CFD and laboratory analysis of axial cross-flow velocity in porous tube packed with differently structured static turbulence promoters

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Abstract
Computational fluid dynamics (CFD) was used for modeling flow regime in a porous tube. This tube is an ultrafiltration membrane filter made from zirconium-oxide which is very effective in the separation of stable oil-in-water micro-emulsions, especially when the tube is filled with static mixer. The results of the CFD analysis were used in the preliminary optimisation of the static mixer's geometry since it has significant effect on the energy requirement of this advanced membrane technology. The self-developed static mixers were tested "*in vitro*" from the aspect of separation quality and process productivity as well to validate CFD results and to develop a cost effective, green method to recover unmanageable oily wastewaters for sustainable development. In this work the results of computational simulation of the fluid velocity and membrane separation experiments are discussed.

Keywords: cross-flow ultrafiltration, oil-in-water emulsion, computational fluid dynamics, static mixers.

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Oil-in-water emulsion is common by-product in chemical-, food-, mechanical- and other type of industries. Nowadays these waste waters cannot be discharged directly into the natural environment to avoid creating a significant ecological problem. With treatment of such waste oil emulsions, fluid can be separated to its components: oil and water. This separation can be done by evaporation too, but this method is very energy-consuming. Furthermore, in case of stable nano- or micro-emulsions the traditional water cleaning technologies are not always enough efficient to ensure the limited oil values in the released water [1]. With ultrafiltration, concentration of the oil in permeate can be reduced below 50 mg L^{-1} (limiting value for discharge to the public sewer in Hungary [2]). After filtration, the concentrated wastewater may contain less than 1/5 of original volume, so final evaporation might need approximately one-fifth of the original energy requirement to separate the water from the oil.

Using Kenics® static mixer inside a tubular membrane during ultrafiltration of an oil-in-water emulsion has a positive effect to permeate flux, retention of the oil and fouling delay [3]. Originally the aim of Kenics® type turbulence promoter's geometry was the cost effective mixing two or more fluids. For this reason this kind of mixer causes big pressure drop along the membrane; due to this phenomena Kenics® mixer can be used only at lower recirculation flow rates for membrane separation to ensure cost-effectiveness [4]. The main aim of this work was to find new turbulence promoter geometry which will result in similar flux and retention improvement, raising tangential velocity, but keep pressure drop along membrane as low as possible.

In the first step, the new shapes were tested with "*in silico*" simulation experiments. Computational fluid dynamics (CFD) is a state-of-the-art numerical technique for solving fluid problems [5]. CFD calculations use a computational grid to solve the governing equations describing fluid flow, *e.g.*, the continuity equation and the set of Navier-Stokes equations, and any additional conservation equations, such as energy balance, across each grid cell by means of an iterative procedure in order to predict and visualize the profiles of velocity, pressure, temperature, etc. Early users of CFD are found in the automotive, aerospace and nuclear industries. With the enhancement of computing power and efficiency and the availability of affordable CFD packages applications of CFD have extended into the food industry for modeling industrial processes, thereby generating comprehensive analyses leading to designing more efficient systems [6].

Lattice Boltzmann methods which were used for CFD analysis in this work are numerical techniques for the simulation of fluid flows [7]. Their strength lies however in the ability to easily represent complex physical phenomena, ranging from multiphase flows to chemical interactions between the fluid and the borders. Indeed, the methods find their origin in a molecular description of a fluid and can directly incorporate physical terms stemming from knowledge of the inter-

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action between molecules. The methods are often regarded as particular discrete representations of the Boltzmann equation. The Boltzmann equation is analogue of the Navier–Stokes equation at a molecular level, where it describes the evolution of the probability distribution function for a molecule to be present at a given point in the space of positions and velocities, the 6-dimensional phase space. The amount of physical phenomena contained in the model at this molecular level of description is larger than at the hydrodynamic level of the Navier–Stokes equation. This is because the Boltzmann equation is not subject to a separation of time scales and has the ability to describe fluids in non-hydrodynamic regimes with large molecular mean free paths. Furthermore, the molecular model is able to capture transport phenomena such as friction, diffusion and temperature transport and derive the corresponding transport coefficients. Boltzmann equation acts on real-valued quantities, but it describes some dynamics in a discrete phase space which can be called lattice [8].

