang-Scholz Model (COMSOL Multiphysics™)	The model should be applied to wetland systems where clogging is considered to be a potential problem.	Particle (usually suspended solids) transportation, retention and distribution	Used for research purposes, currently not commercially available, general methodology is in the public domain
RTD/GPS-X	Design and optimization of deep zones of CW (treatment due to bacterial processes)	a) Characterization of soluble inflow compounds b) Retention time distribution profiles	Used for research purpose, not commercially available but using commercial software GPS-X
RSF_Sim	Dimensioning and optimization of operation of CWs for combined sewer overflow treatment	Measured or simulated dynamic CSO data, filter media characteristics, treatment performances	Open access for scientific purpose, implementation into commercial sewer system software in progress (France)

345

346

347 **3.2.1. Group 1: the HYDRUS Wetland Module and BIO_PORE**

348 On one hand the HYDRUS Wetland Module might be too complex to be directly used for
349 design purposes (table 2), meaning that the money and effort invested into it cannot be easily
350 justified. In some countries standards are limiting the design to be based on rules of thumbs,
351 e.g. the Austrian standard, ÖNORM B 2505 (2009), making the design-purpose use of
352 numerical models with such complexity impossible. For these reasons the HYDRUS Wetland
353 Module can be primarily suggested for research purposes and for creating simplified models
354 based on them. There will always be options to test new fields of application on the edge or
355 outside of the original scopes. For instance, Rizzo et al. (2014) have demonstrated that the
356 HYDRUS Wetland Module with CWM1 is able to adequately simulate performances of
357 laboratory horizontal flow CWs loaded with artificial wastewater that are subjected to
358 unsteady loads using data from Galvao and Matos (2012). Also the studies using CW2D for
359 simulation of CSO-CWs (Dittmer et al., 2005; Meyer et al., 2006; Henrichs et al., 2007, 2009)
360 and for simulating nitrate dynamics in a rural headwater catchment (Smethurst et al., 2013)
361 exceeded the original scope of the model.

362 On the other hand, Pálffy and Langergraber (2014) demonstrated a case in which the
363 HYDRUS Wetland Module with CW2D facilitated the design of a HF CW for polishing the
364 effluent of a sequencing batch reactor with 700 m³ per day peak capacity. This suggests that
365 the scale of the project and the characteristics of the wastewater might justify the use of
366 complex tools similar to CW2D or CWM1.

367 Samsó and García (2014a) pointed out possible weak points of the equations describing
368 biokinetics in ASM-based models (including CWM1 and CW2D) and showed that the
369 BIO_PORE model also includes the possibility to simulate the accumulation of inert organics
370 in long term scenarios.

371 Similar to the HYDRUS Wetland Module, the BIO_PORE software (Samsó and García,
372 2013a) is dedicated to a) simulate the hydraulics and hydrodynamics of wetlands, b) simulate
373 the contribution of plants to the treatment of water, c) predict effluent pollutant concentrations
374 in HFCWs, d) study the location and dynamics of bacterial communities in HFCWs, and e)
375 improve the understanding of wetlands. BIO_PORE was not developed for design purposes,
376 but it supports understanding of the functioning. A special emphasis is given on the prediction
377 of failures, which correspond to the time in which bacterial communities are pushed that
378 much towards the outlet by the accumulation of inert solids that they are not able to consume
379 the desirable proportion of influent pollutants (cartridge theory, Samsó and García, 2014a).
380 The main weakness of BIO_PORE can be found in the missing link between biofilm growth
381 and changes in hydraulics, because it still does not include clogging. Not more than 3 to 5
382 years (after which clogging is generally more evident) can be simulated with certain
383 guarantees.

384 Although it is not yet implemented in BIO_PORE, Samsó (2014c) presents a mathematical
385 formulation to simulate the effects of clogging in the hydraulics and hydrodynamics of CWs,
386 which also allows simulating the runoff generated as a result of severe clogging.

387 In the application of biokinetic reaction models like CWM1 or CW2D, a general limitation is
388 the lack of proper data to verify simulation results. For instance, Rizzo et al. (2014)
389 highlighted that acetate was found as the main effluent COD component during peak influent
390 events. These results could not be validated due to the lack of experimental data for COD
391 fractionation. However, although the experiments by Galvao and Matos (2012) have not been
392 designed with a modelling exercise in mind, Rizzo et al. (2014) could simulate their results.
393 This study also showed that there is a need for planning experiments in a different way (e.g.
394 sampling frequency, parameters analyzed) when dynamic models should be applied.

