Water Research 83 (2015) 396–411

Contents lists available at ScienceDirect

Water Research

journal homepage: www.elsevier.com/locate/watres

iCFD: Interpreted Computational Fluid Dynamics – Degeneration of CFD to one-dimensional advection-dispersion models using statistical experimental design – The secondary clarifier

Estelle Guyonvarch [a], Elham Ramin [a], Murat Kulahci [b, c], Benedek Gy Plósz [a, *]

[a] Department of Environmental Engineering, Technical University of Denmark, Miljøvej, Building 113, 2800 Kgs. Lyngby, Denmark
[b] Department of Applied Mathematics and Computer Science, Technical University of Denmark, Richard Petersens Plads, Building 321, 2800 Kgs. Lyngby, Denmark
[c] Department of Business Administration, Technology and Social Sciences, Luleå University of Technology, SE-97187 Luleå, Sweden

ARTICLE INFO

Article history:
Received 20 December 2014
Received in revised form
12 April 2015
Accepted 8 June 2015
Available online 18 June 2015

Keywords:
Computational Fluid Dynamics (CFD)
One-dimensional advection dispersion model
Interpreted CFD model (iCFD)
Statistical factor screening
Degeneration of model structural complexity
Secondary settling tank

ABSTRACT

The present study aims at using statistically designed computational fluid dynamics (CFD) simulations as numerical experiments for the identification of one-dimensional (1-D) advection-dispersion models – computationally light tools, used e.g., as sub-models in systems analysis. The objective is to develop a new 1-D framework, referred to as interpreted CFD (iCFD) models, in which statistical meta-models are used to calculate the pseudo-dispersion coefficient (*D*) as a function of design and flow boundary conditions. The method – presented in a straightforward and transparent way – is illustrated using the example of a circular secondary settling tank (SST). First, the significant design and flow factors are screened out by applying the statistical method of two-level fractional factorial design of experiments. Second, based on the number of significant factors identified through the factor screening study and system understanding, 50 different sets of design and flow conditions are selected using Latin Hypercube Sampling (LHS). The boundary condition sets are imposed on a 2-D axi-symmetrical CFD simulation model of the SST. In the framework, to degenerate the 2-D model structure, CFD model outputs are approximated by the 1-D model through the calibration of three different model structures for *D*. Correlation equations for the *D* parameter then are identified as a function of the selected design and flow boundary conditions (meta-models), and their accuracy is evaluated against *D* values estimated in each numerical experiment. The evaluation and validation of the iCFD model structure is carried out using scenario simulation results obtained with parameters sampled from the corners of the LHS experimental region. For the studied SST, additional iCFD model development was carried out in terms of (i) assessing different density current sub-models; (ii) implementation of a combined flocculation, hindered, transient and compression settling velocity function; and (iii) assessment of modelling the onset of transient and compression settling. Furthermore, the optimal level of model discretization both in 2-D and 1-D was undertaken. Results suggest that the iCFD model developed for the SST through the proposed methodology is able to predict solid distribution with high accuracy – taking a reasonable computational effort – when compared to multi-dimensional numerical experiments, under a wide range of flow and design conditions. iCFD tools could play a crucial role in reliably predicting systems' performance under normal and shock events.

1. Introduction

System analysis tools typically comprise numerous sub-models, simulating a set of processes demarcated from the environment using a selection of boundary conditions. Sub-models used are identified so that the computational efforts made through system analysis exercises are kept to a minimum (Gujer, 2008). Consequently, detailed information related to, for instance, design boundaries, may be ignored, and their effects may only be accounted for through calibration of model parameters used as catchalls, and by arbitrary amendment of structural uncertainty

* Corresponding author.
E-mail address: beep@env.dtu.dk (B.G. Plósz).

http://dx.doi.org/10.1016/j.watres.2015.06.012
0043-1354/

Abbreviations

1-D	one-dimensional
2-D	two-dimensional
2LFDE	two-level fractional factorial design of experiments
CFD	computational fluid dynamics
D_0-iCFD	iCFD model considering one pseudo-dispersion D_0 constant along the tank
$D_{1,2}$-iCFD	iCFD model considering two pseudo-dispersions D_1 and D_2 in the clarification and in thickening zone respectively
D_f-iCFD	iCFD model considering one pseudo-dispersion D_f just around the feed inlet
iCFD	interpreted computational fluid dynamics
LHS	latin hypercube sampling
RAS	return activated sludge
SBH	sludge blanket height
SHC	solids handling criteria
SSRE	sum of square of relative errors
SST	secondary settling tank
SWD	side water depth
TSS	total suspended solids
WWTP	wastewater treatment plant