As result of this simulation, 5 new geometries have been found which should be interesting for real time experiments. After producing 5 new turbulence promoters their effect on initial flux and retention has been tested.

MATERIALS AND METHODS

For computational fluid dynamics (CFD) open source software based on lattice Boltzmann algorithm was used [8]. Input for this method was textual file with 3D matrix in it where rectangular space around membrane was divided into 0.1 mm cubes. Values in this matrix can be 1 (solid material) or 0 (means in that particle is fluid) (Eq. (1)):

$$a_{i,j,k}, \text{ where } i = 1,2,...,72,\ j = 1,2,...,72,\ k = 1,2,...,500,\quad a = 0 \text{ or } 1 \tag{1}$$

Initial average flow velocity was also given as input parameter. After calculation vorticity and velocity norms are calculated for each particle and the output of this computation is also a matrix in textual (*.vti) file. This file can be visually represented with Paraview open source scientific visualization software [9].

The laboratory experiments were carried out in cross-flow mode, using a conventional ultrafiltration set-up with tubular single-channel module containing a ceramic zirconia (ZrO_2) membrane (Exekia, Pall, USA) (Fig. 1). The ceramic membrane had a nominal pore size of 50 nm, inner diameter of 6.8 mm and the effective membrane area of 50 cm^2.

Inside the tube, membrane static mixers were installed as shown in Fig. 2. Turbulence promoter used as origin for comparison was Kenics® static mixer (Omega, USA) made from polyacetate. Based on CFD simulation, for laboratory testing, 5 new static mixers were produced from stainless steel (Fig. 2).

A stable oil-in-water emulsion was prepared from a commercial cutting lubricant oil additive (Unisol, Mol, Hungary). The oil concentration in the emulsion was 5 mass%. The feed was pumped from a tank to the membrane module and then recirculated (Fig. 1). The recirculated flow rate (*RFR*) and transmembrane pressure (*TMP*) were controlled by means of regulation valves. The recirculated flow rate was 100 L h^{-1} and transmembrane pressure was 2 bar.

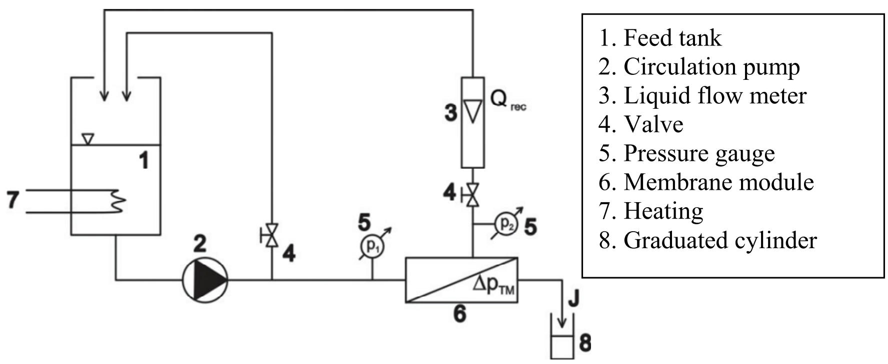

Figure 1. Schematic diagram of the experimental set-up.

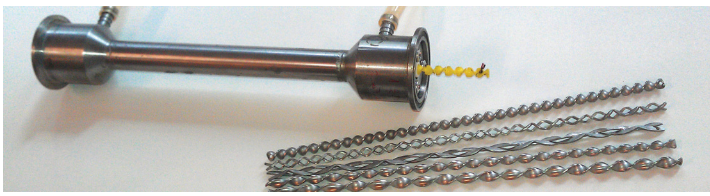

Figure 2. Kenics® static mixer in membrane module (left), 5 new turbulence promoters (right).

The membranes were cleaned according to the recommendations of the manufacturers prior to each experiment and the pure water fluxes of the cleaned membranes were measured. The cleaning procedure was repeated until the original water flux was restored.

