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Development of an ultrafiltration predictive model to estimate the cost of downstream in biorefineries: Effects of epistemic experimental uncertainties

A. Rosengart *, M. Vizzi, F. Manenti, A. Citterio

Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, piazza Leonardo da Vinci 32, 20133 Milano, Italy

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ABSTRACT

Crossflow filtration is a common unit operation for bio-separations, in particular for high volume applications, as biofuel production facilities and other biorefineries. However, the complex mechanism of membrane bio-fouling hinders the development of a general predictive model, to be used for cost and life-cycle evaluations in conceptual design of new processes. To overcome the limited applicability of fully empirical models, a simple though general Darcy model was used to describe flux reduction. The equations representing the additive resistances to flux were defined after a systematic review of the available literature. The developed model was successfully benchmarked with the data from a biorefining pilot plant. Provided the little agreement of literature on the values of the semi-empirical parameters of the model equations, these parameters were considered as fuzzy variables, characterized by an inner uncertainty especially if extended outside their experimental boundaries. Possibility theory was hence applied to study the propagation of uncertainty, from the model parameters to the model output (average flux and filtration cost). The range of variability of the upper cost of filtration was calculated for a biorefinery case study: the resulted estimates are compatible with real industrial filtration costs. The model provides also an indication of the economic risk due to limited experimental knowledge.

1. Introduction

High throughput and contained costs are primary aspects for any downstream operation in the field of biorefinery. Chemical building blocks, monomers and fuels derived from biomass must compete with the low price of oil, though introducing a number of new technological challenges related to seasonality, dilution, non-homogeneous substrates. In particular, bio-products recovery accounts up to the 80% of the final price [1] and the removal of the microorganisms from the fermentation broth becomes one of the most relevant downstream operations [2]. For large-scale applications, crossflow filtration is widely used, as a support to centrifugation or even in its substitution, thanks to a much sharper particle size cut-off and a lower energy consumption. As for many other operations in bioprocesses, the method to scale up filtration units is strongly empirical, because of the variability of filterable substrates and because of the diverse possible operation conditions [3]. However, when assessing the economic feasibility of a new process at its early stage of study, it is not always possible to proceed with the usual empirical approach. Quality by Design (QbD) practice, theorized for pharmaceutical industry but gaining consent also in industrial biotech, requires quick estimations of process layout even at the first stages of bio-chemical routes investigations, when the available data are minimal. In this way, the economic and environmental performances of the future plant are taken into account from the beginning. QbD inspired approaches have been applied to new productions as bio-ethanol [4], bio-butanol [5], polyhydroxy-alcanoates [6].

Unfortunately, the lack of standardized data for ultrafiltration units complicates any predictive approach, which is unavoidable when dealing with preliminary studies or small-scale experimental information.

The problem of representing microorganism suspensions in industrial crossflow filters has been extensively studied, but the results are always strongly dependent on the experimental conditions and little reproducibility has been achieved, even for the same bacterial strains. Tarleton and Wakemann stated in the middle of the 90s that previous studies suffered of "conflicting experimental data", and tried to de-couple the different mechanisms of

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* Corresponding author.
E-mail addresses: alessandro.rosengart@polimi.it (A. Rosengart), mattia.vizzi@mail.polimi.it (M. Vizzi), flavio.manenti@polimi.it (F. Manenti), attilio.citterio@polimi.it (A. Citterio).

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Nomenclature

A	membrane area (m^2)
c	concentration (kg/m^3)
D	diffusion coefficient ($m^2\ s^{-1}$)
d	diameter (m)
J	flux ($m\ s^{-1}$)
K	mass transfer coefficient, cells ($m\ s^{-1}$)
k	mass transfer coefficient, colloids ($m\ s^{-1}$)
L	module length (m)
m	mass (kg)
N	necessity
n	cake compressibility index
P	possible probability distribution
R	resistance (m^{-1})
t	time (s, min, h)
u	cross flow velocity ($m\ s^{-1}$)
V	holdup volume (m^3)
w	cells mass per square meter ($kg\ m^{-2}$)

