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Investigation of Polyethylene glycol-Coated Serpentine Micro Gas Chromatography Columns for Volatile Organic Compounds Separation with Helium Carrier Gas

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Research Article

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Abstract

The current study describes a numerical analysis of serpentine circular micro gas chromatography (μ GC) columns with a polyethylene glycol coating for the separation of VOCs using helium as a carrier gas. Finite element analysis was conducted in COMSOL Multiphysics through the combination of the Laminar Flow and Transport of Diluted Species interface.Two typical analytes, acetone and ethanol, were used, and the effect of geometry on the performance parameters including retention time, theoretical number of plates, height equivalent to a theoretical plate (HETP), resolution, velocity, and pressure were investigated.The simulated serpentine circular microcolumn resulted in retention times between 4.0 to 23.5 seconds, theoretical number of plates of 2.0 to 24.0, HETP of 0.018 to 0.022, resolution of 1.10 to 1.65, velocity ranging from 0.25 to 0.35 ms^{-1}, and pressure drop of 160 Pa to 3.5×10^5 Pa. It is seen from the findings obtained above that longer and narrow columns have more efficient separation capability because of increased analyte stationary-phase interaction, whereas wider diameters of internal dimensions increase fluidic resistance and decrease separation efficiency. The study clearly shows that the serpentine PEG-coated columns possess much better efficiency with great prospects in creating portable μ GCs for VOC analysis.

1. Introduction

The most significant target analytes for environmental monitoring, indoor air quality testing, industrial process analysis, and health-related analysis include volatile organic compounds (VOCs). This is due to the fact that many of these VOCs can elicit adverse physiological responses from exposure, regardless of the concentration level.[1–7] One of the most reliable ways of analyzing VOC samples is by using gas chromatography (GC), which is known to provide highly selective, robust, and versatile separation and detection capabilities.[4,5,8] The limitations associated with existing GC systems include size, cost, and power requirements, making them less suitable for mobile or field use.[9–14] However, such limitations can be effectively addressed through intensive research aimed at reducing the dimensions of the GC device to μGC, where all main components are mounted on miniature chip-based platforms.[6–13] Miniaturized μGC provides benefits like decreased usage of carrier gas and sample, minimized analysis times, low thermal mass, and improved portability; consequently, this technique has been recognized as an ideal solution for on-site VOC detection.[11–13] Recent reports in the journal Lab on a Chip showed how micro-preconcentrators, micro-columns, multi-dimensional systems, and miniature architectures for gas analyses could be achieved through microfabrication techniques.[6–11] Among these constituents, the separation column represents an important component because its geometry, nature of the stationary phase, and operation parameters dictate the separation column parameters like retention factor, bandwidth, theoretical plate number, HETP, and resolution.[11,15] The optimization of the micro-column should be done not only for efficient and selective separation processes, but also for low-pressure drop, small footprint, and ease of construction. Serpentine micro-columns offer great advantages in that respect by allowing large separation channel lengths with small chip dimensions, thus ensuring effective chip integration while preserving separation distance.[10,11,15] The choice of stationary phases is

important for the operation of μGC as well. Poly(ethylene glycol) (PEG) is an established polar stationary phase in GC analysis and has been chosen for oxygen-containing, polar VOCs on account of their interaction with PEG.[14] The representative VOCs acetone and ethanol are expected to exhibit differentiated behavior based on their retention time using the selected PEG stationary phase. Furthermore, the use of helium as a carrier gas due to its inert nature and good diffusibility properties is standard practice in μGC.[12,13] On the other hand, simulations have proven to be an effective technique for the design of microfluidic chips and μGC systems because flow properties, pressure drop, species transport, and dispersion can all be determined before device fabrication using numerical models.[12,13] It should be noted that finite element techniques, such as COMSOL Multiphysics, are especially suited for the design of devices of the sort mentioned above, owing to the capability for coupled flow and species transport analysis in complex channels. In this study, a simulation study of PEG coated serpentine micro GC columns for separation of VOCs using helium carrier gas was conducted. In this simulation, a circular cross section serpentine micro GC column has been designed by utilizing the interfaces in COMSOL Multiphysics software to model helium flow and analyte transport in the column. Acetone and ethanol were chosen as model VOCs and the effect of column dimensions such as length and inner diameter on velocity, pressure, retention time, number of theoretical plates, HETP and resolution have been systematically studied.

