TITLE:

- Videos – CFD-DEM simulations: fluidisation of calcite-pellets in water

SHORT DESCRIPTION:

- Videos – CFD-DEM simulations fluidisation calcium carbonate granules (calcite-pellets 0.8-0.9mm and 1.4-1.7mm) in water

FORMAT:

- MP4 videos (details see below)

CONTACT INFORMATION:

- Tim M.J. Nijssen - t.m.j.nijssen@tue.nl / 0000-0002-2574-8547
- Onno J.I. Kramer - TU Delft (CiTG, 3ME) o.j.i.kramer@tudelft.nl / onno.kramer@waternet.nl 0000-0002-4825-9869

ORGANIZATIONS:

- Eindhoven University of Technology, Department of Chemical Engineering & Chemistry, Multiphase Reactors Group
- Delft University of Technology, Faculty of Civil Engineering and Geosciences, Department of Water Management
- Delft University of Technology, Faculty of Mechanical, Maritime and Materials Engineering, Department of Process and Energy
- Waternet, Amsterdam (funder)
- HU University of Applied Sciences Utrecht, Institute for Life Science and Chemistry
- Queen Mary University of London, Division of Chemical Engineering, School of Engineering and Materials Science

SUBJECT:

- Hydraulic modelling of multiphase flow systems

KEYWORDS:

- multiphase phenomena
- computational fluid dynamics modelling
- liquid-solid fluidisation
- drinking water treatment
- circular sustainable processes
- water softening
- calcite pellets
- CFD-DEM
- numerical simulations
- fluidization

METHODOLOGICAL INFORMATION:

- CFDEMcoupling framework, relying on LIGGGHTS and OpenFOAM.
- The simulations in this work were conducted using the model described in detail by (Nijssen et al.,

2020). This model couples Computational Fluid Dynamics (CFD) and the Discrete Element Method (DEM), allowing for simultaneous description of the water phase and the suspended particles. This work employs the unresolved CFD-DEM methodology, which resolves the fluid flow at a length scale larger than the particles. This allows for the simulation of a large number of particles ($\lessapprox 10^6$) but requires interaction models to evaluate the force exerted by the fluid on the particles and vice versa. The model by Nijssen et al. is especially suited for simulation of LSF beds as it includes closures for the drag, lift, as well as virtual mass and Basset forces. The addition of the Basset force is a significant improvement over the classical drag-only CFD-DEM approach, which is more suited for gas-solid systems (Nijssen et al., 2020). For a complete description of the model, the reader is referred to the original work. The parameters and settings used in the simulations are summarised in Table 1. The fluid properties are taken at 20 °C.

- Nijssen, T.M.J., Kuipers, J.A.M., van der Stel, J., Adema, A.T., Buist, K.A., 2020. Complete liquid-solid momentum coupling for unresolved CFD-DEM simulations. International Journal of Multiphase Flow 132. https://doi.org/10.1016/j.ijmultiphaseflow.2020.103425
- Kramer, O.J.I., van Schaik, C., Nijssen, T.M.J., 2020d. Videos of fluidisation of calcite-pellets 0.8-0.9mm and 1.4-1.7 mm in water for various flow rates [Data set] 4TU.Centre for Research Data. 4TU.ResearchData, The Netherlands. https://doi.org/10.4121/13277246.v1
- Kramer, O.J.I., Castrejon-Pita, J.R., Boek, E.S., 2020a. Videos (high speed camera) - liquid-solid fluidisation experiments (calcite-pellets 1.4-1.7 mm in water) [Data set] 4TU.Centre for Research Data. 4TU.Centre for Research Data, Amsterdam, The Netherlands. https://doi.org/10.4121/uuid:41556e6c-b599-42cd-9f1d-bcf01dbe8576
- Kramer, O.J.I., de Moel, P.J., Padding, J.T., Baars, E.T., el Hasadi, Y.M.F., Boek, E.S., van der Hoek, J.P., 2020b. Accurate voidage prediction in fluidisation systems for full-scale drinking water pellet softening reactors using data driven models. Journal of Water Process Engineering 37, 1–15. https://doi.org/10.1016/j.jwpe.2020.101481
- Kramer, O.J.I., Padding, J.T., van Vugt, W.H., de Moel, P.J., Baars, E.T., Boek, E.S., van der Hoek, J.P., 2020c. Improvement of voidage prediction in liquid-solid fluidized beds by inclusion of the Froude number in effective drag relations. International Journal of Multiphase Flow 127. https://doi.org/10.1016/j.ijmultiphaseflow.2020.103261

ADDITIONAL TECHNICAL INFORMATION:

- Videos include outside views of the reactor representing each particle by its diameter, as well as cross-sectional view of the local voidage.
- Particle size distributions are Gaussian distributions:
  - Fraction A: $\langle d_p \rangle$ = 0.9 mm, σ_p = 0.08 mm
    - fraction_A_particles.mp4
  - Fraction B: $\langle d_p \rangle$ = 1.55 mm, σ_p = 0.16 mm
    - fraction_B_particles.mp4
- The superficial liquid velocities used are:
  - Fraction A: 30 mm/s
    - fraction_A_voidage.mp4
  - Fraction B: 15, 30, 61, 87, 142 mm/s
    - fraction_B_voidage.mp4

- Remaining simulation settings are given in the table below.

Variable	Symbol	Value	Unit
Column diameter	D	0.057	[m]
Column length	H	2.0	[m]
CFD cell size	Δx	4.65	[mm]
CFD time step	Δt_{CFD}	10^{-3}	[s]
DEM time step	Δt_{DEM}	10^{-5}	[s]
Fluid density	ρ_f	998.20	[kg/m^3]
Fluid dynamic viscosity	η_f	$1.005 \cdot 10^{-3}$	[Pa s]
Gravitational acceleration	g	9.81	[m/s^2]
Particle density	ρ_p	2575	[kg/m^3]
Total particle mass	m_p	0.87	[kg]
Particle Young's modulus	Y_p	5.0	[MPa]
Particle Poisson ratio	ν_p	0.45	[-]
Particle coefficient of restitution	e_p	0.3	[-]
Particle coefficient of friction	μ_p	0.05	[-]

PROJECT:

- This research is part of the project "Hydraulic modelling of liquid-solid fluidisation in drinking water treatment processes" carried out by Waternet, Delft University of Technology, and HU University of Applied Sciences Utrecht. Financial support came from Waternet Drinking Water Production Department.
- Part of this research was carried out under project number S16046 in the framework of the Partnership Program of the Materials innovation institute M2i (www.m2i.nl) and the Technology Foundation STW (www.stw.nl), which is part of the Netherlands Organisation for Scientific Research (www.nwo.nl).

- Simulation in this work were carried out using the CFDEMcoupling framework, relying on LIGGGHTS and OpenFOAM.

SHARING AND ACCESS INFORMATION:

- 4TU.ResearchData
- Delft, 28 January 2021