Greek symbols

α	specific cake resistance ($m\ kg^{-1}$)
$\alpha cuts$	alpha-cuts
β	time constant (s^{-1})
$\dot{\gamma}$	shear rate (s^{-1})
ΔP	pressure difference (Pa)
δ	cake thickness (m)
ε	cake porosity (–)
μ	dynamic viscosity (Pa s)
Π	possibility
ρ	density (kg/m^3)
Φ	solidosity (particle volume fraction) K

Superscripts

bulk	bulk phase
gel	membrane gel layer
cake	cake
StSt	steady state

Subscripts

0	reference
ads	adsorption
c	cake
cells	cells
h	hydraulic
K	experimental coefficient
mat	material
p	permeate
pol	concentration polarization
shear	shear
TM	trans membrane
x	colloid

biological fouling [7]. The main obstacles for a good modelling were later identified in the complexity of biological solutions, the weakness of the theoretical models and the non-linear interactions between different causes [8].

The easiest representation of the flux of permeate in a filter is the Darcy law with additive resistance contribution, as reported in Eq. (1).

$$J_p = \frac{\Delta P_{TM}}{\mu_p \sum_{i=1}^{n} R_i} \tag{1}$$

where ΔP_{TM} is the applied transmembrane pressure, μ_p is the dynamic viscosity of the permeate and R_i is the resistances to the flux due to the specific fouling mechanism. The research activity of the late 80s and first half of the 90s was mainly devoted in recognizing which phenomena contribute to membrane bio-fouling (for example bio-film formation, polarization, or others) [9], with some first attempts to model the effects [10]. The main aspects of the fouling mechanism were qualitatively understood, but a general paradigm valid for any type of microorganism was far from being achieved. For this reason, subsequent research efforts changed approach, directing to different purposes.

A first trend in modern filter modelling is the characterization of very specific filtration applications, using adaptive models (Standard Blocking, Complete Blocking and Intermediate Blocking models are some of the most popular) to represent empirical data. The representation is good in most of the applications [11], but the results are highly context dependent, as for yeast filtration in beer industry [12]. Another trend is the development of highly detailed computational fluid dynamics (CFD) simulations of cross-flow filters, to gain a deep and detailed insight of the system [13]. CFD simulations, however, are both computationally and time demanding, applicable only to simplified systems. Also, due to the evasiveness of the fouling mechanisms, another approach is the one of using artificial neural network models [14]. For conceptual design estimations, neither fully adaptive models, nor CFD simulations are suitable due to their lack of flexibility. Instead, a model with a sound physical interpretation, but with few and constrained parameters as Darcy equation, could provide reasonable values to predict the performances of complex (and little investigated) fermentation broths, as some uncertainty is tolerable for preliminary estimates. The uncertainty in the calculated quantities derives from the application of a semi-empirical model whose experimental parameters have been only roughly estimated or have been extended for analogy from similar systems. This lack of knowledge is defined “epistemic uncertainty” and requires statistical concepts from the field of Possibility theory. In this framework, an original and flexible model for representing the biological fouling in cross-flow ultrafiltration units is proposed, with the purpose of estimating filtration costs. An uncertainty propagation algorithm, based on the possibility theory, is implemented to deal with the lack of experimental knowledge of certain biological systems. To the authors’ knowledge, this is the first study that applies possibility theory as a supporting tool to process conceptual design, in the field of industrial bio-filtration.

2. Theory of filter fouling and model development

The permeate flux reduction due to membrane fouling is determined mainly by three aspects: the type of filtration equipment, the operation mode, and the fouling properties of the filtrate.

For the first two, the model will consider the unit layout with fed-batch operation presented in Fig. 1: each feed pump is assumed to serve 24 parallel membrane modules, and each recirculation pump 4 modules (equipment detail will be described in the next sections). This layout is a simplification of the real possible dispositions (multiple array with booster pumps, Christmas-tree network, etc.), which allow an optimization of the pumping expenses [15]: this level of detail is not advisable during conceptual design. Also, the variability of the filter geometries is remarkable, with alternatives such as hollow fiber, spiral wound, flat sheet, tubular and capillary filters [3]. Several technological solutions have applied to enhance filter performances (e.g. vibrating

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