Mathematical framework for modelling reactive crystallisation of struvite from wastewater

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stream

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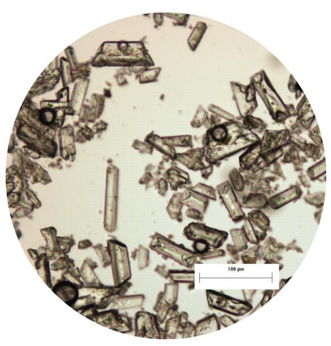
Introduction

Magnesium ammonium phosphate is a crystalline substance often treated as a problem in wastewater treatment facilities. Spontaneous reactive crystallisation or precipitation of struvite can cause scaling on pipes in the treatment works and current treatment methods for such scaling are expensive and time consuming.

Use of struvite as fertiliser in agriculture has been highly praised, hence novel methods of recovery are needed in order to have more sustainable and environmentally friendly treatment works.



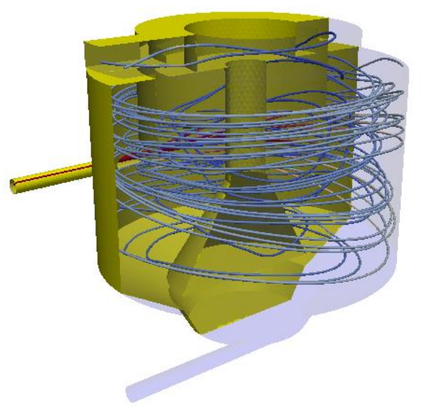
Aims

Hydrodynamic vortex separator is a compact, energy efficient solid-liquid separator developed by Hydro International. Using Computational Fluid Dynamics, we aim to simulate precipitation of struvite inside such device.

Challenges

Modelling precipitation covers three areas: hydrodynamics, reaction dynamics, and precipitation dynamics or crystal growth.

Mathematical framework for each separate component is clear, so the challenging part of the project at the moment is about choosing and implementing correct coupling procedures, assumptions, and algorithms.



Hydrodynamics

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

Currently no turbulence model is used, but an appropriate one will be picked for the final simulations.

Drift Flux Model[1] is often used to capture sludge settling and coupling to the fluid. The system of interest satisfies the conditions needed for the model, so DFM will used to couple the formation of new particulates and the fluid.

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

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

Reaction dynamics

Currently a single reaction system is used to model reaction processes in the system. More complex reaction mechanisms might be used later in the project.
Assuming that all reactants and products are dissolved, the **scalar transport equations** for the species are passive, i.e. one-way coupled.

Liquid phase reaction thermodynamics had to be implemented into the OpenFOAM® framework to correctly model energetic changes in the system due to the **chemical reaction**.

Reaction

$$Mg^{2+} + NH_4^+ + H_n PO_4^{3-n} + 6H_2O \leftrightarrow$$

$$\leftrightarrow MgNH_4PO_4 \cdot 6H_2O \downarrow + nH^+$$

Species transport

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

Precipitation dynamics

Crystal formation is treated using a population balance modelling approach. Crystal Size Distribution is treated as a pseudo scalar field $n(\xi,x,t)$ and transported using a **transport equation**.
Extended quadrature-based moment method[2] is used to approximate and solve CSD in terms of it's statistical moments $m_j(\xi,x,t)$. This approach is chosen due to it's robustness and stability.

Coupling with hydrodynamics (Drift Flux Model) and reaction dynamics (with appropriate source terms) will be done later in the project.

Moments transport

$$\frac{\partial m_j}{\partial t} + \nabla \cdot \left(U m_j\right) - \nabla \cdot \left(\Gamma \nabla m_j\right) = J_0^j \dot{n}_0 + jG m_{j-1} +$$

$$+ [B^a - D^a + B^d - D^b]$$

Moments transformation

$$n(\xi, x, t,) = \sum_{j=0}^{N} w_j m_j$$

References

[1] D. Brennan, 2001, The numerical simulation of Two-Phase Flows in Settling Tanks, 2001, PhD Thesis, Imperial College of Science, Technology and Medicine

[2] E. Madadi-Kandjani, A. Passalacqua, An extended quadrature-based moment method with log-normal kernel density functions, Chemical Engineering Science, Volume 131, 2015, 232-339, doi:10.1016/j.ces.2015.04.005

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