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Influence of operation conditions on cake structure in dead-end membrane filtration: Monte Carlo simulations and a force model

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ABSTRACT

Understanding the cake structure during filtration is important to minimizing fouling and reducing cleaning operation. Here, a Monte Carlo model is proposed to investigate the effect of Hamaker constant, zeta potential, particle size, ionic strength and applied pressure on the profile of the particle volume fraction of the cake structure. A scaling relationship between the local deposit solid volume fraction and various operation conditions in the micro-scale is presented. This result can be well explained by a force balance model based on the two simple particle distributions. Combining this scaling relationship and a developed force accumulation and transfer model allows a better determination of the reversibility of the deposit layer, and also provides insight into selecting appropriate cleaning strategies.

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1. Introduction

Microfiltration and ultrafiltration are now used in a wide range of industrial applications (in the food, biotechnology, pharmaceutical, water industries and waste-water treatment). For these processes, fouling is an unavoidable deleterious phenomenon that causes serious permeate flux decline. This can be typically classified into two processes: concentration polarization (CP) layer and cake layer formation on the membrane surface. The CP layer reaches its steady state after a short time period when the filtration process begins. Thereafter, suspended particles continuously accumulate and form a dense cake layer which becomes the major resistance to the permeate water flux (Aimar and Bacchin, 2010; Bacchin and Aimar, 2005; Bacchin et al., 2002a; Beyer et al., 2010; Chen et al., 1997; Daniel et al., 2011; Field and Wu, 2011; Zhang and Ding, 2015). Several studies on permeate flux decline indicate that particle accumulation during membrane filtration is affected by physical and chemical characteristics of the particle system, such as particle size, ionic strength, zeta potential as well as hydrodynamic operating conditions (Chan and Chen, 2001; Chen et al., 2005; Harmant

and Aimar, 1996, 1998; Jia et al., 2015; Kim and Hoek, 2002; Kühnl et al., 2010; Li et al., 2011a; Vigneswaran and Kwon, 2014).

Four classical mechanistic models have been applied to explain the membrane fouling: standard pore blocking, complete pore blocking, intermediate pore blocking and cake filtration. Some combined models that integrate two or more of the above, which could provide suitable fits of experimental data (Cao et al., 2015; Duclos-Orsello et al., 2006; Grenier et al., 2008; Ho and Zydny, 2000; Vela et al., 2008). In order to understand membrane fouling in depth, some online measurements (Ding et al., 2016; Dreszer et al., 2014; Gao et al., 2014; Li et al., 2012, 2014a, 2014b; Mendret et al., 2009, 2007; Sung et al., 2003; Tarabara et al., 2004) have been proposed to relate the properties of the deposit cake layer and the decline of the filtration flux.

Besides experimental investigations, numerical models (Ando et al., 2012; Bacchin et al., 2006b, 2002a; Bowen and Sharif, 2002; Bowen and Williams, 2007; Broeckmann et al., 2006; Bugge et al., 2012; Chang et al., 2006; Chen and Kim, 2006; Chen et al., 2011; Duclos-Orsello et al., 2004; Griffiths et al., 2014; Günther et al., 2012; Han et al., 2017; Li et al., 2011b; Mendret et al., 2010; Mignard and Glass, 2001; Redkar et al., 1996; Shin et al., 2013; Tien and Ramarao, 2013; Wang et al., 2014; Wang and Li, 2012, 2014) can promisingly help in finding the best directions to improve the process efficiency, at a lower cost than carrying out systematic experimental explorations of the processing parameter

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space. But the accuracy of these models depends on the development of predictive models that can inter-link solution properties and operating conditions to filtration performance. In the macroscopic scale, film theory, gel layer, osmotic pressure and boundary layer resistance models are several of the theoretical approaches that have been developed (Bacchin et al., 2006a, 2002b; Elimelech and Bhattacharjee, 1998; Romero and Davis, 1990; Song and Elimelech, 1995; van den Berg and Smolders, 1990; Welsch et al., 1995). These models can simulate the filtration process and investigate the influence of process parameters on permeate flux decline. However, the reality of these theoretical and numerical models highly depends on the knowledge of the cake structure in the micro-scale. In most practical applications, the profile of the cake volume fraction is rarely and not easily measurable. On the contrary, the microscopic models with consideration of the particle-fluid and inter-particle interactions can naturally reveals the true structure of the cake layer.

Among various numerical models in microscopic scale (Bowen and Sharif, 2002; Bowen et al., 2001; Chen et al., 2005, 2011; Chen and Kim, 2004, 2006; Kim and Hoek, 2002; Kim and Liu, 2008), Monte Carlo simulation may be one computationally efficient algorithm for multi-particle interactions (Chen and Kim, 2004). Kim's group had provided the complete details of Monte Carlo method for dead-end and cross-flow filtration (Chen et al., 2005; Chen and Kim, 2006; Kim and Hoek, 2002; Kim and Liu, 2008). Their models usually included inter-particle interaction based on Derjaguin–Landau–Verwey–Overweek (DLVO) theory (Derjaguin, 1941; Verwey et al., 1948) and hydrodynamic drag force, and successfully investigated the influence of the filtration processing parameters on the cake structure and filtration flux.

