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CT scanning of membrane feed spacers – Impact of spacer model accuracy on hydrodynamic and solute transport modeling in membrane feed channels

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ABSTRACT

This study evaluated the impact of precise representation of spacer geometry on numerical simulations of hydrodynamics and solute transport in feed channels of membrane processes. Three levels of increasing geometry accuracy were assessed: i) cylindrical filaments, ii) filaments with circular sections of variable diameter based on microscopic measurements, and iii) geometries obtained from X-ray computed tomography (CT scans) in three resolutions (22 µm, 11 µm, and 5.5 µm). The three-dimensional CT scans revealed quasi-elliptic, not circular, cross-sections of the filaments. Microscopic measurements fail to account for this ellipticity, resulting in overestimation of pressure drop calculated at industry-typical average velocities (0.07–0.15 m s^{-1}) by a factor of 1.8 compared to CT-based geometries. On the other hand, the cylindrical spacer filaments representation overestimates concentration polarization at the membrane surface compared to CT-based geometries. Experimental results of pressure drop and particle deposition were in close agreement with simulations using CT scanned geometries. This work demonstrates that modeling results depend significantly on the spacer geometry accuracy. Within the investigated CT scan accuracies 20 µm was found sufficient for modeling hydrodynamics and solute transport in spacer-filled feed channels. The results may be useful for reliable investigation and development of novel spacer geometries.

1. Introduction

Feed spacers are used in spiral-wound membrane modules to create a flow channel between two sheets of adjacent membrane leaves and to potentially enhance feed water mixing so that the build-up of concentration polarization at the membrane surface is attenuated [1]. The most widely applied spacer geometry in practice is the bi-planar net made of extruded polypropylene. It comprises two layers of parallel filaments (non-woven), which commonly form a diamond-shaped layout at a thickness of typically 0.6–0.9 mm (24–36 mil) [2,3]. Spacer filaments deviate from a straight cylindrical shape and exhibit varying thickness ("necking") with the largest diameters at the intersection points [3,4]. Therefore, spacers exhibit a rather complex and irregular geometry.

Spacer geometry is critical to module performance as it directly relates to hydrodynamic and solute transport [5]. The flow field also determines the local distribution of foulants [6]. Thus, for quantitatively reliable fluid flow and solute transport simulations employing computational fluid dynamics (CFD), spacer model geometries close to the original conditions are crucial. However, current spacer geometry modeling is still carried out using far-ranging simplification of the geometry. Two-dimensional (2-D) representations of the cross-flow channel that are used to quickly obtain qualitative results (e.g., by modeling the spacer as an array of circular flow obstacles) were reported to oversimplify the intricate three-dimensional (3-D) hydrodynamics within cross-flow channels [7,8]. Various 3-D CFD studies were conducted to overcome the insufficiency of 2-D models, but were largely limited to simple cylindrical spacer representations [8,9], thus neglecting the variability of the filament diameters. A more accurate representation of spacer geometry was proposed by Picioreanu et al. [7]. In that work, the non-uniform spacer filaments were measured by optical microscopy and the conventionally applied cylindrical strands

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were replaced by an array of truncated cones with varying diameters. The study revealed that for instance pressure drop computed with the more complex spacer geometry could be twice as high as the one resulting from a simple cylindrical approximation, at flow rates typically applied in engineering practice [7]. This modeling method was further refined, so that the spacers were not only assembled out of truncated cones with edges at the contact boundaries, but also modeled by use of characteristic dimensions and cubic extrusion guides creating smooth filament surfaces [6]. At the same time, measurement techniques also evolved and recently scanning electron microscopy (SEM) was employed to more accurately assess the characteristic dimensions of spacer geometry [4,6].

The latest development in the evolution of spacer geometry accuracy was proposed by Haaksman et al. [10]. In that work, an X-ray computed tomography (CT) scan was carried out to obtain accurate 3-D geometries for any given spacer design. CFD results revealed that the CT scan approach allows for a better quantification of local distribution of velocity and shear [10]. However, a study that simulates solute transport on CT scanned spacer geometries is still lacking, while recent studies aiming on CFD modeling and mass transfer still use the cylindrical geometry [11,12]. Also, a conclusive assessment on how the CT scan accuracy effects hydrodynamics and solute transport simulations in the feed channel is missing. Siddiqui et al. [13] investigated the accuracy of different porosity quantification methods of spacer-filled feed channels and the impact on hydrodynamic predictions. Results showed that the microscopic techniques deviate significantly from the more accurate methods for feed-channel porosity measurements (i.e., volume displacement technique, weight and density technique, CT scanning technique) [13]. Deviations in porosity measurement accuracy can result in a significantly different prediction of the pressure drop of − 31% to 43%, with CT scanning being the recommended porosity measurement technique aimed for numerical studies [13]. However, the accuracy of geometry (and thus, porosity) determination depends heavily on the CT scan resolution. Thus, this study aims (i) to validate the proposed CT scanning approach by modeling hydrodynamics, particle deposition and solute transport within the feed channel, (ii) to verify modeling results of pressure drop and particle deposition through experimental tests, and (iii) to apply the most accurate CT scan up to date to investigate the influence of the CT scan accuracy on CFD and solute transport simulations. In addition, we present here a simplified workflow of converting raw CT scan data to solid shape data to generate the model geometry usable in CFD and solute transport simulations. The development of a periodic computational domain, which is also delineated within this work, allows to reconstruct a spacer net and is applied for numerically efficient particle deposition and solute transport modeling.

