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Towards predictive modeling of crystallization fouling: A pseudo-dynamic approach

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ABSTRACT

In this work, a new computational fluid dynamics (CFD) model is developed to characterize a crystallization fouling process mathematically. The introduced method incorporates a pseudo-dynamic scheme where the dynamic fouling process is approximated as a set of sequential steady-state processes taken place in a continuously varying geometric domain. This unique approach allows the characterization of mass, momentum and heat conservations of a continuous flow of liquid over a growing fouling layer. Dynamic evolution of the fouling layer surface (even with a complex shape) and its intricate interactions with hydrodynamics and fouling kinetics can then be rigorously taken into account. The introduced model was validated using the experimental data for a calcium sulphate fouling system. Furthermore, the effects of the solution chemistry and operating conditions on fouling resistance evolution were quantified through a comprehensive parametric study. As a predictive tool, this model could be especially useful for the identification of effective fouling mitigation or even elimination strategies.

1. Introduction

Fouling of heat exchangers is still an ongoing problem that causes tremendous energy loss and substantial costs in a wide variety of industries, although continuous progresses have been made to understand fouling mechanisms and pursue fouling mitigation approaches (Kazi et al., 2009; Zhao and Chen, 2013). In the past decades, numerous studies have been carried out to explore how surface characteristics, solution chemistry, and operating conditions can be manipulated to inhibit fouling layer growth (Forster and Bohnet, 2000; Zhao and Chen, 2013), which usually require laborious and lengthy experimental schemes. Those efforts may be greatly facilitated if a predictive model is available. The comprehensive 3D dynamic data offered by the model, most of which are not easily attainable using current experimental techniques, could improve our fundamental understanding of fouling mechanisms. Moreover, thorough and systematic in silico experiments can be designed to identify the most effective fouling inhibition pathways.

The complex process of fouling involves several stages, i.e., initiation, transport, attachment, removal and ageing (Bohnet, 1987). In each stage, multiple interconnected physical and chemical phenomena occur simultaneously at multiple scales, which include heat, mass and momentum transfer in the solution domain, and crystal nucleation and growth in the fouling layer domain, etc. The intrinsic multistage, multiphysics and multiscale feature of fouling makes predictive model development an extremely challenging task. Yang et al. (2012) developed a simple lumped parameter model based on the fractional surface coverage to correlate experimental data in the initiation/induction stage. Ishiyama et al. (2010, 2011), Coletti et al. (2010) and Sileri et al. (2011) characterized the ageing stage and explored the effect of ageing on thermal and

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Nomenclature

C_{fs}	surface concentration (mol/m^3)
C_{in}	inlet concentration (mol/m^3)
C_{sat}	saturation concentration (mol/m^3)
D	diffusion coefficient (m^2/s)
g	gravitational acceleration (m/s^2)
h_f	height of the fouling layer (m)
k_R	rate constant of reaction (m^4/(kg s))
K_1	a constant
m_d	deposition mass per unit area (kg/m^2)
m_f	total mass per unit area (kg/m^2)
m_r	removal mass per unit area (kg/m^2)
n	reaction order
q	input heat flux (kW/m^2)
$\dot{r}$	growth rate of the fouling layer (m/s)
Re	Reynolds number
R_f	fouling resistance (m^2 K/W)
$\bar{R}_f$	mean overall fouling resistance (m^2 K/W)
R_g	universal gas constant (J/(mol K))
S_c	supersaturation ratio
t	time (s)
t_{end}	ending time (s)
Δt	time step (s)
T_{fs}	surface temperature of the fouling layer (K)
T_{in}	temperature of the inlet solution (K)
v_{in}	inlet velocity (m/s)
λ_f	thermal conductivity of the fouling layer (W/(m K))
λ_{solid}	thermal conductivity of deposit (W/(m K))
λ_w	thermal conductivity of the fluid (W/(m K))
μ_w	viscosity of the fluid (Pa s)
ρ_{air}	density of air (kg/m^3)
ρ_f	density of the fouling layer (kg/m^3)
ρ_{solid}	density of the deposit (kg/m^3)
ρ_w	density of the fluid (kg/m^3)
σ_f	shear resistance (N/m^2)
τ	shear stress (N/m^2)
$\bar{\tau}$	mean shear stress (N/m^2)
ω	porosity
Ω_e	solution domain
Ω_f	fouling layer domain
$\partial\Omega_{e-f}$	solution-fouling layer interface