2. Materials and Methods

2.1 Microcolumn geometries and simulation strategy

μGC column geometries for several microfluidic channels were simulated by the finite element method (FEM) in COMSOL Multiphysics® software for studying the carrier gas flow, analyte transport, concentration profile, and output separation. Three different microcolumn structures were chosen as representative cases to analyze their influence on chromatographic transport: (i) a straight microchannel with circular cross-section; (ii) a straight microchannel with trapezoidal cross-section; and (iii) a serpentine microchannel with circular cross-section.[7–9]

Parametric studies for the circular cross-sectioned columns were carried out in two scenarios for straight and serpentine columns, respectively. In one scenario, the variation was performed on the internal diameter (ID), which was varied from 50 to 600 μm in 50 μm increments while the column length was kept constant at 15 cm. In another scenario, the variation was done on the length of the column, which was varied from 10 to 100 cm in 10 cm increments while the ID was kept constant at 250 μm. For the trapezoidal straight microcolumn, a hydraulic diameter of 250 μm was considered constant while the length of the column was varied from 10 to 100 cm in 10 cm increments. Also, for the second trapezoidal column set, a length of 15 cm was taken constant while the hydraulic diameter was varied from 50 to 600 μm in 50 μm increments. A constant thickness of 5 μm for the stationary phase was maintained in all cases for comparison purposes.[10]

The initial step taken was that of constructing a benchmark model of a straight tube in order to test the validity of the modelling method in relation to the well-known trends in terms of fluid flow and mass transfer in the analytical chromatographic system prior to applying the modelling approach to serpentine systems. This initial test allowed us to check whether our modelling framework would be able to predict the right trends in retention and band broadening depending on the column length and diameter.[11–12]

2.2 Physics interfaces and numerical implementation

The simulations were conducted using COMSOL Multiphysics® by implementing the Laminar Flow (spf) interface available in the Fluid Flow Module and the Transport of Diluted Species (tds) interface present in the Chemical Species Transport Module. The flow module was employed to determine the hydrodynamic field of the system, while the latter was utilized for the analysis of the species transport during the transient regime, taking into account axial dispersion and species-wall interaction in the presence of a carrier gas flowing through the microchannels.[7,14]

Outlet pressure was held constant at 0 Pa gauge pressure for all geometrical configurations. For the transient analysis of species transport, the initial time, time increment, and final time were taken as 0 s, 0.5 s, and 10 s, respectively. The reason behind such time discretization was that it was essential for studying the dynamics of injected pulses of analyte and the resulting concentrations at the outlet necessary for the evaluation of column performance parameters. Convection of the analyte species was modelled based on the velocity field derived through laminar flow simulation.[15,16]

2.3 Material properties and stationary-phase representation

He gas was chosen based on the properties of its inertness, high diffusivity, and wide use as the carrier gas in gas and μGC techniques. In the current model, helium was characterized by a density of 0.164 kgm^{-3} and dynamic viscosity of $1.96x10^{-5}$ Pas. The values were in agreement with available data on the gas properties at ambient temperature. The choice of acetone and ethanol as example volatile organic compounds (VOCs) was made. Acetone and ethanol diffusion rates in the stationary phase made up 2.5×10^{-10} m^2/s and 2.0×10^{-10} m^2/s, respectively. Additionally, partition coefficients of the VOCs in PEG/helium mixture were chosen as equal to 90 for acetone and 190 for ethanol. The choice was done on the basis of better affinity between ethanol and polar PEG surfaces.[17,18]

A thin wall boundary condition representing the internal wall surface of the microcolumn was applied for PEG stationary phase implementation. 5 μm coating thickness was chosen to represent the PEG stationary phase in all parametric calculations. Partition coefficients, analyte-specific, describing the gas-stationary phase equilibrium, were adopted from literature. Equilibrium constant K, in terms of concentrations at the gas-solid interface equilibrium state, was the ratio of analyte concentration in the stationary phase to that in the gas phase.[19] For microfabricated capillaries, the equilibrium constant was linked to the apparent retention factor using the phase ratio concept, dependent on the channel radius and the thickness of the stationary layer. Calculated phase ratio corresponding to the channel inner

diameter of 250 μm and the PEG coating of 5 μm provided retention characteristics indicating higher retention for ethanol than acetone, thus suggesting the feasibility of the selected partition coefficients.[8,9]

