Numerical simulations on the flow fields of dynamic axial compression columns in chromatography processes

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Abstract. Dynamic axial compression (DAC) columns are key elements in Simulated Moving Bed, which is a chromatography process in drug industry and chemical engineering. In this study, we apply the computational fluid dynamics (CFD) technique to analyze the flow fields in the DAC column and propose rules for distributor design based on mass conservation in fluid dynamics. Computer aided design (CAD) is used in constructing the numerical 3D modelling for the mesh system. The laminar flow fields with Darcy’s law to model the porous zone are governed by the Navier-Stokes equations and employed to describe the porous flow fields. Experimental works have been conducted as the benchmark for us to choose feasible porous parameters for CFD. Besides, numerical treatments are elaborated to avoid calculation divergence resulting from large source terms. Results show that CFD combined with CAD is a good approach to investigate detailed flow fields in DAC columns and the design for distributors is straightforward.

1. Introduction

Simulated moving bed (SMB) chromatography process, which is a multicoloumn chromatography process, has been applied to various industrial fields, such as foods, petrochemicals, fine chemicals, and pharmaceuticals [1]. The counter current movement of the adsorbent bed is simulated by periodically shifting the inlet and outlet nodes to the direction of the flow during each switching period. Therefore, the SMB process can achieve high productivity and low solvent consumption [2] and allows significantly higher yield and purity compared to a batch chromatography [3, 4]. Generally, the performance of chromatography depends on the combined effects of DAC column dynamics and the pre and post column geometry. In the beginning of the column, an even fluid distribution must be achieved cross sectionally through careful design in order to give satisfactory separation efficiency [5]. At the same time appropriate packing materials have to be chosen and the column has to be carefully packed to maintain the flow pattern as close as possible to a plug flow[6]. The above mentioned factors are especially important to columns with large diameter. If these factors were not considered, band distortion and unsymmetrical peaks would be observed because flow misdistribution can result from faulty header design [7, 8].

CFD has well been known for more than 20 years as a pragmatic and reliable tool to describe local hydrodynamics in various reactors and separation processes [9]. Its modelling has been applied to investigate the transport phenomena in the preparative chromatography column [10-12]. Therefore, based on the recent advances of flow characterisation by CFD, it is proposed to characterize in detail hydrodynamics of DAC columns, and then to deduce numerical treatments that can be beneficial to
simulations. We use CFD to access the internal information inside the DAC column and the flow is considered to be laminar due to low flow speed in the micro-particle packed column [13, 14]. In this study, we present the governing equations for the physical problem and introduce CAD and CFD techniques to simulate flow fields in the DAC column in section 2. Results and discussions are stated in section 3, which includes numerical treatments for enhancing calculation convergence and CFD code validations. Rules to design distributors at the header of the DAC columns, are also proposed in this section. Remarks are concluded in the final section, which includes the present contributions and future works.

2. Methodology
The present simulation is simplified as an incompressible laminar flow of a single species that does not generate heat. Inside the DAC column, no-slip boundary conditions are used for the walls and the packed bed is viewed as a porous medium in which the flow of a Newtonian fluid is known to follow Darcy’s law at a low Reynolds number. The flowchart for the design of DAC columns in this study is illustrated in figure 1.

2.1. Governing equations

2.1.1. Equations in physical domain. The conservation equation for transport of a scalar quantity \( \phi \) is demonstrated by the following equation written in integral form for an arbitrary control volume \( V \) as follows [15]:

\[
\int \rho \phi \mathbf{v} \cdot d\mathbf{A} = \int \Gamma \nabla \phi \cdot d\mathbf{A} + \int_V S_\phi dV
\]  

(1)
where $\rho$ indicates density; $\vec{v}$ is velocity vector; $\vec{A}$ is surface area vector; $V$ is volume; $\Gamma$ is the diffusion coefficient for $\phi$ and $S_\phi$ is source term of $\phi$ per unit volume. The symbol $\phi$ can be replaced by 1 for the continuity equation, and $u$, $v$, and $w$ are the momentum equations in the $X$, $Y$ and $Z$ directions, respectively. Inside the DAC column, the packed bed can be simulated by a porous medium, which is expressed as extra source terms including viscous loss (Darcy’s law) and inertial loss. The added source terms to model the porous effect are expressed as

$$S_j = -\left(\frac{\mu}{\alpha} |v_j| + C'\frac{1}{2}\rho |v_j|^3\right)$$

(2)

where $\alpha$ is permeability ($1/\alpha$ is viscous resistance); $C'$ indicate inertial resistance factor and $|v|$ is the magnitude of velocity.

2.1.2. Equations in computational domain. Since the fluid used in this study is IPA (Isopropyl alcohol), the density is assumed to be constant in the flow field. Equation (1) can be expressed in generalized coordinates using the finite volume method approach for simulations. The discretized formulation for each cell (control volume) based on Eq. (1) yields

$$\sum_{f} N_f \phi f A_f = \sum_{f} \Gamma f (\nabla \phi f)_{e} A_f + S_{\phi} V$$

(3)

where $f$ denotes face of the control volume; $N_f$ is number of faces enclosing cell.