Symbols

α_i	correlation coefficients corresponding to the contribution f_i
θ_{cb}	inclination angle between the Crosby baffle and the horizontal, °
b	intercept of the correlation between D and the contribution f_i, m^2/d
D	pseudo-dispersion coefficient, m^2/d
D_0	pseudo-dispersion coefficient constant along the tank, m^2/d
D_1	pseudo-dispersion coefficient in the clarification zone, m^2/d
D_2	pseudo-dispersion coefficient in the thickening zone, m^2/d
D_f	pseudo-dispersion coefficient around the feed layer, m^2/d
f_i	factor or interactions between factors correlated to D
H	tank's average depth, m
H_b	length of the inlet baffle, m
H_{cb}	vertical distance between the effluent weir and the Crosby baffle attachment point, m
H_{in}	vertical distance between the top of the tank and the inlet aperture, m
M_{tot}	total sludge mass stored in the tank, kg
M_tot_{1D}	$Mtot$ calculated with the 1-D model, kg
M_tot_{CFD}	$Mtot$ calculated with the CFD model, kg
Q_{in}	inlet flowrate, m^3/d
Q_{ov}	overflow rate, m^3/d
Q_{under}	underflow rate, m^3/d
R	recycle ratio, dimensionless
R^2	coefficient of determination, dimensionless
R_b	horizontal distance between the feed wall and inlet baffle, m
SBH_{1D}	SBH calculated with the 1-D model, m
SBH_{CFD}	SBH calculated with the CFD model, m
v	bulk velocity, m/s
v_s	sludge settling velocity, m/s
X	sludge concentration, kg/m^3
X_{eff}	effluent sludge concentration, kg/m^3
X_eff_{1D}	X_{eff} calculated with the 1-D model, kg/m^3
X_eff_{CFD}	X_{eff} calculated with the CFD model, kg/m^3
X_{feed_layer}	sludge concentration of the feed layer, kg/m^3
X_{in}	inlet concentration, kg/m^3
X_{RAS}	underflow sludge concentration, kg/m^3
X_RAS_{1D}	X_{RAS} calculated with the 1-D model, kg/m^3
X_RAS_{CFD}	X_{RAS} calculated with the CFD model, kg/m^3
X_{TC}	transient/compression sludge concentration threshold, kg/m^3
z	vertical direction variable, m
z_{crit}	critical distance with z_{feed} where D_f shall be considered, m
z_{feed}	feed layer height, m

propagations to outputs. An example for such practice is the hydrodynamic simulation models of bioengineered wastewater treatment systems, comprising bioreactors and the secondary settling tank (SST). SSTs, used as a case study in this paper, play three crucial roles in conventional wastewater treatment plants (WWTP): effluent clarifier, thickener of the sludge to be recycled (RAS) and sludge storage during high loading conditions (Ekama et al., 1997). The settling characteristics of activated sludge, the design of the tank, and the flow conditions in SSTs can influence the solid-liquid separation process. Thus, in principle, these boundary conditions need to be considered to predict the capacity of SSTs and consequently the permissible flow into the WWTP. SSTs are known to be the main hydraulic bottleneck of the wastewater treatment process, and thus, it is of key importance to properly model these units, and understand the involved fluid dynamic processes. Computational fluid dynamics (CFD) is a powerful tool allowing for a better understanding of numerous process units, such as SSTs, and thus potentially leading to a more rational design (Water Environment Federation, 2005). Two- and three-dimensional CFD models are able to handle numerous phenomena, and thereby to accurately predict solids' distribution. However, they usually require a high computational time. Therefore, for dynamic simulations and for the simulation of a more extensive system, simpler one-dimensional (1-D) models (Li and Stenstrom, 2014), or grammar-based genetic programming with an encoding to represent hydraulic models as program trees (Dürrenmatt and Gujer, 2012) can be used. In the case of 1-D SSTs, predictions made on systems, comprising bioreactors connected to SSTs, are highly dependent on the 1-D SST model structure and parameters (Plósz et al., 2011; Ramin et al., 2014a). Following first-order SST models (e.g., Takács et al., 1991), more recent research attempted to develop 1-D models based on 1-D advection-dispersion partial differential equations (Bürger et al., 2011, 2005; De Clercq et al., 2003; Hamilton et al., 1992; Plósz et al., 2007; Watts et al., 1996), which include a second-order dispersion term in the solids transport equation (see Eq. (1)).

$$\frac{\partial X}{\partial t}+\frac{\partial (v\cdot X)}{\partial z}+\frac{\partial (v_s\cdot X)}{\partial z}-\frac{\partial}{\partial z}\left(D\cdot\frac{\partial X}{\partial z}\right)=0 \quad (1)$$

where X is the solid concentration, z is the vertical direction variable, v is the bulk velocity, v_S is the sludge settling velocity and D is the pseudo-dispersion coefficient. The upward integrated and discretized form of Eq. (1) is given in Table 1.

The introduction of the pseudo-dispersion coefficient D, by analogy to Fick's law, helps to distinguish the effects of sludge settleability from other hydraulic effects on the SST performance (Ekama et al., 1997). This coefficient is named “pseudo-dispersion”,