Verification study of Computational Fluid Dynamics solver for struvite precipitation

Bernardas Jankauskas[1]; Prof Gavin Tabor[1]; Dr Daniel Jarman[2]
University of Exeter[1]; Hydro International[2]

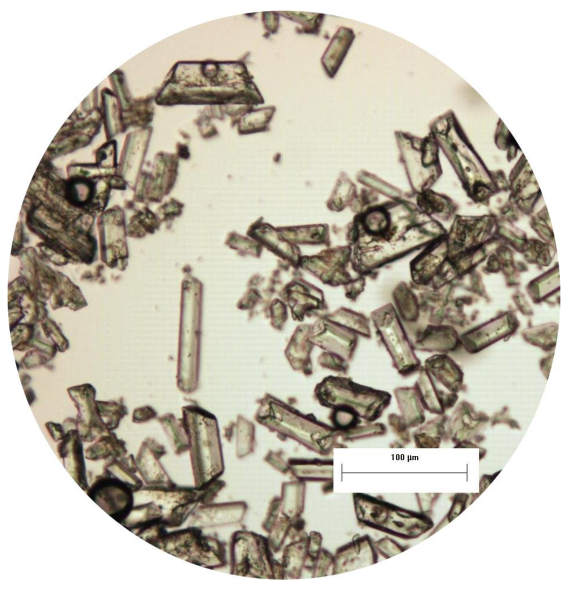
Stream

The Industrial Doctorate Centre for the Water Sector

Motivation

Struvite is a crystalline substance often treated as a problem in wastewater treatment facilities. Spontaneous reactive crystallisation or precipitation of struvite can cause scale formation on the pipe walls. Descaling procedures for the pipes are costly and time consuming.

In addition to scaling issues, slow-release fertiliser potential of struvite in agriculture has been highly praised. Novel methods of struvite recovery from wastewater are in high demand and are also required in order to have a more sustainable and environmentally friendly wastewater industry.



Aims

Hydrodynamic vortex separator is a compact, passive, energy efficient solid-liquid separator developed by Hydro International.

We deploy Computational Fluid Dynamics methods, aiming to study the potential of this device for use as a reaction vessel for struvite precipitation processes.

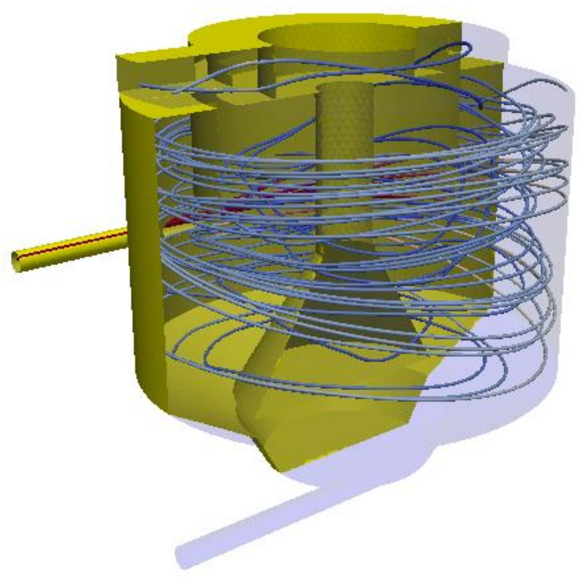
CFD framework

OpenFOAM® framework is used to perform the simulations. The PIMPLE algorithm is used to solve pressure-velocity equations.

Drift Flux Model[1] is used to capture sludge settling and void fraction coupling to the fluid.

Arrhenius reaction rate based reaction model is used to capture species transport in the system.

Precipitation kinetics are modelled with Population Balance equation modelling. Extended Quadrature method of moments[2] algorithm is used to discretise, solve PBE evolution equations and recover relevant parameters of the crystal size distribution.



Mathematical model

Momentum transport

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) = -\nabla \mathrm{p} + \nabla \cdot \Gamma \nabla U - \nabla \cdot U_{rel} + \rho g$$

Mass conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$

Species transport

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i U) = \nabla \cdot \Gamma \nabla Y_i + S_i$$

Population Balance

$$\frac{\partial n}{\partial t} + \nabla_{\boldsymbol{x}} \cdot [n\boldsymbol{U}] - \nabla_{\boldsymbol{x}} \cdot [\Gamma \nabla_x n] + \nabla_{\xi} \cdot [\mathrm{G}(\xi) n] = \bar{B}^a - \bar{D}^a + \bar{B}^b - \bar{D}^b + N$$

Reaction solver verification case

Solver verification is a key part of CFD modelling. It is necessary in order to understand whether the algorithms that implemented are doing what they are supposed to do.