2.4 Boundary conditions and analyte injection

Inlet volumetric flow rate of the fluid was considered as 0.6 SCCM, which translates to1.0×10^{-8} m^3s^{-1}. Fully developed laminar flow was used as the inlet and outlet boundary condition on the fluid flow model. Additionally, the outlet pressure was constrained to 0 Pa gauge. With regard to the species transport analysis, the inlet concentrations of the analytes (acetone and ethanol) were assumed to be 4.4×10^{-5} $molm^{-3}$. The analyte injection was simulated by employing the following expression: $0.5\times gp_1$ (t). Here, gp_1 (t) is the time dependent Gaussian distribution utilized to simulate an injection plug.[20]

2.5 Meshing and numerical accuracy

Meshes customized for each of the geometries considered were used for all the simulations, with meshing conducted both radially and axially to resolve gradients in velocity adjacent to walls and analyte concentration gradients adjacent to the stationary phase. A particular focus was placed on meshing within the curved regions of the serpentine microcolumn due to the presence of streamline variations in those regions, along with differences in the distribution of species. Figure 2 shows a typical example of meshed geometry. Discretization was accomplished through a P1 + P1 finite element formulation of the coupled solution fields. Mesh convergence analysis was conducted to ensure that the output from the simulations was independent of mesh density.[21]

2.6 Performance metrics

Chromatographic efficiency of micro-columns considered was estimated using parameters such as retention time, resolution, HETP (Height Equivalent to Theoretical Plate) and N – theoretical plates, commonly used to determine column efficiency for GC and μGC techniques. Retention time was found according to the peak appearance of the outlet concentration of the corresponding component. Resolution was analyzed by estimating how well the output peaks of acetone and ethanol were separated taking into account the width of each of them. Theoretical plate number was calculated from the analysis of peak shapes and retention properties. HETP was calculated by dividing the length of column by the number of theoretical plates.[22]

2.7 Scope of the parametric study

This was possible due to the fact that the same conditions were considered for carrier gases and stationary phases when simulating both circular straight and serpentine microcolumns, as well as straight microcolumns with trapezoidal cross sections. Changing parameters such as length and diameter of the channels allowed studying the effect of geometrical parameters on the helium flow velocity, pressure drop, solutes retention, and separation efficiency. The use of the thin wall PEG approximation allowed estimating the impact of stationary phase on retention and mass transport of solutes without meshing the entire volume of the coating layer.[23]

3. Result and Discussion

Figure 1(A) demonstrates the total meshing of the serpentine microcolumn, which constitutes the entire computational domain. Figure 1(B) represents an enlarged meshing in the channel part, where fine meshes are employed to account for better flow and mass transport. Figure 1(C) is a representation of the meshing at the curved part, where higher velocity gradients and concentration differences are expected.[24,25]

In Fig. 2, the simulation scheme used in COMSOL for the flow of acetone-ethanol through the serpentine microcolumn is demonstrated in three Fig. 2(A) through Fig. 2(C) showing the total model, channel cross-section, and direction of transport of the species, respectively. It demonstrates the interaction of the species with the helium gas and PEG coated stationary phase in the micro-channel during separation.[26,27]

Figure 3 depicts the velocity field of helium gas in the serpentine microcolumn, with Fig. 3(A) showing the complete velocity field and Fig. 3(B) illustrating the velocity field close to the inlet and curved channel sections. The high velocity close to the inlet and the variations along the curves demonstrate the effect of the serpentine configuration on flow development.[28,29]

The velocity distribution for helium flow inside the serpentine microcolumn is displayed in Fig. 4, where Fig. 4(A) depicts the general flow pattern and Fig. 4(B) focuses on the velocity variations at the curvature of the channel. The contour plots clearly demonstrate that the flow is well-channelled through the serpentine structure while producing local velocity variations at the curvatures.[30,31]