hydraulic performance of heat transfer devices. In contrast to the limited work on the stages of initiation and ageing, the other three stages have been investigated more vigorously. The multicomponent transport of all ionic species involved in a carbonic fouling system was described using a rigorous kinetic model by Segev et al. (2012). Their model cannot address the growth and removal of a fouling layer as well as its effect on the thermal and hydraulic behavior of heat transfer devices. A model for fouling layer formation was developed and continuously expanded by Bohnet's group at the Technical University of Braunschweig (Brahim et al., 2003, 2004; Bohnet, 2005). Simplified heat and mass transfer models were adopted and preliminarily coupled to describe the transport, attachment and removal stages of fouling. A major contribution of their efforts is to consider the interaction between fluid flow and geometric evolution of the fouling layer using a scheme called "fictitious crystal growth" (Brahim et al., 2003). The above listed models have improved our quantitative understanding of the fouling process. However, there is still a need to have a comprehensive predictive model that can describe both macro- and micro-scale phenomena throughout the complete multi-stage fouling process.

In this work, aiming at a comprehensive predictive tool, we develop a generic framework for guiding crystallization fouling modeling. The module-based framework assists the identification and development of necessary models at different length scales meanwhile assures the flexibility and integrity of the overall model. As the first key component in this framework, a macroscopic computational fluid dynamics (CFD) model for fouling layer formation is presented with an emphasis on its unique features and capabilities. Example calculations on the calcium sulphate fouling system will demonstrate the validity and effectiveness of our method. Furthermore, parametric analyses will be carried out to reveal quantitatively the effect of the solution chemistry and operating conditions on fouling layer growth. Discussions on the need for the development of microscopic crystallization models, promising scale coupling approaches, as well as specific fouling models for the initiation and ageing stages will be given in the end.

2. Modeling methodology

A general framework has been constructed to guide the development of fouling models. Fig. 1 illustrates the model system that consists of two key domains, i.e., the solution domain (Ω_e) and the fouling layer domain (Ω_f) above a heat transfer surface. Moreover, the model framework contains two layers of modeling blocks, which are bi-directionally coupled.

Within the solution domain, mass, momentum and heat transfer coupled with homogeneous bulk reactions need to be characterized to obtain the chemical, thermal and hydrodynamic environment. The localized fouling environment then serves as an input for the models in the fouling layer domain, where surface reactions determine the flux of reactive species across the solution-fouling layer interface ($\partial\Omega_{e-f}$) as well as the change of the interface location (i.e., fouling layer removal or growth). Thus, they provide the boundary condition and boundary location for the solution domain models. Note that the heat transfer surface serves as a bottom boundary of the fouling layer, where a constant heat flux or a constant temperature can be specified. In this section, general methods for most modeling tasks listed in the framework are presented with an emphasis on their interrelationships. Specifically, the unique pseudo-dynamic scheme for fouling layer growth is introduced in detail. Model implementation methods are also delineated.

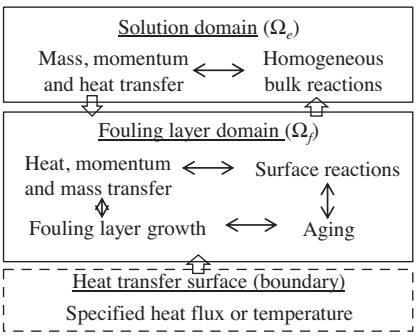

Fig. 1 – Fouling model framework and simulation domain decomposition.