2.2. CAD for 3D modelling

For most preparative and process scale chromatographic columns, DAC column ends include distributors (or collectors) and frits to distribute (or collect) fluid over the cross section of the column. Figure 2 displays CAD diagrams of the DAC column (2a) and the components of its header part (2b) by SoldWorks 3D CAD software. The 3D solid modellings from CAD are imported into the pre-processor in ANSYS MESHING for building the mesh system [16]. Figure 3 displays grid coordinates (left-hand side; LHS) and the grid distribution around column header (right-hand side; RHS) in the mesh system by the grid generation technique. The mesh is unstructured grid system with mixed hexahedra and tetrahedral grids. To effectively compute the present flow fields, the flow domain was split into smaller subdomains. We employed the mixed grid types to build the mesh around the distributor and collector. In the packed bed zone, structured hexahedral grids were used to fit the space inside the column. Moreover, finer grids were imposed along boundary walls to resolve the laminar boundary layer. The grid number for our parameter study was determined to be 0.8 million from grid independent tests and validated with experiments.

2.3. CFD for detailed flow fields

The equations governing the present incompressible flow fields have no link between the continuity and momentum equations due to lack of the equation of state. To solve the set of algebraic equations derived from the governing equations, the SIMPLE algorithm was employed to carry out the calculations [16, 17]. SIMPLE is an acronym for Semi-Implicit Method for Pressure Linked Equations. SIMPLE actually solves the pressure correction equation, which is derived from combining the discrete continuity and momentum equations. Therefore, the set of momentum and continuity equations are coupled and nonlinear so we solve the equations iteratively. The momentum equations are solved for the velocities; however, the newly obtained velocities don’t satisfy continuity. Corrections to velocities and pressure are proposed to satisfy the discrete continuity equation in SIMPLE algorithm. After iterations for the above correction computations, the final solution can be obtained if the estimated residuals approach within required tolerances. In this study, the 3D numerical geometry model for the DAC column is created based from the engineering drawing as shown in figure 2. Then we use CFD pre-processor, ANSYS MESHING to transform the geometry model to the mesh system as shown in figure 3. After the mesh system is imported to the CFD FLUENT solver,
numerical parameters, such as fluid properties, initial and boundary conditions have to be input. Besides, parameters for computation iterations and post processing for contour plotting need to be provided.

![Figure 3](image)

**Figure 3.** Grids in the mesh system: coordinates (LHS) and grids around the column header (RHS) by the grid generation.

3. Results and discussions

3.1. Numerical treatments

In this study, when the standard solution procedures and solution parameter settings were used, we found that the rate of convergence in computations slowed down if the pressure drop was relatively large in the flow direction in a porous region. This slow convergence can occur because the pressure drop of porous media appears as a momentum source term, which yields a loss of diagonal dominance in the matrix of discretized equations solved. The best remedy for poor convergence of a problem involving a porous medium is to supply a good initial guess for the pressure drop across the medium. Another possible way to deal with poor convergence in computation is to temporarily disable the porous media model and obtain an initial flow field without the effect of the porous region. With the porous media model turned off, FLUENT will treat the porous zone as a fluid zone and calculate the flow field accordingly. Once an initial solution is obtained, or the calculation is proceeding steadily to convergence, we thus enable the porous media model and continue the calculation with the porous region included. Based on the Kozeny-Carman correlation in Eq. (4) and following the solution strategies as mentioned above, we can obtain the convergent calculations as anticipated.

![Figure 4](image)

**Figure 4.** Seeking the appropriate viscous resistance via CFD.

![Figure 5](image)

**Figure 5.** Pressure drop versus inlet flowrate for the DAC column.

The Kozeny-Carman correlation is represented by the following equation [14]:

\[
\alpha = \frac{d_p^2 \cdot \varepsilon^2}{150(1 - \varepsilon)^3}
\]
where $\alpha$ is permeability; $\varepsilon$ is porosity and $d_p$ is diameter of packing particles. The porosity is the volume fraction of fluid within the porous region (i.e., the open volume fraction of the medium). The porosity is set to be 1.0 (or permeability $\alpha \to \infty$; viscous resistance $1/\alpha \to 0$) if the medium is treated as merely the IPA fluid. According to data from the manufacturer of the DAC column; $d_p = 50 \times 10^{-6}$ m; $\varepsilon = 0.37$; $\alpha = 5.75 \times 10^{-12}$ m$^2$. Therefore, the viscous resistance is evaluated to be $1.74 \times 10^{11}$ m$^{-2}$.

Thus at the beginning of calculations, this value is a trial to seek the appropriate one which meets the experimental data within the required tolerance as illustrated in figure 4. In figure 4, the experimental datum was searched out via the CFD by the trial value as an initial input from right-hand side to left in the horizontal axis. In fact, the process is a kind of reverse engineering to obtain the values we anticipate.