395

396 **3.2.2. Group 2: Process-dedicated models**

397 In contrast to ‘black box’ approaches such as multiple regression modelling, principal
398 component analysis, redundancy analysis, and the self-organizing map modelling (Dong et al,
399 2012), process-dedicated models offer a better understanding of the underlying science within
400 a wetland. For example, within the Wang-Scholz Model, the particle sedimentation process
401 and its effect on clogging can be modeled predominantly based on SS accumulation inside the
402 CWs.

403 Clogging processes within constructed wetlands are complex. They are difficult to be
404 quantified by representative values without destroying the wetland filter or interfering with its
405 operation. Values obtained from the literature have been used for parameters where no
406 measurements were available. The experimental CWs do not operate in continuous inflow
407 mode, because they are drained and refilled at fixed intervals. For simplification, a pseudo
408 convection velocity of wastewater is assumed to represent the average rate of the water
409 change in the whole year.

410 The Wang-Scholz Model has been applied to simulate the SS sedimentation processes within
411 experimental CWs. The relatively good results (Sani et al., 2013) demonstrate that the four
412 mechanisms (i.e. diffusion, convection, sedimentation and pebble surface adsorption) may
413 play the main role in the SS transport in vertical-flow wetland systems. It can be seen from
414 the characterized modelling parameters that the pebble surface adsorption takes the most
415 prominent effect on SS filtering or interception. An average approach ignoring the varied
416 particle sizes and the discontinuous inflow works effectively for modelling the water
417 treatment using small scale vertical-flow wetland systems. However, the Wang-Scholz Model
418 consistently under-predicts the SS concentrations within the litter zones. This can be
419 explained by the fact that the model does not account for biological growth and decay of plant
420 matter. Nevertheless, the model is also useful to distinguish between physical and
421 biochemical process influences.

422 The diphasic model Diph_M is a research oriented type of mechanistic model. It is focusing
423 on single process understanding (2nd stage kinds of VFCWs), without any aim of sizing or
424 even treatment yields estimation. It was validated separately for flow and transport
425 phenomena using experimental data. Results gave better insights on oxygen transport inside
426 VFCWs (Forquet et al., 2009, Petitjean et al. 2012). Apart from that, the benefits of
427 development can be found in a long-term perspective when this specific part will be
428 implemented into more general mechanistic models. Right now it is used to evaluate the
429 prominence of processes as a sound tool for the study of systems in which strongly
430 interdependent phenomena are occurring.

431 The P-hydroslag model shall be used to a) predict P concentration evolution at the outlet of a
432 slag filter, b) predict concentration evolution of other compounds of interest (pH, Ca, etc), c)
433 predict the longevity [d] and the retention capacity [mg P / g slag] of a given slag filter, and d)
434 evaluate the influence of operating parameters as the type of slag, hydraulic retention, type of
435 voids and the composition of wastewater on the performance and longevity of the system.
436 Limits of this first approach can be found in the fact that the actual model does not consider
437 porosity reduction of the filter related to precipitate accumulation. It also does not consider
438 the limiting effect of crystal accumulation on slag dissolution. Accordingly the actual model
439 probably overestimates longevity and retention capacity.

440 In order to reach a high number of users, the P-hydroslag the model is reasonably complex as
441 it involves simplifications which are: i) the wide variability of slag composition resulting in
442 different reactivity is simplified by a CaO dissolution reaction with a rate decreasing over
443 time, ii) precipitation rates are simplified to basis expressions with good experimental fitting,
444 and iii) the initial model considered only hydroxyapatite, but its accuracy was greatly
445 improved when monetite and its transformation to hydroxyapatite were added (Claveau-
446 Mallet et al., 2014).

447 The dual-porosity model (DPM) uses a larger number of hydraulic parameters than the simple
448 hydraulic model (equilibrium model) in HYDRUS-1D, which makes it more complex to use.
449 Moreover, among those parameters, some are difficult or even impossible to measure. Only a
450 calibration carried out from outflow data combined with tracer tests as well as measurements
451 of water contents and pressure heads within the filter allows their determination. In DPM, no
452 flow in the immobile phase is considered. Only exchanges between mobile and immobile
453 phases are taken into account. The dual-permeability model simulates flows in both phases,
454 but it involves a larger number of hydraulic parameters to be calibrated, which further
455 complicates their determination. On the other hand, as the water flow through a first-stage of
456 French VFCW is mainly gravity-driven (in the macro pores), it may be preferable to turn
457 towards models where preferential flows are described by the Kinematic Wave equation
458 (Larsbo and Jarvis, 2003). These models are tailored to soils with macro pores or heavy clay
459 soils with distinct shrinkage cracks.

