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The Bürger-Diehl model: The right integrator for the right model

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Introduction

The settling tank is a critical process of most activated sludge wastewater treatment systems. Therefore, important studies have been performed on its modelling. Empirical settling tank models can be as simple as point settlers where sludge is separated from water based on a fixed coefficient. However, nowadays, one of the most widely used settling models is the conceptual model proposed by Takács et al. (1991). While this model was considered as the state-of-the-art at the time of its conception, it is still subject to various shortcomings which has led to the development of a more advanced settling model: the Bürger-Diehl (BD) model (Bürger et al., 2011)

Methodology

Extensive literature describes the BD model, but still, many modelers hesitate to use it because of its complexity and its computational cost. In this work, we apply the BD model with hindered settling, inlet dispersion and compression settling to the Benchmark Simulation Model 1 (BSM1) to study the computational cost that comes with the use of the BD model configuration and with the solver used for the simulation. The simulation was performed both at steady state (constant inputs) and with a storm weather influent (14 days with storms during days 8 and 10).

In the scope of the simulation software Tornado/WEST (www.mikebydhi.com), the BD model, which was originally conceived as a set of partial differential equations (PDEs), is transformed to a set of ordinary differential equations (ODEs) by the method of lines. At this step, the spatial discretization of the BD model must be chosen, since we know that a very fine discretization offers a great accuracy, but at the cost of a high computational load due to the larger number of equations to solve and to the constraints on time steps posed by the Courant–Friedrichs–Lewy (CFL) stability condition. The influence of this discretization is studied in this work by testing four different configurations with 30, 50, 90 and 200 layers.

When comparing numerical methods for simulation, the concept of efficiency is usually used. One method is more efficient than another if the computational cost is less for a given tolerance. Since the spatial discretization of the BD model produces an error that is less than first order, the additional error produced by the time discretization when using an ODE solver of order one or higher is negligible (Diehl et al., 2015). Therefore, we can focus on the computational cost when comparing time solvers.

The maximum time step given by the CFL condition guarantees numerical stability for an explicit solver and is approximately proportional to the square of the layer's thickness of the spatial discretization (Bürger et al., 2013). While it is possible to use small step sizes to meet the CFL condition, solvers with adaptive step-size control estimate the error and do not need the CFL condition. Furthermore, the so-called implicit solvers possess intrinsic stability properties that remove the CFL condition, thus alleviating the computational cost and allowing for taking much larger time steps.

In this study, four solvers were used to perform the simulation without the use of the CFL condition. The first is an explicit Runge-Kutta method of fourth order with an adaptive step control strategy, described by Press et al. (2007) and named RK4ASC. This solver is known to be very efficient on wastewater models, thanks to its low cost per time step but, as an explicit solver, very small time step may have to be imposed when applied to stiff models. The second, third and fourth solvers are all based on the CVODE solver from the SUNDIALS library (https://computation.llnl.gov/casc/sundials/main.html). CVODE offers a large number of options to solve large-scale models. For non-stiff models, it uses the Adams-Moulton Formulas (AMF) while for stiff models the Backward Differential Formulas (BDF) are available. Furthermore, the CVODE solver requires solving internally large systems of implicit equations. To do so, two techniques were evaluated in this work: the pre-conditioned Krylov method SPGMR and the Newton-Raphson method based on the full Jacobian matrix (hereafter called the Dense method). In total, four state-of-the-art solvers (RK4ASC, CVODE-AMF-SPGMR, CVODE-BDF-SPGMR, CVODE-BDF-Dense) were chosen for their ability to cover the most common numerical situations in ODEs of wastewater systems. Finally, to compare results, the accuracy settings of all solvers have been set to constrain the error by the following condition:

$$err_{x_i} \leq RTol * |x_i| + ATol$$

Where err_{x_i} is the error estimated internally by the solver on the state variable x_i, $RTol$ and $ATol$ are the relative and absolute tolerances provided by the user. In all simulations, $RTol$ was fixed at 1E-5 and $ATol$ at 1E-3.

Selected results

As expected, the choice of the solver settings influenced the simulation results only within the tolerance requested. Therefore, each setting was capable of providing similar results. The spatial discretization of the BD model, however, significantly affected the simulated effluent quality, as can be observed in Figure 1.