Beside permeate flux, and retention of the oil, one of the most important parameter from an economical point is pressure drop along the membrane, because it has direct effect to specific energy consumption (E in (J m^{-3}) defined as the power dissipated per unit volume of permeate. The hydraulic dissipated power is directly related to the pressure drop along the membrane module (Δp in Pa) and the specific energy consumption can be calculated as:

$$E = \frac{RFR\Delta p}{J_p A} \tag{2}$$

where J_p (L m^{-2} h^{-1}) is the permeate flux, A (m^2) is the membrane surface area and RFR (L h^{-1}) represents the recirculated flow rate.

The permeate flux was calculated from the experimental data with the following classical equation:

$$J_p = \frac{V}{tA} \tag{3}$$

where V (L) is the volume of permeate and t (h) is for time.

The oil concentrations in the feed and the permeate solutions were analysed using UV spectrophotometer on 600 nm wave length. Measured absorbency was converted to concentration using calibration curve.

RESULTS

CFD Analysis

In Fig. 3 the CFD analysis of the 6 different packing is demonstrated, from 1 to 6. In each figure the vorticity norm (norm of the vorticity vector in 3D) distribution (based on discrete particle motion) can be found on the left, the matrix of the turbulence promoter is the middle one and on the left the structure of static mixer is illustrated. The green colour shows low vorticity values compared to blue surface where the vorticity is increased. In Figs. 3–7 it can be seen that Kenics® static mixer causes very big turbulence because of high friction of fluid with turbulence promoter. As a result this phenomenon causes enormous pressure drop along membrane. This pressure change has direct effect on specific energy consumption of ultrafiltration (Eq. (2)). Static mixers Nos. 1 and 2 on Fig. 3 doesn't ensure very intensive promotion of turbulence (compared to Kenics® type mixer), but the problem is still the high pressure drop caused by the geometry. Spiral--ribbon mixer (Fig. 3, No. 3) could be optimal solutions for turbulence promotion since the velocity increase caused by them does not results in higher pressure drop along the module. However the shaping is crucial with these types of mixers; when the spiral's pitch is too large and the size (diameter and thickness) is small the mixing efficiency is very limited.

Laboratory UF experiments

The method to simulate permeation through the pores of a given membrane with CFD is still under

Figure 3. CFD pictures generated with ParaView [8] static mixers: 1) zigzag h/d = 2, 2) zigzag .h/d = 1.2, 3) spiral h/d = 1, 4) spiral h/d = 1.5, 5) spiral h/d = 2, 6) Kenics® static mixer.

development thus the effect on the flux or retention of the membrane cannot be seen in the figures. Because of this the next step was the test of the turbulence promoters in real environment from the aspect of oil retention, but also flux and pressure-drop. The results of this ultrafiltration experiments with new static mixers are presented in Figs. 5–7. In Fig. 5 the flux increasing effect of inline static mixers can be seen. If the flux-enhancement is the standalone target, Kenics® type mixer (6.) and the dense spiral mixer (3.) are the best choices, but the zigzag mixer (2.) is very good as well. Noticeable fact, that the permeate flux of an ultrafilter could be raised up to 3–4 times higher with appropriate static turbulence promoter packing. In Fig. 6 it is well understood that mixer No. 6 causes great promotion in the fluid which generates flow resistance and leads to drastically increased energy requirement. The promoter No. 6 was developed for mixing reasons and due to this its application for membrane filtration enhancement is not advisable. Comparatively, the turbulence promoters which were developed for membrane applications behave more like the empty tube – except No. 2 zigzag mixer. From energy consumption point of view the No. 2 significantly increases the energy usage of the operation.

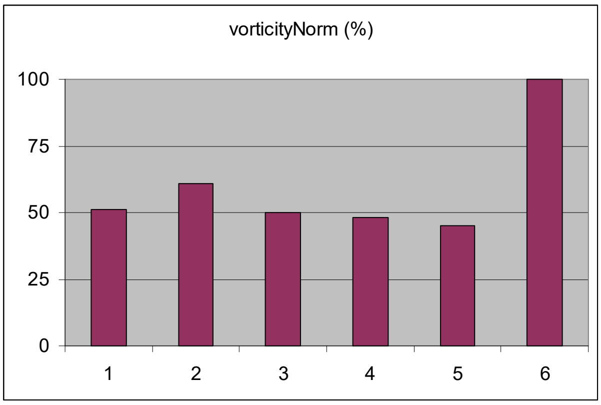

Figure 4. Vorticity Norm peaks in % compared to Kenics® static mixer.

