Improving CFD modelling of drinking water reactors

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**Project duration**  
6-9 months

**Research field**  
Hydraulic modelling of liquid-solid fluidisation in drinking water treatment processes

**Subject title**  
Improved CFD modelling of irregularly shaped particles in drinking water hydraulic reactors

**Introduction**

**Softening**

In the Netherlands, an annual 400 million m³ drinking water is softened in treatment plants with fluidised bed pellet reactors (Figure 1). The reasons for softening drinking water concern the protection of public health, the protection of the environment, the economy and increased comfort for users.

**Water cycle**

Waternet is Amsterdam’s water cycle company that controls the area’s water cycle in an integral and socially responsible manner, based on four values: safety, customer orientation, sustainability and innovation. It means that Waternet focuses on providing inexpensive and clean water to its customers and at the same time aims to increase the sustainability of water treatment. In particular, one of Waternet’s strategic goals is the completion of CO₂ neutral water treatment plants by 2020. However, in order to achieve this goal, the water treatment plant needs to be operated in an efficient way that would minimise the impact on the environment. As a result, re-use of materials and minimisation of the use of chemicals in all water treatment steps is necessary. Waternet has an annual 90 million m³ production of drinking water and uses liquid-solid (Figure 2) fluidised bed pellet softening reactors. This takes place at the Leiduin and Weesperkarspel water treatment plants and is aimed to reduce the calcium content of drinking water.

**Softening process**

The softening process involves the dosing, which leads to an alteration of the calcium carbonate equilibrium in which the solubility product is exceeded. The reactor is filled with seeding material and calcium carbonate (CaCO₃) pellets (Figure 3). The large specific surface area in the reactor causes the CaCO₃ to crystallise on the particles, called pellets, as a result of which these grow in size and become increasingly round. Since larger particles will migrate to the lower region of the reactor bed, a stratified bed will evolve. To retain the right fluidisation conditions, it is important to prevent situations that lead to a fixed bed state. Therefore, the largest pellets (usually those that are larger than 1-2 mm) are extracted from the reactor and used as a by-product in other processes, for instance in industrial and agricultural processes.

**Sustainability**

Pellet-softening in a fluidised bed reactor was developed and introduced in the Netherlands in the late 1980s, and by the end of 2017 almost all Dutch drinking water will be softened with the help of this technique. For more than 30 years, crystal and garnet sand have been used as a seeding material. To meet sustainability goals and to promote the
development of a circular economy, water companies have modified their pellet-softening processes, in which garnet sand has been replaced by calcite seeding particles that are based on re-used ground, dried and sieved calcium carbonate pellets. The garnet core inside the pellets hinders their potential application in market segments such as the glass, paper, food and feed industries, and it hinders their direct re-use in the pellet reactor itself when it comes to ensuring a more sustainable and circular process. The pellet market value and the sustainability of the softening process can be increased through the substitution of the sand grain by a calcite grain of 0.5 mm (100% calcium carbonate). If the calcite pellets are ground and sieved, they can be re-used as a seeding material.

Traditional models
All traditional fluidisation prediction models are based on perfectly round particles with a one-dimensional particle diameter $d_p$. For water treatment processes, the Carman-Kozeny equation is the most frequently used model to predict fluid dynamics such as bed porosity and pressure drop of a fluid flowing through a reactor’s packed bed of grains. For the derivation of this model, several assumptions have been introduced. From a modelling departure point, the reactor bed is divided into a collection of curved passages or capillary tubes. Then the actual or interstitial fluid velocity between the particles is introduced. In addition, to compensate for permeability, a tortuosity factor is proposed as a correction factor. Accordingly, the pressure difference can be calculated using Hagen-Poiseuille’s law describing laminar fluid flow in straight, circular section pipes. However, the equation is only valid for laminar flow. With an adjusted Reynolds number, the model can be modified and evolve into an expression consisting of a laminar group and a second group, enabling us to represent more turbulent regimes. The result is an expression to estimate the total pressure difference or drag. In a reactor filled with fluidised particles, the frictional pressure drop is constant and independent of the superficial velocity.