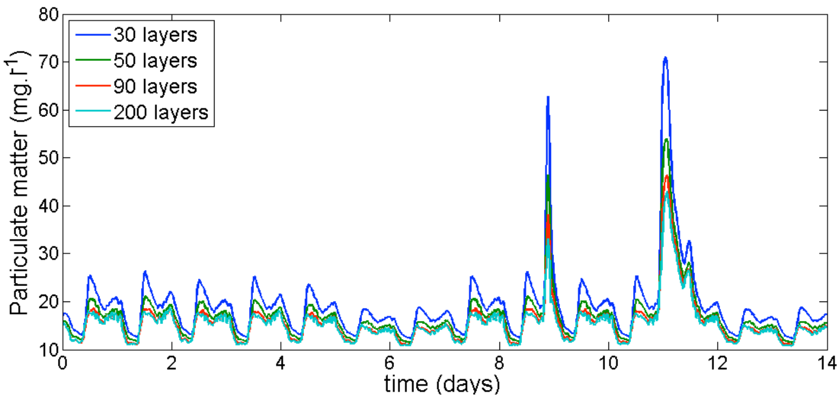

Figure 1: Particulate matter concentration exiting the secondary clarifier. The four spatial discretizations of the Bürger-Diehl model are presented: 30, 50, 90 and 200 layers.

Figure 1 shows that the concentration of particulate matter exiting the secondary clarifier follows the same dynamics irrespectively of the number of layers in the spatial discretization. However, coarser discretizations generate larger amplitude of the dynamics modelled. The simulation time, in turn, depends greatly on the choice of the solver and its options. Table 1 regroups the number of model evaluations (computation of the right-hand side of the ODE) required for each simulation along with the total simulation time.

The fastest solver at steady state is the CVODE-BDF-Dense method. This solver can take full advantage of the computational time invested in the calculation of the Jacobian matrix by taking very large time steps as the transient solution converges to steady state. In contrast, RK4ASC struggles to keep the solution accurate (therefore stable), exhibiting a small and constant average time step throughout the simulation. The two last options offer decent performances, but the SPGMR solver is not precise enough to allow stable long time steps.

Table 1 Computational cost of the four solver configurations tested. The "Model eval." refers to the number of model evaluations performed by the solver and the "Total time" is the computation time required to complete the simulation. Only the steady state results of the two more challenging spatial discretizations are shown and results for all four spatial discretizations are shown for the dynamic simulation. Fastest simulation results for each discretization are highlighted in bold.

No Layer		RK4ASC	CVODE-AMF-SPGMR	CVODE-BDF-SPGMR	CVODE-BDF-Dense
Steady State simulation					
90	Model eval.	3 977 555	410 651	186 833	**1 606**
	Total Time (s)	125	18	8	**0**
200	Model eval.	19 050 997	1 883 610	762 347	**8 440**
	Total Time (s)	1 123	131	54	**1**
Dynamic simulation					
30	Model eval.	229 483	**91 390**	156 763	3 382 232
	Total Time (s)	5	**3**	4	72
50	Model eval.	270 534	**112 074**	247 643	7 332 415
	Total Time (s)	7	**4**	9	201
90	Model eval.	691 384	**271 673**	513 999	14 317 022
	Total Time (s)	26	**14**	26	563
200	Model eval.	3 001 611	**759 123**	1 400 534	39 621 899
	Total Time (s)	193	**58**	116	2 742

When moving to the dynamic simulation, however, the results are highly different. The clear winner of the steady state simulation becomes the slowest competitor by up to two orders of magnitude. The Jacobian matrix is too variable and must be computed an excessive number of times, leading to unacceptable computational cost. During these simulations, the fastest solver configuration has been CVODE-AMF-SPGMR, but RK4ASC and CVODE-BDF-SPGMR remain within an order of magnitude. Noteworthy, even with a BD model discretized in 200 layers, the model was deemed non-stiff by CVODE and the AMF performed better than the BDF. RK4ASC required at least twice as many model evaluations in each case, but was not distanced unacceptably.

Discussion and conclusion

Modellers like to invest their time in actual modelling. However, one should not forget that complex numerical methods are required to obtain an acceptably accurate solution at reasonable speed. This study highlighted the advantage of using stiff solvers for steady state calculation. CVODE-BDF-Dense should always be considered for steady state calculation, leaving the other options for specific models that might require additional fine-tuning of the solver. The dynamic simulations did not provide such clear answers, but still suggest that fine-tuning is possible and can reduce computation times by an appreciable factor. Finally, other parameters can significantly affect computation times such as the requested accuracy or the stiffness of the model (depending on the choice of constitutive functions for phenomena such as hindered settling, compression and dispersion). Therefore, choosing an appropriate time solver for a model is an art that should not be overlooked.

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