In Fig. 7 oil retentions of the membrane are introduced. Consecutively the No. 3 promoter showed the best, industrially acceptable separation of emulsified oil droplets, especially on 100 L/h and 1 bar TMP. It is also

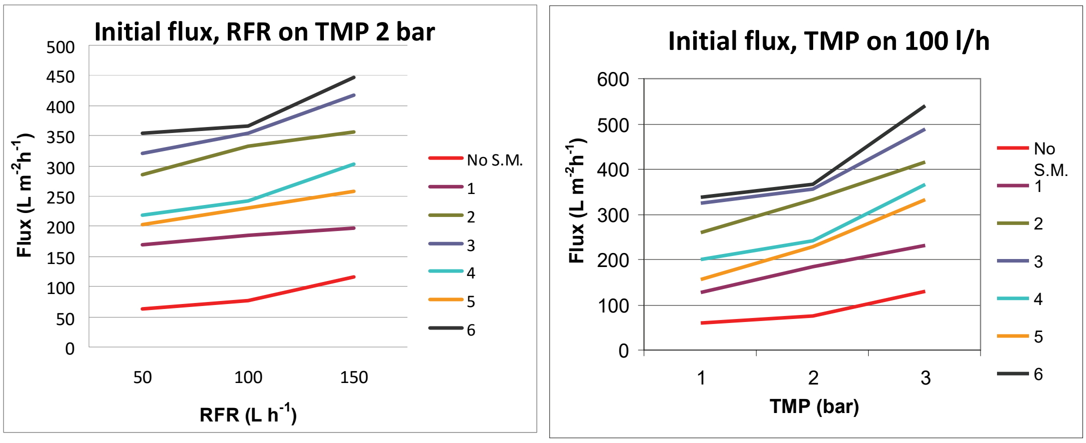

Figure 5. Initial flux vs RFR (left), Initial flux vs. TMP (right).

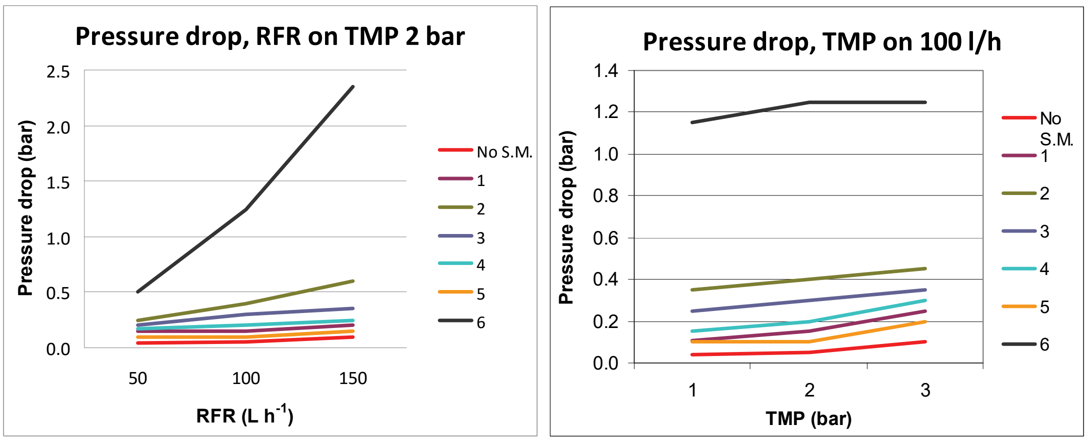

Figure 6. Pressure drop along membrane vs. RFR (left) and pressure drop vs. TMP (right).

