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iCFD modeling of final settlers – developing consistent and effective simulation model structures

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Summary of key findings

The concept of interpreted computational fluid dynamic (iCFD) process modelling approach is presented (Fig. 1, Guyonvarch *et al.*, 2015). The 1-D advection-dispersion model along with the

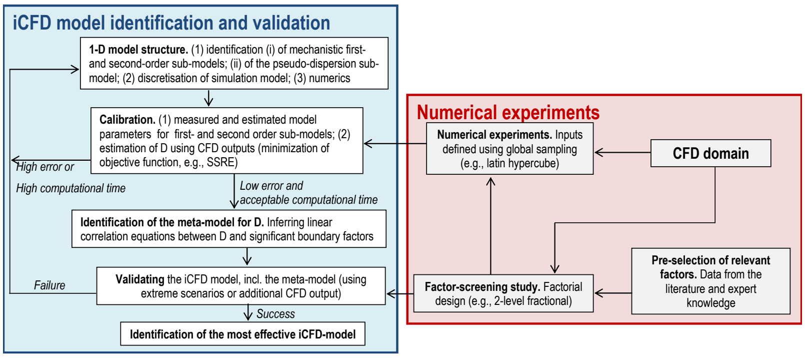

Figure 1 Overview of the methodology applied to the case of secondary clarifier for the development of an interpreted computational fluid dynamic (iCFD) model.

statistically generated meta-model for pseudo-dispersion constitutes the newly developed iCFD concept. The case of secondary settling tanks (SSTs) is used to demonstrate the methodological steps using a validated CFD model with the hindered-transient-compression settling velocity model by (Ramin *et al.*, 2014). Factor screening and latin hypercube sampling (LSH) are used to degenerate a 2-D axi-symmetrical CFD model structure (Ramin *et al.*, 2014) into a one-dimensional (1-D) advection-dispersion model structure. The boundary condition sets, obtained in the LHS, are imposed on the 2-D 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,* the pseudo-dispersion coefficient. Correlation equations for the *D* parameter (meta-models) are then identified as a function of the selected design and flow boundary conditions, and their accuracy is evaluated against the *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. The iCFD models developed are intended to comply with the consistent modelling methodology (Bürger *et al.*, 2011).

Background and relevance

System analysis tools typically comprise numerous sub-models, identified so that the computational effort taken through system analysis exercises is 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 amendments of structural uncertainty propagations to outputs. An example for such practice is the 1-D simulation models of SSTs. This study aims at using statistically designed CFD simulation scenarios with different design and flow boundary conditions to identify consistent and effective 1-D structures. A correlation analysis is carried out between *D* values and the determinant boundaries using LHS.

Results

Factor screening. Factor screening is carried out by imposing statistically designed (software: JMP®, SAS, USA) moderate (under-loaded) and extreme (under-, critical and overloaded) operational boundary conditions on the 2-D CFD SST model (software: OpenFOAM-*settlingFoam* solver, 8). Results obtained in the statistical analysis of the CFD outputs in the extreme scenario suggest that the loading conditions characterised with feed solid concentration (X_{in}), SST overflow rate (Q_{ov}), recycle ratio (R), and, to a minor extent, the inlet height (H_{in}), are the four significant factors, impacting the SST performance, in terms of sludge blanket height (*SBH*), solids concentration in recycle of activated sludge (X_{RAS}) and solids concentration in SST effluent (X_{eff}). Statistical results obtained in the moderate scenario indicate five factors significantly influencing the SST performance, i.e. X_{in}, Q_{ov}, R, sidewater depth (*SWD*) and H_{in}. Baffles installed in the SST inlet and outlet, are found to have negligible effect on X_{eff}, compared to the aforementioned five factors.

LHS. Based on the screening study, the five significant factors used in the subsequent LHS are X_{in}, Q_{ov}, R, *SWD* and H_{in}. Based on the LHS 50 CFD steady-state simulation outputs, in terms of *SBH*, X_{RAS}, X_{eff}, total amount of solids in SST (M_{tot}) values, are used to for iCFD model identification.

iCFD model identification. We assess the 1-D model structure in terms of setting the feed location (layer) and transient/compression threshold concentration, X_{TC} (software: MATLAB®, Mathwork, USA). Using the CFD outputs from LHS, we assessed nine different model structures based on literature (Bürger et al., 2011; Dupon & Dahl, 1995; De Clercq, 2006; Ramin *et al.*, 2014; Plósz *et al.*, 2007) and on more recent considerations (Fig. 2a). Validation tests were done using