460

461 **3.2.3. Group 3: Design support models**

462 The RTD/GPS-X model (Soric et al., 2013) allows a) predicting C and N concentrations at
463 different depths of the biofilters, b) predicting actual and dead volumes evolution i.e.
464 hydraulic behavior taking into account biofilm development and saturation conditions, and c)
465 evaluating the influence of hydraulic loading rate on TOC and TN removal. By this, the
466 model aims to be used to improve wetland design and operation. So far, RTD/GPS-X has
467 been calibrated with experimental data from a biofilm reactor fed with surrogate-filtered
468 wastewater (no particles), so mass transfers were only correlated to soluble substrates. The
469 only clogging process taken into account was biological clogging due to biofilm development.
470 The contribution of the plants was not taken into account, so RTD/GPS-X is only applicable
471 to the deep zones of CWs and for bacterial activity yet. As soluble C and N are removed

472 essentially by bacterial processes, this model should provide good simulation results for CW
473 design regarding this kind of species.

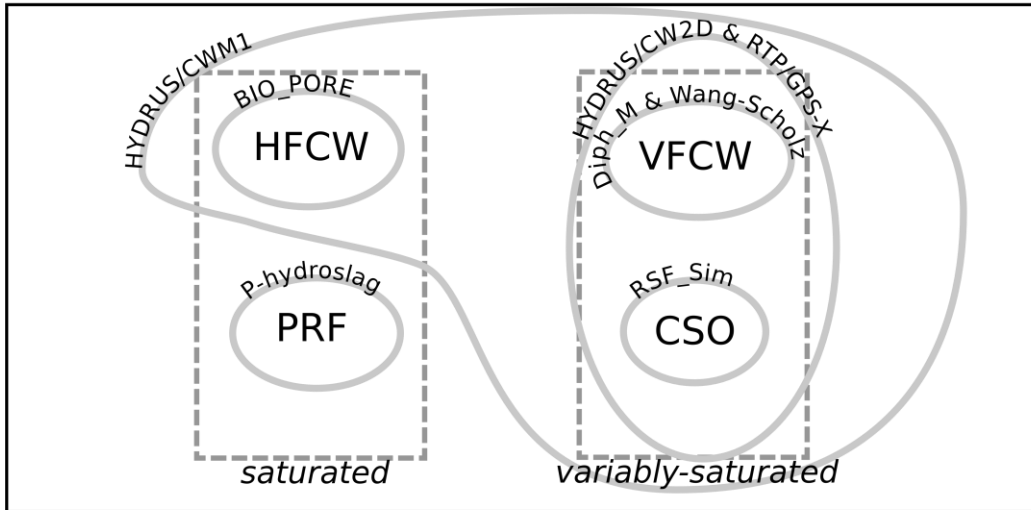
474 The main aim of RSF_Sim can be found in long-term estimations of RSF performances. This
475 seems to be useful due to the fact that RSF design is always requiring sewer system
476 simulation (Meyer et al., 2013, 2014). Whereas nowadays hydraulic loads are considered as
477 main design criteria, future approaches should take the pollutant loads and treatment
478 capabilities into account. The according new engineering tool needs simple usage, even with a
479 sophisticated background originated from the application of mechanistic models. The number
480 of required input parameters was kept very small, and initial values can be found easily in
481 literature sources. The tool can be used with measured data, as well as with input originated
482 from pollution load sewer system simulations.

483 The application of RSF_Sim allows estimating treatment performances in a long-term view.
484 Successful applications of RSF_Sim are based on the existing high number of calibrations and
485 validations. Single events can be calibrated on additional measured data, but a detailed
486 prediction of treatment failures will never be possible. It needs to be considered, that CSOs
487 and treatment wetlands underlie local variations. Thus, under-performances need to be
488 expected within a certain range, and safety factors should be considered. In a global view, the
489 accuracy of CSO-CW simulation results is heavily depending on the quality of the sewer
490 system simulations. Thereby, the filter operation cannot be described more accurately than the
491 according sewer system, including assumptions concerning the catchment area.