Figure 5 represents the simulated contour plots for pressure within the serpentine microcolumn, with Fig. 5(A) representing the total pressure profile, while Fig. 5(B) indicates the pressure difference around the bends in the channel. Pressure decreases as the flow progresses, and the bends in the channel also cause pressure differences, which is significant since pressure drop influences carrier-gas flow and GC system efficiency.[32,33]

Figure 6 demonstrates that there is a significant dependence of the helium flow through the serpentine microcolumn on the geometrical parameters of the microcolumn. With the increase of column length from 10 cm to 100 cm with fixed ID, the velocity changes in the range of 0.38 – 0.25 ms^{-1} with simultaneous growth of pressure in the range 180–450 Pa reaching a stable value. However, with an increase in ID from 50 μm to 600 μm at fixed length, the velocity changes drastically in the range 9.8–0 m/s with pressure reduction to almost zero from 3.5×10^5 Pa.[34,35]

From Fig. 7 below, one can note that there is a direct relationship between the retention time and theoretical plates in relation to increasing column length and a decrease in internal diameter.[36] Qualitatively, this is because increasing column length means more time is spent by the analytes in contact with the PEG stationary phase whereas decreasing the internal diameter means stronger

confinement and interaction of the analytes with the column walls leading to effective separation of acetone from ethanol.[37,38] Quantitatively, as seen in Fig. 7(A) and 7(B), there is an increase in the retention time and the theoretical plate numbers from 6 s and 2,000 respectively to 21 s and 24,000 when the column length increases from 10 cm to 100 cm while in Fig. 7(C) and 7(D), there is an increase in the retention time and the theoretical plates from 6.5 s and 1,800-2,600 respectively to 8.5–9.3 s and 3,500-4,800 respectively.[39,40]

4. Conclusion

The current research involved the development of a simulation model using the FEM-based software environment COMSOL for the investigation of helium gas flow and acetone-ethanol mixture separation processes in serpentine circular PEG-coated micro-GC columns. Numerical studies revealed that the proposed optimized serpentine geometry provided retention times of 4.0-23.5 s, theoretical plate numbers of 2.0–24.0, HETP of 0.018–0.022, resolution of 1.10–1.65, velocity of 0.25–0.35 m s-1, and pressure drop of 160 Pa to 3.5×10^5 Pa, showing higher efficiency of the separation process. The obtained results have also indicated the importance of the column parameters in enhancing chromatographic efficiency since the increase in column length led to an enhancement of both retention and plate number, and the decrease in internal diameter increased efficiency while reducing pressure drop considerably. Consequently, there exists a compromise between chromatographic efficiency and hydraulic resistance in the micro-column. Overall, serpentine circular PEG-coated micro-GCs may serve as prospective devices for VOC separation in laboratory-scale studies. One of the tasks for future work is the fabrication and experimental validation of the optimized microcolumn.

Declarations

Ethical approval statement

The research used purely computational techniques and simulations. This study did not involve any participants or samples from humans and any living or dead animal tissue. Hence, no ethical approval or informed consent was needed for the experiment to proceed.

Conflicts of interest

The author declares no conflicts of interest.

Financial disclosure statement

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Author contributions

The manuscript was developed by one author. The author did all the conceptualization, designing of the simulation, COMSOL modeling, implementation, parametric studies, graphs plotting, data analysis, result analysis, writing, and editing of the manuscript.

Data availability statement

The data for this study can be obtained from the author upon reasonable request. These include numerical simulations, their processing, and their visual representations, which have been performed during the course of the current study by using COMSOL Multiphysics.

References to unpublished works

The manuscript does not cite unpublished works.

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Optional single-author note

This work was conducted independently by the author as part of doctoral research.