In the present work, we have used MC simulation to investigate the possibility of describing the influence of various operation conditions on cake structure in a more general way. We have attempted to use a simple force balance model to explain the observed scaling laws. Finally, the scaling laws coupling with a developed force accumulation and transfer model is used to predict and compare with the reported experimental data (Harmant and Aimar, 1996).

2. Model

2.1. Governing equations

The model system is composed of charged, spherical particles interacting via a DLVO pair potential, which is comprised of attractive Lifshitz-van der Waals (VDW) and repulsive electrostatic double layer (EDL) interactions (Hunter, 2001).

$$V_{DLVO} = V_{VDW} + V_{ELE} \quad (1)$$

where V_{VDW} is the van der Waals' potential and V_{EDL} the electrostatic double layer potential. The attractive van der Waals potential between equal-sized particles can be modeled by many available expressions. In this study, it is calculated by

$$V_{VDW} = -\frac{A}{6} \left(\frac{2}{s^2 - 4} + \frac{2}{s^2} + \ln \frac{s^2 - 4}{s^2} \right) \quad (2)$$

$$\text{with } s = \frac{2r + h}{r}$$

where h is the minimum separation between the particle surfaces, r the particle radius, and A the Hamaker constant (Hamaker, 1937; Hunter, 2001). The electrostatic interaction potential between the particles is calculated from the linear superposition approximation (Hong, 1998; Horn, 1990):

$$V_{ELE} = 64\pi\epsilon_r\epsilon_0 \left(\frac{RT}{zF} \right)^2 \times \tanh \left(\frac{zF\psi_1}{4RT} \right) \times \tanh \left(\frac{zF\psi_2}{4RT} \right) \times \frac{r_1 r_2}{r_1 + r_2} e^{-\kappa h} \quad (3)$$

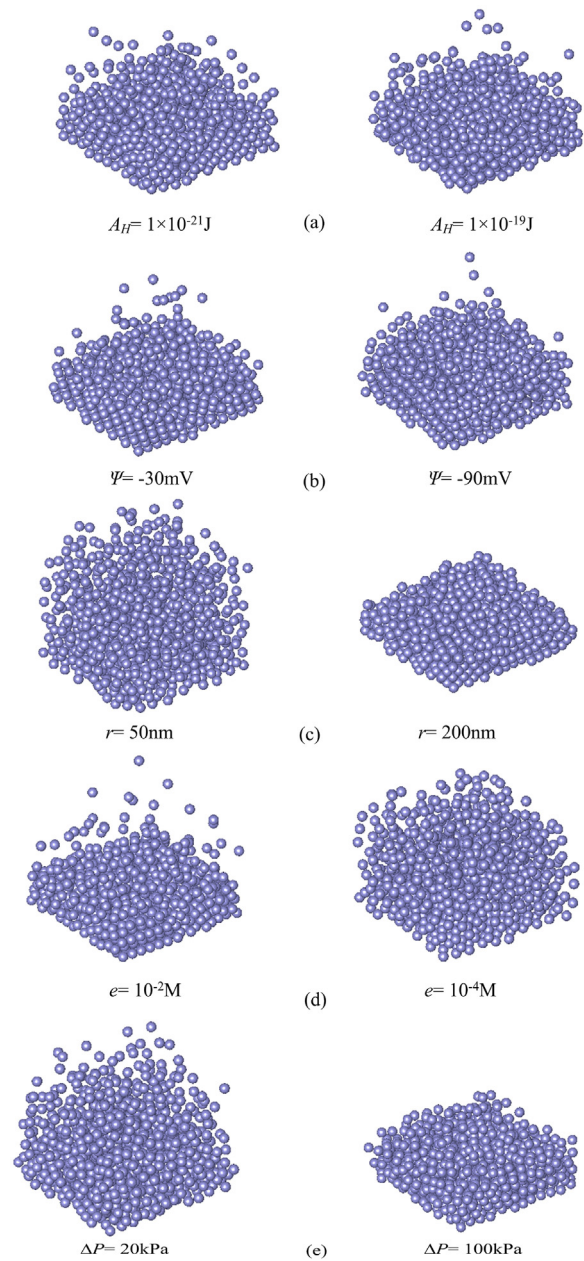


Fig. 1 – Snapshots of MC simulation results for various operation conditions, other processing parameters values are adopted the asterisked values in Table 1: varied (a) Hamaker constant, (b) zeta potential, (c) particle radius, (d) ionic strength of solution and (e) applied pressure.

in which ψ_1 and ψ_2 are the zeta potentials. κ is the Debye–Huckel parameter where κ^{-1} represents the characteristic thickness of the double layer, can be given by

$$\kappa^2 = \frac{2000e^2 N_A I}{\epsilon_r \epsilon_0 k_B T} \quad (4)$$

F is the Faraday constant, z the valence of the electrolyte, ϵ_r the dielectric constant of the medium, ϵ_0 the permittivity of vacuum, k_B Boltzmann's constant, R the gas constant, e is the charge on the electron, N_A the Avogadro's number and I the ionic strength of the solution, respectively.

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