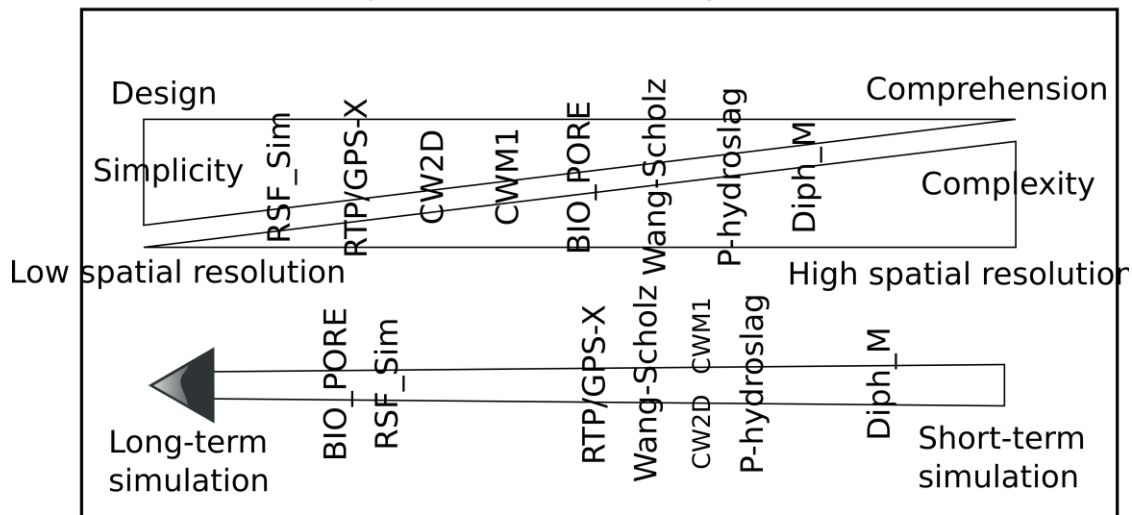
492

493 3.3. Graphical comparison and model selection support

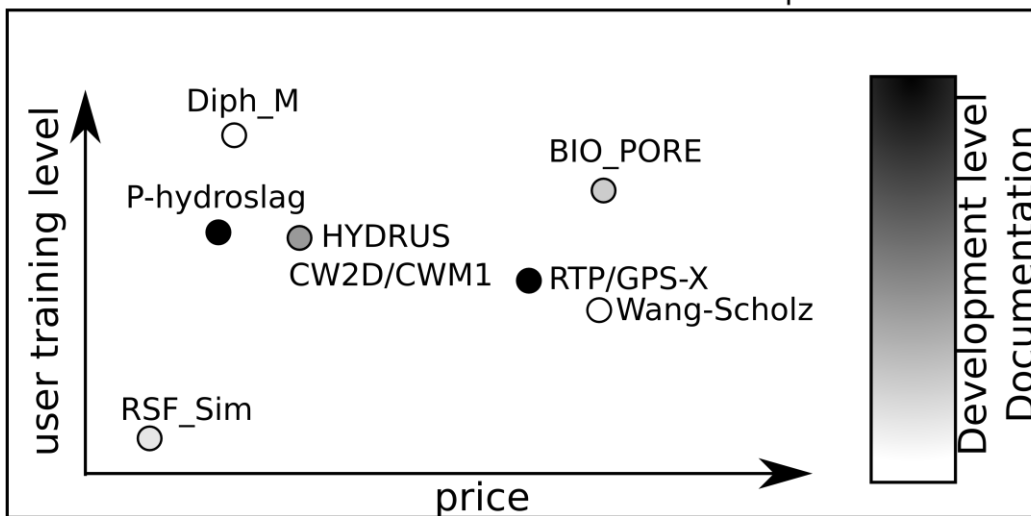
Step 1: Which model for your system?



Step 2: Which model fits your needs?



STEP 3: Which resources are required?



494

495 Figure 1: Flow chart of proper model selection

496

497 4. Discussion and outlook

498 4.1. Balancing complexity and practicable handling

499 From a basic point of view, model complexity needs to be increased in order to get closer to
500 reality. By this also the number of equations and thereby the number of required input
501 parameters increases. Considering the efforts for investigation and selection of proper input
502 values, the increase of complexity can be seen as the opposite of practicable handling. High
503 quality models show a reasonable balance.