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Figures

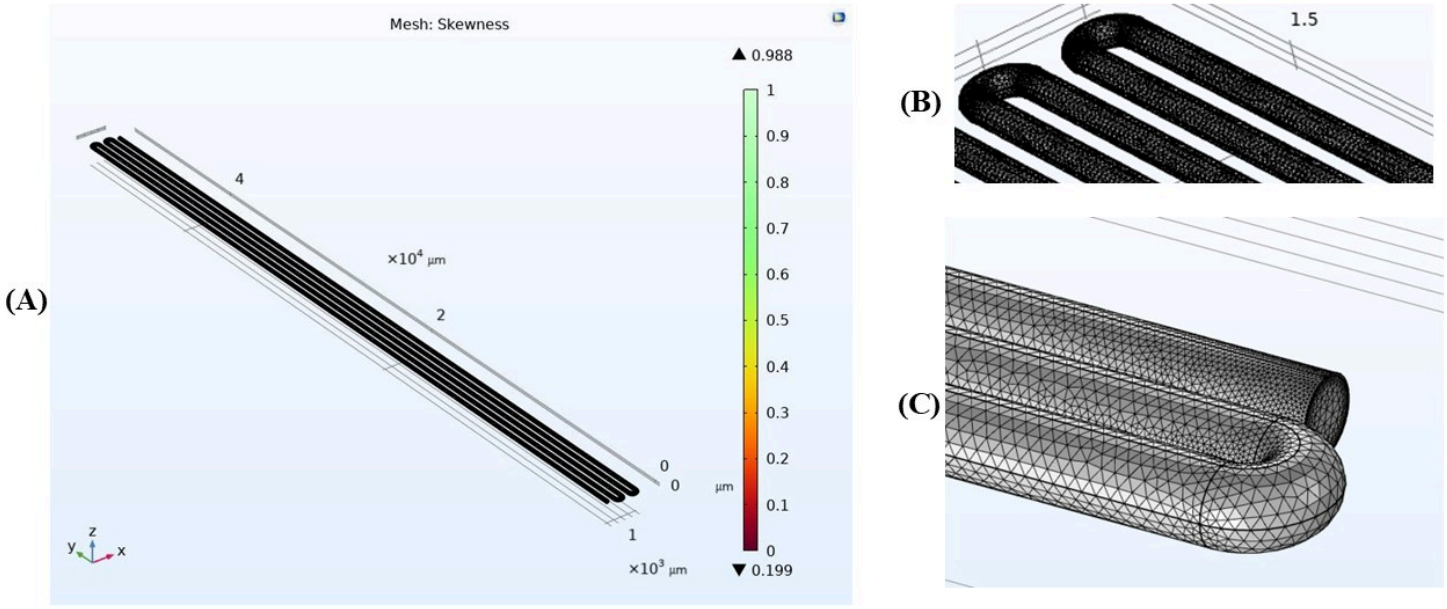


Figure 1

Meshing of the serpentine microcolumn showing (A) complete geometry, (B) zoomed view of the channel mesh, and (C) refined mesh distribution at the bend section.