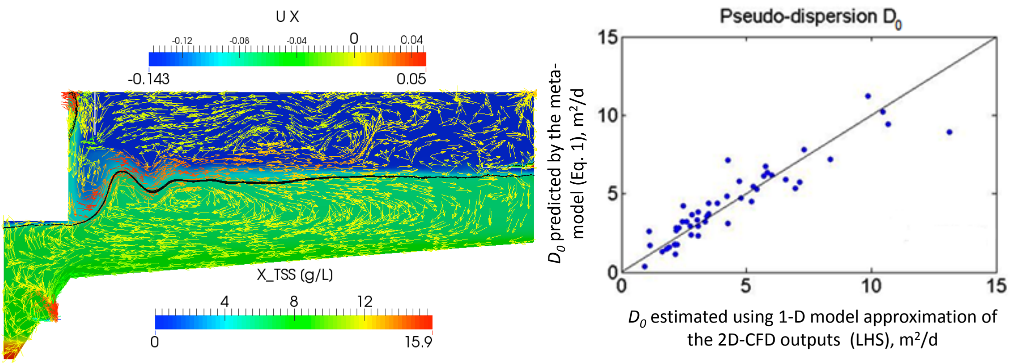

Figure 2 (A-left) Illustration of the influent density current based on 2-D axi-symmetric CFD simulation and the rationale for feed-layer selection through 1-D SST modelling. (B-right) Evaluation of the accuracy of meta-model to predict *D* using D_0-iCFD, simulation model.

the CFD outputs from extreme scenarios. The most effective model structure (relatively low the sum of square of relative errors, SSRE, and computational time) obtained is that in which the X_{TC} is set at the concentration of the layer just below the feed-layer. The feed-layer location is set to the highest location where $X > X_{in}$ (solids concentration in SST influent). An effective discretization level (trade-off between computational time and numerical error) is assessed by approximating the LHS outputs with an iCFD model discretised using 10, 30, 45, 60, 90 and 200 layers. Solutions obtained show convergence, and the discretisation scheme with 60 layers seems to be an effective trade-off.

Identification and validation of the *D*-model. To identify a formulation for the pseudo-dispersion coefficient in the iCFD model, we tested three structural scenarios by defining (i) one single pseudo-dispersion coefficient (D_0) for all the layers; (ii) one pseudo-dispersion coefficient (D_1) above and another pseudo-dispersion coefficient (D_2) below the feed-layer; (iii) one pseudo-dispersion coefficient (D_f) just around the feed-layer. These scenarios were inspired by literature (Bürger et al., 2011; De Clercq, 2006; Plósz *et al.*, 2007). As for the D_0–iCFD model, values of SSRE obtained are below 1 with an average SSRE=0.206. The simulation model thus can predict the solids distribution inside the tank with a satisfactory accuracy. Averaged relative errors of 8.1 %, 3.1 %, 16.1 % and 11.8 % are observed for *SBH*, X_{RAS}, X_{eff} and M_{tot}, respectively.

A statistical analysis of the calibrated D_0 compared to the five input factors is performed. In addition to the elementary factors, four interactions are found significant: X_{in}^2, $X_{in}*H_{in}$, $R*H_{in}$ and $X_{in}*Q_{ov}$. A correlation is obtained between the loading and design factors and D_0 with an R^2 of 0.853, i.e.

$$D_0 = \left|\beta_0 + \beta_1 \cdot X_{in} + \beta_2 \cdot R + \beta_3 \cdot H_{in} + \beta_4 \cdot Q_{ov} + \beta_5 \cdot SWD + \beta_{11} \cdot {X_{in}}^2 + \beta_{12} \cdot R \cdot H_{in} + \beta_{13} \cdot X_{in} \cdot H_{in} + \beta_{14} \cdot X_{in} \cdot Q_{ov}\right| , \quad (1)$$

where β_1, β_2, β_3, β_4, β_5, β_{11}, β_{12}, β_{13}, β_{14} denote the correlation coefficients obtained. The D_0 values predicted with Eq. 1 are compared to the values estimated using 1-D model approximation of the 50 CFD outputs, and results suggest a relatively effective correlation as well (Fig. 2b). The three iCFD models, employing different formulations for *D*, calibrated using the meta-models (Eq. 1 for D_0), are used to approximate the CFD outputs obtained in the extreme scenarios. Using the D_0-iCFD model, the solid distribution at the corners of the LHS experimental region can be predicted with the highest accuracy (average SSRE=0.71), thereby validating the simulation model. For $D_{1,2}$-iCFD, the meta-model is limited in calculating *D*, and the model fails the validation test using the extreme scenario (SSRE=386). Using the D_f-iCFD model, the predictive accuracy obtained is comparable with that obtained with the D_0-iCFD (compare 1.73 to 0.71). The computational time required through simulation with D_f-iCFD, however, is significantly higher than that obtained with the D_0-iCFD (on average 3.5 times longer). Therefore, this study concludes that, considering the capability and usability – in terms of complexity and computational time requirements – the D_0-iCFD model is preferred over the $D_{1,2}$- and the D_f-iCFD models.

Discussion

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 an important role in reliably predicting WWTP performance under normal and shock-loading (Jeppsson et al., 2013; Plósz et al., 2009).

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