504 CW2D and CWM1 have been widely applied in the past, and convincing simulation results
505 increased the acceptance of CW models in general. Although both CW2D and CWM1 are
506 complex process-based tools, they should be improved in some aspects. CW2D does not
507 involve anaerobic processes which is already a limitation of the application field.
508 Incorporating these processes might decrease the practicable handling as other functional
509 bacterial groups and COD fractions should be added. CWM1 was intended to be a general
510 tool for CW modelling and it already includes anaerobic processes, bacterial groups and the
511 suitable COD fractionation. Increasing model complexity with adding phosphorus forms to
512 the components could broaden possible application fields and would not decrease
513 practicability. Samsó and Garcia (2013a,b) state that BIO_PORE is a model intended for
514 scientific purposes, so the more complexity and the more processes considered the better.
515 With the current computational capacity, the maximum possible complexity is only limited by
516 the users' capacity to interpret the results (Samsó et al., 2014b).

517 The developers of the process dedicated models (group 2) state that their scientific approaches
518 do not aim at practicable handling on first hand, but some see it as an important characteristic.
519 For Diph_M a very detailed description is targeted, and a high number of parameters is
520 accepted. In comparison, the Wang-Scholz Model could be developed further; e.g., a
521 decreased model complexity will make the model more focused and therefore relevant to

522 more practitioners. The P-hydroslag model can be easily upgraded with additional equations
523 when needed, by example calcite precipitation if the wastewater contains a high concentration
524 of inorganic carbon. The main complexity challenge can be found in the description of crystal
525 structures within the filter affecting the dissolution rate of slag (Claveau-Mallet et al.; 2012).
526 As hydroxyapatite crystal structures are diversified (hydroxyapatite is also a biological
527 product!), finding a realistic and simple mathematical equation that represents the "crystal
528 barrier" for slag dissolution is challenging.

529 For the design support models like and RSF_Sim (group 3) the idea was to develop easy to
530 use tools with good balances between simplification and simulation result quality. RTD/GPS-
531 X model is based on user-friendly software that makes it easy to use once it has been
532 accurately calibrated. The calibration step can be complex but the final use of the model
533 should remain easy. However the model needs to be upgraded with particulate matter
534 equations to fit full-size treatment units. For RSF_Sim, the low level of complexity can be
535 seen as a main quality. In this way, an increased complexity would counter the model
536 purpose. On the other hand, a more detailed background based on stochastic data analysis –
537 not affecting the usability – would give benefits to the application.

538

539 4.2. Current fields of model improvement and extended application

540 The latest verification of the CWM1 implementation in the HYDRUS Wetland Module (Pálffy
541 and Langergraber, 2013) needed three parameters to be adjusted for each experimental
542 column: (1) initial bacterial concentrations, (2) initial adsorbed NH₄-N concentrations, and
543 (3) cRoot, the parameter determining root re-aeration rate. Bacterium concentrations have a
544 great effect on wetland performance. A method which can measure the concentration of active
545 bacteria in microcosms and link the activity to groups identical to those found in process-

546 based numerical models could help to decrease uncertainty around biokinetic parameter
547 values and changes in bacterium communities.

548 Results from Rizzo et al. (2014) suggest that the HYDRUS Wetland Module is a suitable tool
549 to study HFCWs under time-variable flows, opening new possible future applications. Among
550 these, the stochastic behavior of HFCW outflows is of great interest. Indeed, the randomness
551 of HF CW effluent is generally neglected during the typical design procedure, and the HFCW
552 size should be highly overestimated to face real outflow variability (Kadlec and Wallace,
553 2009). In this context, HFCW effluent stochastics could be simulated by HYDRUS-CWM1.
554 For instance, a HFCW could be forced by stochastic influent loads modeled as noisy signals
555 (Ridolfi et al., 2011), allowing to investigate if the randomness of effluent is driven by the
556 variability of inflows. Moreover, users could investigate if the implementation of noisy signal
557 technique could improve the HFCW design procedure.

558 Needs for further development of the HYDRUS wetland module can be found in a clogging
559 model (particle transport and influence on hydraulic properties), in a dual-porosity flow
560 model coupled with Wetland Module to simulate preferential flow, and finally in active and
561 passive uptake functions of HYDRUS to be made available in the HYDRUS Wetland
562 Module.

563 In BIO_PORE, the biokinetic models are considered to be the most important part, just as
564 bacteria are the most important component on CWs. Therefore better CWs require better
565 biokinetic models. In this regard Samsó and García (2013b,c) believe that a single biokinetic
566 model would help decrease model divergence and concentrate efforts on a single platform,
567 just as in ASMs (Samsó et al., 2014b). In future, special emphasis will be put on clogging,
568 micro-scale bacterial models, and chemical reactions

569 For Diph_M the input parameter estimation is currently under investigation. The model
570 should be implemented into general CW models when VFCW are operated with ponding.