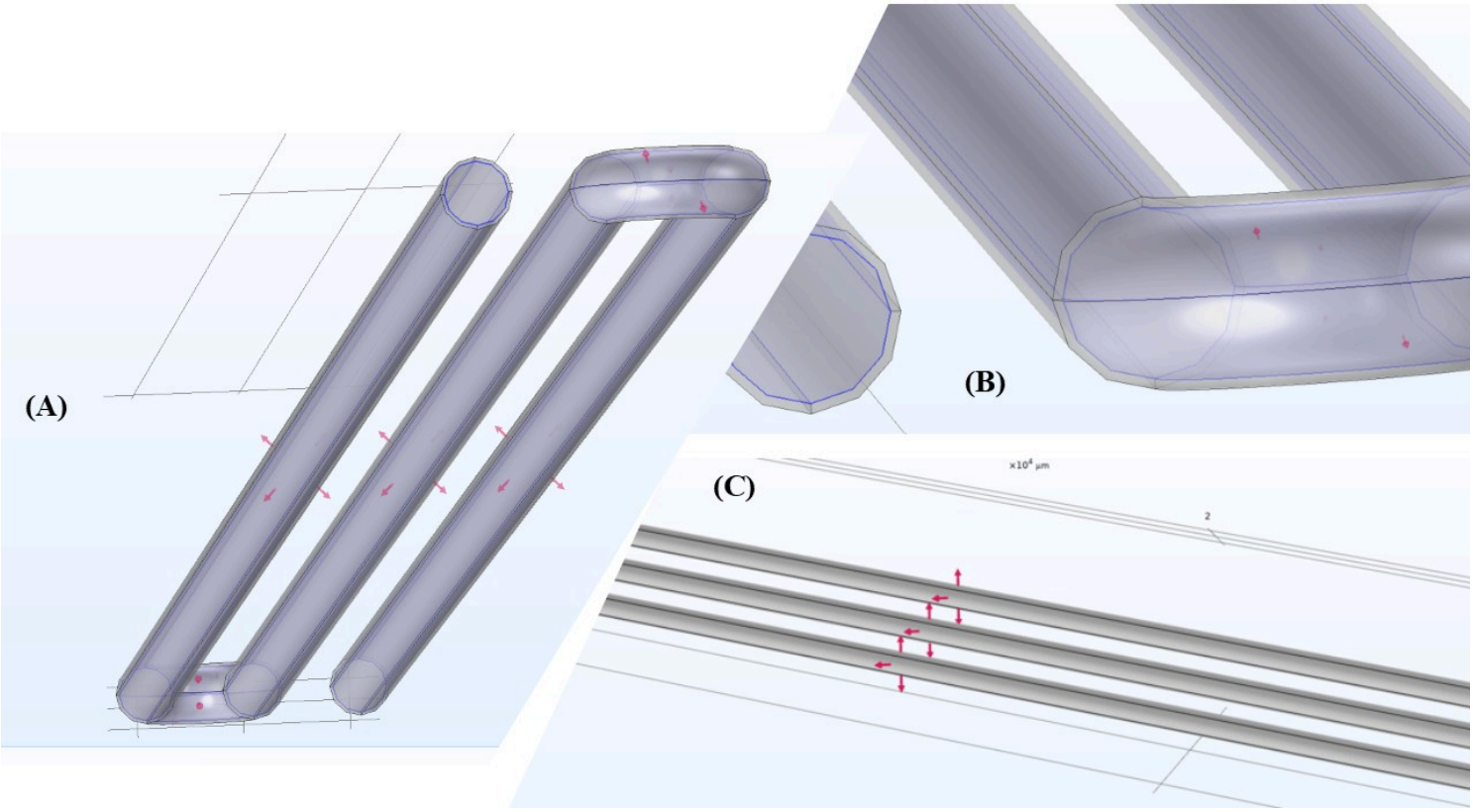


Figure 2

COMSOL-based simulation of acetone–ethanol partitioning between helium carrier gas and PEG stationary phase in the serpentine microcolumn: (A) complete model, (B) channel cross-section, and (C) transport direction of species.

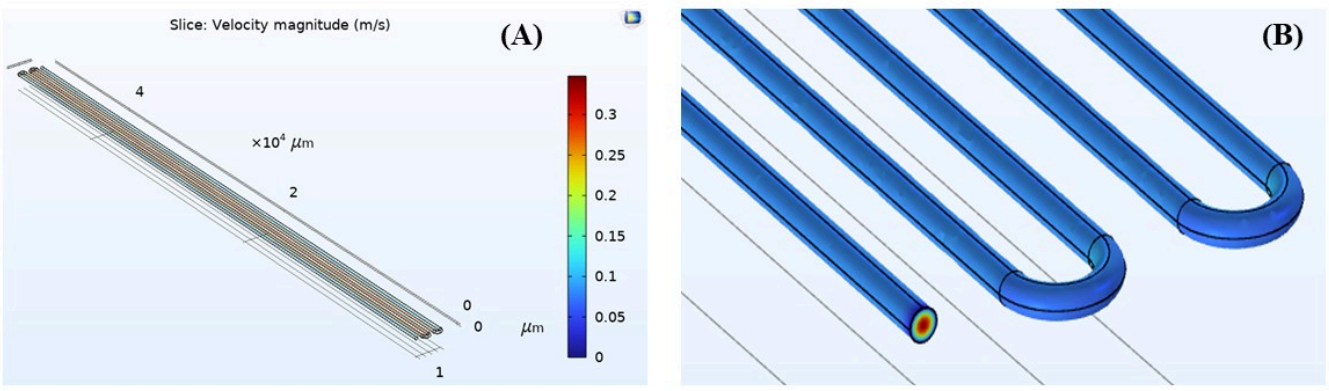


Figure 3

Velocity field of helium carrier gas in the serpentine microcolumn showing (A) overall velocity distribution and (B) detailed flow profile near the inlet and curved channel regions.