3.2. Code validation

The experiments were conducted in the Center for Advanced Chromatographic Processing at I-Shou University. Table 1 lists experiment parameters and these data are also applied for boundary conditions in CFD simulations. The working fluid is IPA, which dissolves a wide range of non-polar compounds, and is relatively non-toxic as compared to other solvents.

| Property                | Value                  | Used in exp. or CFD |
|-------------------------|------------------------|---------------------|
| Viscosity               | 0.0023703kg/m-s        | Exp. & CFD          |
| Density                 | 786kg/m$^3$            | Exp. & CFD          |
| Inlet velocity (exp.)   | 0.1062m/s; 0.2122m/s; 0.3183m/s; 0.4244m/s | Exp. & CFD |
| Porosity (DAC)          | 0.37                   | Exp. & CFD          |
| Viscous resistance      | Frit: $3.5 \times 10^{11}$ m$^{-2}$; Packed bed: $3 \times 10^{11}$ m$^{-2}$ | CFD |
| Pressure                | 0〜200 bar             | Exp. & CFD          |

According to our experiment setup, the velocity flowrate at the inlet can be adjusted by the air compressor, which supplies the loading pressure for the hydraulic cylinder to push downward the working fluid through the packed bed. The gauge pressure to provide the driving force in experiments can be reached to as high as 200 bar. Figure 5 illustrates the relationship of pressure drop versus inlet flowrate for the specific DAC column in experiments and CFD calculations. Experimental and CFD data agree well and the curve reflects their linear property. A linear function is proposed to correlate the CFD data for further applications. The correlation equation referring to pressure drops versus inlet flowrates for the present column can be expressed as

$$Y = 7.45 \times 10^{-9} + 4.26 \times 10^{-3} X \approx 4.26 \times 10^{-3} X$$

(5)

where $Y$ denotes pressure drop (bar); $X$ is inlet flowrate (ml/min). In fact, in porous media, pressure drop is typically proportional to velocity, which is described by the Darcy’s law.

3.3. Rules for distributor design

A distributor (collector) plays a key role to make the plug flow in a DAC column. Manufacturers in this field have been devoted to improving the distributor’s performance to raise the efficiency of their DAC column products [18, 19]. In this study, we have found the CFD is a good alternative way to design distributors in analytic approaches. Figure 6 shows the comparison of velocity vectors before the frit at the column header without a distributor (LHS) and with a distributor (RHS). Obviously, the distributor helps to forming plug flow at inlet and CFD helps to providing the visualization of vector fields to see the distributor’s contribution. In addition, we have employed the CFD to investigate the flow features from two different distributors. Figure 7 displays an original distributor (LHS) we used and the modified one (RHS) we proposed. Axial velocity vectors for various locations in the column
header from CFD have shown that the fluid speed is very low compared to the inlet velocity. Based on the same locations around the headers, we compare the average axial velocities (using log scale) from both distributors’ CFD results for two inlet velocities (V1 and V2) as shown in figure 8. The analytic axial velocities were computed at the middle location of the DAC column based on the given inlet flowrate and the mass conservation law. It reveals that the average axial velocity of using the modified distributor approaches to the analytic value faster than using the original distributor for either V1 or V2. Obviously, the modified distributor performs better than the original one because of mass conservation considered in the design process.

The modified distributor was designed according to some rules proposed by this study. The rules are on the assumption that the plug flow is inviscid without circulation existing in channels of the distributor. The rules are made by satisfying the law of mass conservation and stated as follows:

1. Draw a radial line from the center of the distributor surface to get a radius and evenly divide the radius to N segments.
2. Make N-1 concentric circles on the surface to form N-1 rings and an inner circle in which the feed tube (inlet) is located. Calculate the areas and denote them S1 to SN from inner to outer region on the distributor surface.
3. Determine Mn (n=1 to N-1) uniformly spaced distribution openings surrounding each ring. Denote the opening area as An (No restrictions for the shape of the opening).
4. Make sure opening-area density, (∑A)/(SN), on each ring (n) have the same value; it will keep the same total flowrate for each ring.
5. Denote the segment lengths of each channel (including its branch) from the inlet to the opening as Lj (j=1~J, J denotes total segments), then make sure total length (∑Lj) is the same for each channel on the surface. Besides, the cross-sectional area from the inlet to the opening along the channel keep invariant to make flowrate conservation.

Following the step of rules, the previous modified distributor and the example model with new pattern of opening distribution were proposed in figure 9. In figure 9, N is three; Mn is four; J is two with open-area density equal to 8.83%.

Figure 6. Velocity vectors without a distributor (LHS) and with a distributor (RHS) around headers.

Figure 7. An original distributor (LHS) and the modified one (RHS).

Figure 8. Average velocity distributions in the axial direction.

Figure 9. An example model for the distributor by proposed rules.
4. Concluding remarks

In this study, we have provided evidences by CFD simulations to show that the distributor plays a key role on velocity profile at inlet of the DAC column. Besides, the parameter of viscous resistance in packed bed can be numerically determined via the procedure of reverse engineering. Experimental and numerical data suggest the correlation equation for the relationship about pressure drop versus inlet flowrate for the present DAC column. Moreover, rules for designing the distributor have been proposed according to mass conservation law. New distributors thus can be designed based on the rules and an example model is presented. It is anticipated that based on the present study, transient cases involving concentration transport for columns with low length-to-diameter aspect ratios are worth further researches.

5. References

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