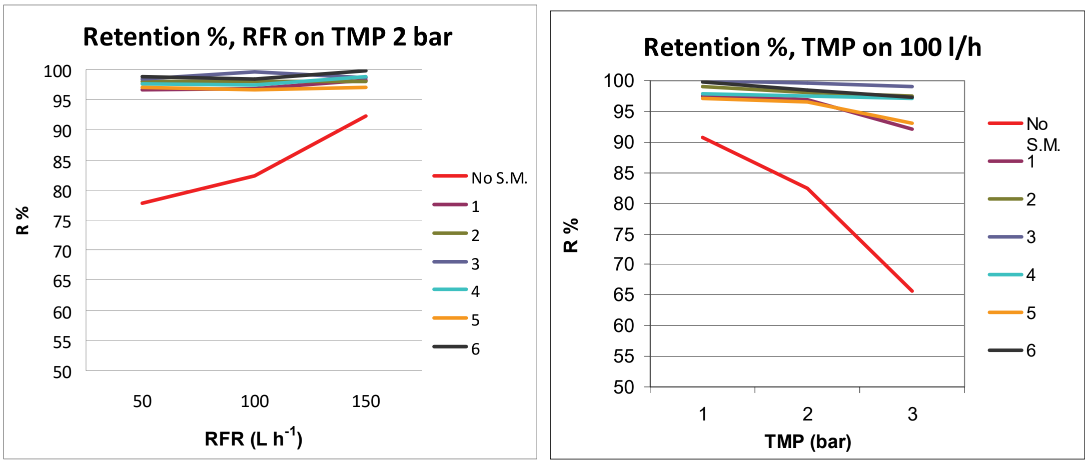

Figure 7. Retention % vs. RFR (left) and Retention % vs. TMP (right).

obvious that the traditionally used empty tube membrane could not ensure satisfying separation of the oil (No S.M.). It can be also seen in Fig. 7 that all of the package could greatly increase retention of the membrane, but since the environmental limit is very strict, some of the results are still not good enough.

Based on the above mentioned result, because of its high flux, low energy demand and high increase of oil retention, static mixer No. 3 is an ideal choice, if productive and sustainable technology is required for stable oil-in-water emulsion separation. The results of CFD analysis is validated with laboratory experiments.

CONCLUSIONS

Computational fluid dynamics is a method with great potential in the prediction of turbulence intensity inside a tubular membrane filter. In present work cross-flow velocity was modelled successfully within a tube packed with differently shaped static turbulence promoters. The model could help to better understand flow regime phenomena caused by different inline static mixers. The method pointed clearly out the adventage of Kenics® FMX type promoter in operations where mixing is a main target, but the simulation also suggested the solution for membrane separation purposes. As far as the CFD still not including the transport through the pores of the membrane, so this is an area with a need for further development in recent algorithms. In future work, the pressure analysis of the same problem with CFD is planned. In order to validate CFD results, the laboratory experiments were also carried out. Within the investigated range, using any of 5 new static mixers showed good improvement for permeate flux and retention of the oil and pressure drop along membrane was significantly reduced using optimised types of turbulence promoters compared with Kenics® static mixer and the empty tube. The experimental data suggests that, for ultrafiltration of stable oil-in-water microemulsion, turbulence promoter No. 3 has best performance (spiral, $d \cong h$).

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IZVOD

CFD I LABORATORIJSKA ANALIZA AKSIJALNE BRZINE PROTOKA KROZ POROZNE CEVI SA PROMOTERIMA TURBULENCIJE RAZLIČITE GEOMETRIJE

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(Naučni rad)

Kompjuterska dinamika fluida (*computational fluid dynamics*, CFD) je primenjena za modelovanje režima protoka u poroznoj cevi. Porozna cev je membrana sa aktivnim slojem od cirkonijum-oksida, koja služi za razdvajanje stabilne mikroemulzije ulje-u-vodi, a čija se efikasnost povećava kada se u cev ubace statički mešači. Rezultati CFD analize su primenjeni za preliminarnu optimizaciju geometrije statičkog mešača, budući da ona ima značajan uticaj na količinu utrošene energije pri unakrsnoj ultrafiltraciji. Statički mešači razvijeni u našoj laboratoriji, eksperimentalno su testirani sa aspekta kvaliteta i efikasnosti procesa separacije i dobijeni rezultati su upoređeni sa rezultatima CFD analize, a sve sa ciljem da se razvije ekonomski efikasan i ekološki prihvatljiv način prečišćavanja otpadnih zauljenih voda. U radu se diskutuju rezultati dobijeni kompjuterskom simulacijom protoka i brzine fluida i eksperimentalni rezultati membranske separacije uz primenu statičkih mešača.

Ključne reči: Ultrafiltracija • Emulzija ulje-u-vodi • Kompjuterska dinamika fluida • Statički mešači