2. Materials and methods

2.1. CT scanning procedure

The geometry of a commercially available diamond-shaped spacer (Toray Industries, Inc., Tokyo, Japan) with a thickness of 34 mil (0.86 mm) was assessed by use of computed tomography (CT) scans. The scan of a piece of this spacer comprising 2 × 3 full rhomboidal mesh elements was executed with a ZEISS Xradia 500 Versa X-ray CT microscope (Carl Zeiss AG, Oberkochen, Germany), using the cone beam of a transmission tube (nt100, Nordson Dage) at a voltage of 60 kVp, power of 4.5 W with a tungsten target and no additional filter. 3601 projections were collected for full (360°) rotation of the sample. The sample was mounted with polystyrene on the sample holder. Fig. 1 displays images of the investigated spacer mesh and the fixed layout of the measurement in the X-ray microscope. The region of interest (ROI) for all measurements was the mesh element nearest the support but still uncovered by the polystyrene (avoidance of potential movement of the spacer during measurement). The data reconstruction was done with the Scout-and-Scan™ Control System Reconstructor (version 11.1.5707) and saved in digital imaging and communications in medicine (DICOM) format as attenuation values. The DICOM data where read into VGStudio MAX (version 2.0, Volume Graphics GmbH, Heidelberg, Germany), converted into isosurfaces by thresholding, and stored as 3-D stereo lithography (STL) file.

The ZEISS Xradia 500 Versa CT microscope uses a two-step magnification of the sample. A geometric magnification of the sample projection onto a scintillator screen is done via the source to object distance (SOD), and the object to scintillator distance (OSD). With the SOD fixed at 70 mm and the OSD at 18 mm, the geometric magnification was $M_{geo} = (SOD + OSD)/SOD = 1.26$ in all experiments. The scintillator converts X-rays into visible light. Switchable magnifying optics between scintillator and detector (iKon-L DW936N BV, Andor) magnifies the scintillator image further. The 4× optical magnification (M_{opt}) of the ZEISS CT microscope was used in the experiment due to the optimal combination of resolution and scintillator efficiency. The detector has 2048 × 2048 pixels of 13.5 × 13.5 µm. Binning into 1024 × 1024 pixel of 27 × 27 µm (bin2), 512 × 512 pixel of 54 × 54 µm (bin4) and 256 × 256 pixel of 108 × 108 µm (bin8) was performed for the three measurements at the three effective, i.e. binned, pixel sizes $r_D = 27$, 54 and 108 µm. The spot size of the X-ray source was determined by the knife-edge method to be $S = 2.2$ µm at 60 kVp and 4.5 W. Due to the small geometric magnification, this spot size S has only a minor effect on the effective voxel size r_{eff} of the reconstruction (Eq. (1)).

$$r_{eff} = \frac{\sqrt{\left(\frac{r_D}{M_{opt}}\right)^2 + S^2 \cdot (M_{geo} - 1)}}{M_{geo}} \tag{1}$$

with r_D the binned detector pixel size, S the spot size of the X-ray source, M_{opt} the optical magnification ($M_{opt} = 4$) and M_{geo} the geometric magnification ($M_{geo} = 1.26$). Repeating the tomography with changed detector pixel sizes r_D by binning, the resolution was changed without changing the other parameters of the measurement. The effective voxel size of the reconstructed object was $r_{eff} = 5.44$ µm (bin2), 10.77 µm (bin4) and 21.50 µm (bin8), referred to in the following as 5.5, 11 and 22 µm CT scan accuracies.

2.2. Surface fitting of the CT scanned feed spacer, solid shape and periodic geometry conversion

The transformed output data format of the CT scanner, a 3-D STL file of the spacer specimen, was not directly usable within the employed CFD software, COMSOL Multiphysics (version 5.3, Comsol Inc., Burlington, MA, USA). Moreover, the STL mesh deviated slightly from the geometric periodicity of the repetitive spacer mesh pattern, possibly due to a slight heterogeneity of the extruded polypropylene fibers resulted during the manufacturing process. However, a periodic geometry is highly desirable for CFD simulations because it allows a significant reduction in the size of a representative computational domain. A solution strategy to overcome these impediments is to precisely remodel the complex geometry, so that a perfectly periodic geometry is created while the utmost of the CT scan accuracy is preserved. This was achieved by use of the Geomagic Design X (3D Systems Inc., Rock Hill, SC, USA) mesh healing and surfacing functionalities, which allow creating solids from a non-uniform polygon mesh. First, the mesh was aligned in an XY-plane and all irrelevant point clouds (due to background noise during CT scanning) lying outside of the spacer geometry were removed via cutting operations. Afterwards the spacer surface was cleared of any holes and defects were repaired (as in [10]), which was done with the further meshing functionalities of Geomagic. To create a precise freeform geometry true to the original scan output, the “Auto Surface Function” of Geomagic was used. This function was able to achieve a high accuracy in the conversion from STL surface triangles