At this stage of our research we perform a verification study for the reaction part of the solver. A trivial reactive system has been used for this study, which has been chosen because an analytical solution for such simplified system is easy to obtain.

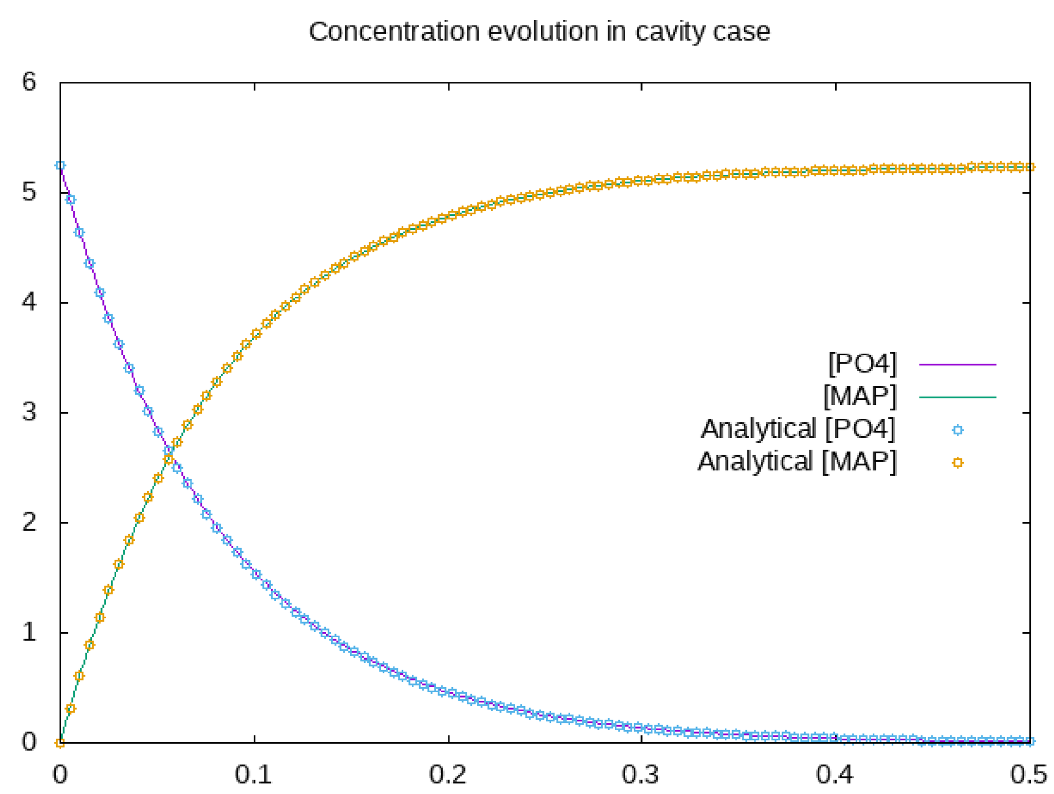
Verification reaction and forwards reaction rate:

$$A \rightarrow B$$

$$k_f = AT^{\beta} \exp(-\frac{E_A}{T})$$

Verification study results

CFD results from the simulation are as expected and match the analytical results exactly. The concentrations for reactants and products are balanced out and no unphysical results are observed.



Further work

Further work requires implementation of a two way coupling between fluid transport and population balance equation solution.

Two way coupling is necessary to achieve correct physical representation of the system. According to the reaction system, appropriate equation source terms for particle growth, nucleation, agglomeration and breakup will be used.

Solver will be validated against the experimental data on barium sulphate precipitation available from the literature.

Additionally, PBE part of the solver will be verified against analytical results available from the literature.

References

[1] D. Brennan, The Numerical Simulation of Two-Phase Flows in Settling Tanks (Doctoral Thesis), University of London, 2001
[2] C. Yuan, F. Laurent, R.O. Fox, An extended quadrature method of moments for population balance equations, Journal of Aerosol Science, Vol. 51, September 2012, Pages 1-23

Sponsors:

www.stream-idc.net

UNIVERSITY OF EXETER | Hydro International® | EPSRC

Contact details:

Postal Address: Harrison Bldg., Rm110, University of Exeter, N Park Rd, Exeter, Devon, EX4 4QF

Further information: bj255@exeter.ac.uk