In case of perfectly round spheres, the drag can be calculated rather accurately. However, the model’s prediction accuracy decreases significantly in case irregularly shaped particles are used. This is due to their complexity, or in most cases, the impossibility to correctly determine the uniquely defined irregularly shaped particles of practical interest. A pragmatic approach is to introduce so-called shape correction factors. One of these is sphericity, which is frequently used as a measure of how closely the shape of an irregularly shaped particle approaches that of a mathematically perfect sphere. Still, using shape factors leads to two rather awkward scenarios: well-defined shape factors (e.g. $\phi \approx 0.8$) work well in a fixed bed state, but when a fluidised bed state appears, the shape factor approaches ($\phi \approx 1$) for the same particle-fluid system. The explanation for this is rather straightforward. In a fixed bed state, irregularly shaped particles are randomly ordered or have random orientations corresponding with a specific drag larger than the theoretically predicted value for round spheres (Figure 4). So, in case fluid velocity is increased, particles re-orientate in a more vertical direction, and the corresponding drag decreases and approaches the theoretically value. In case fluid velocity goes up even further, the drag increases again due to a re-orientation of particles in a more horizontal direction, caused by the greater distance between the particles. This has been demonstrated through fluidisation expansion experiments in an experimental set-up with different sieved particles.

Assignment
The assignment starts with a thorough literature survey to obtain a comprehensive overview of the proposed assumptions and adjustments regarding the Carman, Kozeny and Ergun models. From the field of porous media and hydraulics, existing and state-of-the-art tortuosity models will be examined which can be used to improve the current model.
The assignment focuses on the improvement of the Carman-Kozeny prediction model for optimisation and process control purposes while taking irregularly shaped particles into account. The project’s aim is to obtain new insights and therefore substantially increased knowledge regarding the hydraulics of drinking water treatment processes (liquid-solid fluidisation) through the synthesis of more accurate prediction models and the use of computational dynamic modelling.

**Knowledge gap**

It is not clear how the dimensions of irregularly shaped particles can be used in traditional predicting models.

**Hypothesis**

We expect that Computational Fluid Dynamic modelling will enable us to better quantify particle shape or area in liquid-solid fluidisation prediction models for drinking water softening purposes.

**Research questions**

- To what extent can hydraulic models be improved through applying the drag influences exerted on particles in liquid-solid systems instead of using a pragmatic attempt to compensate irregularity? This particularly includes shape factors in models derived for perfectly round spheres in which the hydraulic effects of particle orientation, rotation and classification are considered.
- Is it possible to explain the observed deviation of naturally irregularly shaped natural particles in terminal settling conditions?
- Is it possible to use spheroids or rods in the Carman-Kozeny model for a simplified expression for irregularly shaped particles?
- What is a suitable definition of irregularly shaped particles in a liquid-solid fluidisation system?
- Can particle sphericity be determined easily through specific experiments?
- Which CFD model is suitable for modelling purposes? Direct Numerical Simulations with embedded particles?
- What is a suitable net drag relation for non-spherical particles? The Hölzer-Sommerfeld relation?

**Modelling**

This assignment is mainly focused on Computational Fluid Dynamic modelling.

**Product**

The output of this study is a specified and quantitative analysis and advisory report for Waternet.

**Experiments**

Experiments can be carried out at the pilot plant facility at Waternet (Weesperkarspel production plant) in Amsterdam. A novel fluidisation and filtration pilot set-up has been put in place for this research project. The acquired mathematical prediction model can also be compared and evaluated for natural, imperfectly round grains applied in full-scale drinking water treatment installations of Waternet.

**Requirements**

“C” competences of the student: the student has to be inquisitive and eager to learn, committed, connective, constructive, and he/she should be able to report on work done in a comprehensive yet concise manner.
**Technical data**

Drinking water production: 30 (Weesperkarspel) + 6 0 million (Leiduin) m$^3$/y for more than 1 million citizens.
Homogeneous liquid-solid fluidised bed reactors: 8 (Weesperkarspel) + 12 (Leiduin).
Reactor height: 5.5 (Weesperkarspel) + 6.0 (Leiduin).
Reactor diameter: 2.6 (Weesperkarspel) + 3.0 (Leiduin).
Water temperature range: 5-25 °C.
Superficial fluid velocity: 60-90 m/h.
Granular seeding material: 0.4-0.6 mm.
Granular calcium carbonate pellets: 0.8-1.2 mm.
Caustic soda dosed concentration 25% w/w.
Raw water total hardness: 2.4 mmol/L.
Softened drinking water total hardness: 1.4 mmol/L.
Total numbers of nozzles in sandwich bottom plate: 189 (Weesperkarspel) + 247 (Leiduin).

**Contact information**

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