571 Future developments on mechanistic models should take the influence of biomass growth on

572 hydraulics into account; similar to like it was described by Samsó and García (2014a) for
573 HFCW.

574 The Wang-Scholz Model would benefit from a long-term modelling study of a 'real' wetland
575 becoming more mature until it requires decommissioning, which might, however, take as long
576 as 20 years. As an improvement of the model itself, the microbial removal processes
577 responsible for ammonia-nitrogen, nitrate-nitrogen and plant-originating SS reduction should
578 be implemented. However, access to long-term wetland system data is rather unrealistic
579 considering that most research projects are based on up to three years of data (Dong et al.,
580 2012).

581 The P-hydroslag model was originally based on dissolution and precipitation rates that lead to
582 prediction of slag filter longevity and retention capacity, the methodology based on a simple
583 batch test and a simple and free numerical tool (PHREEQC). Currently the application for any
584 kind of alkaline slag is under approval. In future, the calibration on controlled slag filters and
585 later on real filters is scheduled in preparation to implementation of P-hydroslag into 2D filter
586 models.

587 RSF_Sim was developed for the German type of CSO-CWs. Currently it is under validation
588 for the French system (Meyer et al., 2013). Especially the role of a permanently saturated
589 water layer needs to be investigated in real operation first, and implemented into the model
590 afterwards. The feeding with raw CSO as a further main difference might have an influence
591 on the treatment process description. For both of the CSO-CW systems a horizontal
592 discretization of the filter media layer is needed to identify the effects and importance of
593 shortcut flows. In general, a collection of available input data is in progress in order to
594 increase the reliability of performance predictions.

595 In RTD/GPS-X it is scheduled to determine the biofilm thickness with more accuracy. Also
596 kinetic parameters of N removal processes (anoxic), gas emission of the reactor for mass

597 balance accuracy, and finally non-soluble substrate and inert particles shall be taken into
598 account for full-scale application.

599

600 5. Conclusions and Recommendations

601 During the last two decades a couple of models were developed for CWs with differing
602 purposes. Meanwhile the usage of this kind of tool is generally accepted, but the misuse of the
603 models still confirms the skepticism. Generally three groups of models can be distinguished:
604 (1) On one hand mechanistic models try to display the complex and diffuse interaction of
605 occurring processes, (2) on the other hand the same kind of models are used to investigate
606 single processes. New kinds of ‘simplified’ approaches (3) – well appreciated by engineers -
607 try to display system performances without going to deep into details. All types are valuable –
608 some more for scientific usage, others more for engineering – and all support their users, but
609 all require skills of the users.

610 Big differences can be found in the model availabilities. Whereas some of the compared
611 software packages are purchasable without limitation, some others are only accessible on their
612 platform level, and some can be seen as secret property. From the experience of the authors it
613 can be summarized, that research groups starting modelling / simulation studies usually tend
614 to either buy a software package or to start from scratch with their own ideas. Adaptations of
615 existing approaches or ‘tool’ sharing are uncommon. This leads to a waste of time, energy and
616 money – both because modelling is time-consuming and older approaches start to disappear
617 immediately after their developers focus on other topics.

618 In order to find the best simulation tool for specific needs, the authors would like to
619 recommend the following procedure:

- 620 1. Define tasks and challenges and do a review in order to find similar cases.
- 621 2. Get into contact with the model developers and check the availability of approaches.

622 3. Try to use older models and find out their limits (figure 1).

623 4. Create ideas for improvements and share them.

624 In addition to the accessibility of tools, simulation studies often suffer from a lack of data.
625 When the use of dynamic models is aimed at the experiments have to be planned in a way that
626 data for model calibration and validation are available. Data requirements are different for
627 different models but include careful planning of sampling frequency and parameters analyzed.
628 Additionally, scientific institutions as well as private enterprises usually publish their best
629 results of research or technology application. Even if you can find high quality publications,
630 the utilization of data is inhibited due to missing details. The authors would like to encourage
631 an intensified data and knowledge exchange, especially because simulation studies including
632 data exploitation is barely funded. From a modelers point of view, the examples of
633 operational failure in practice are sometimes more interesting than the ‘showcases’, because
634 limits of technological application or system performance become visible. This becomes
635 particularly true for the hottest topic of current model development: clogging.

636

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