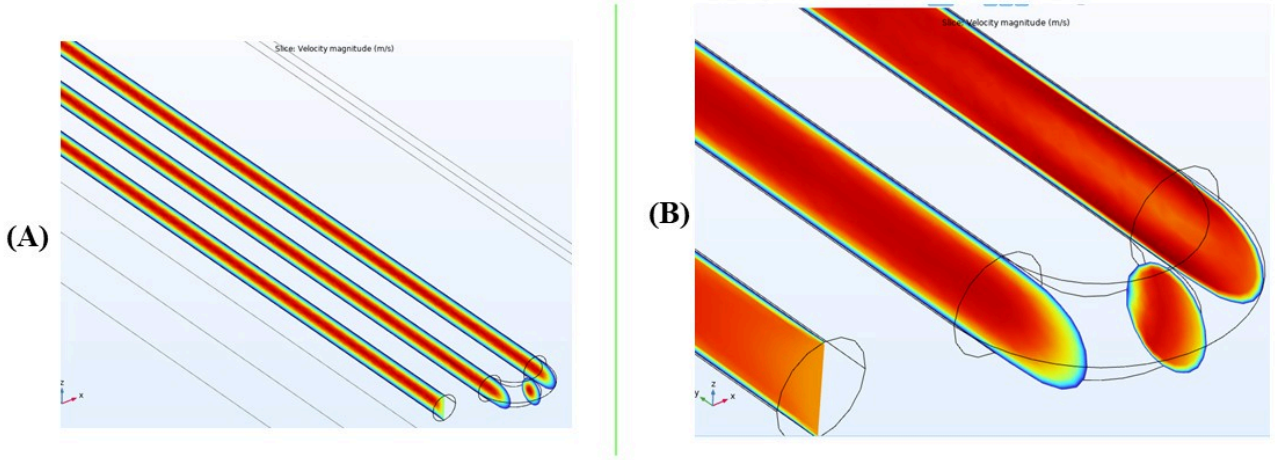


Figure 4

Helium velocity contours in the serpentine microcolumn: (A) overall flow distribution and (B) detailed velocity variation near the curved channel sections.

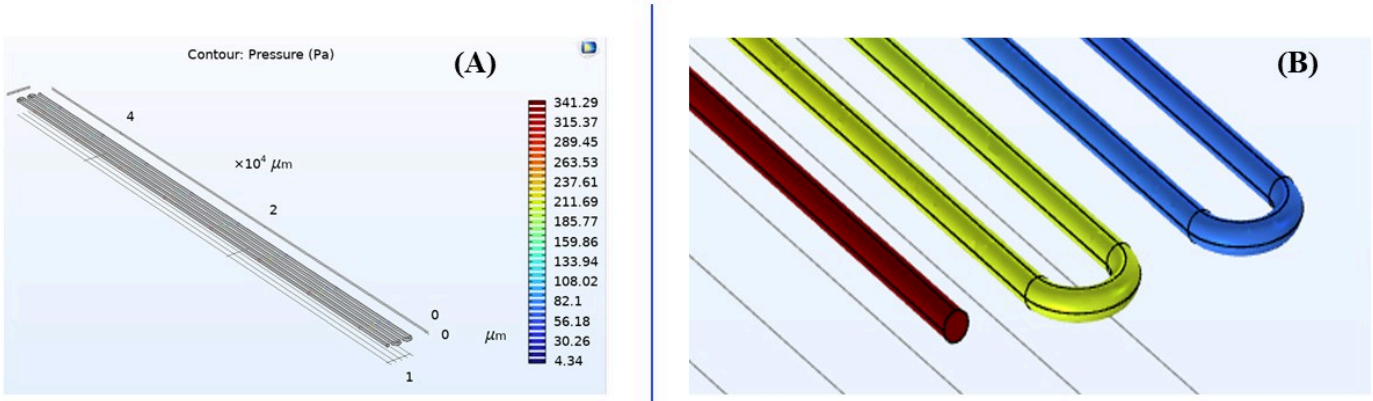


Figure 5

Simulated pressure contours in the serpentine microcolumn showing (A) overall pressure distribution and (B) detailed pressure variation near the channel bends.

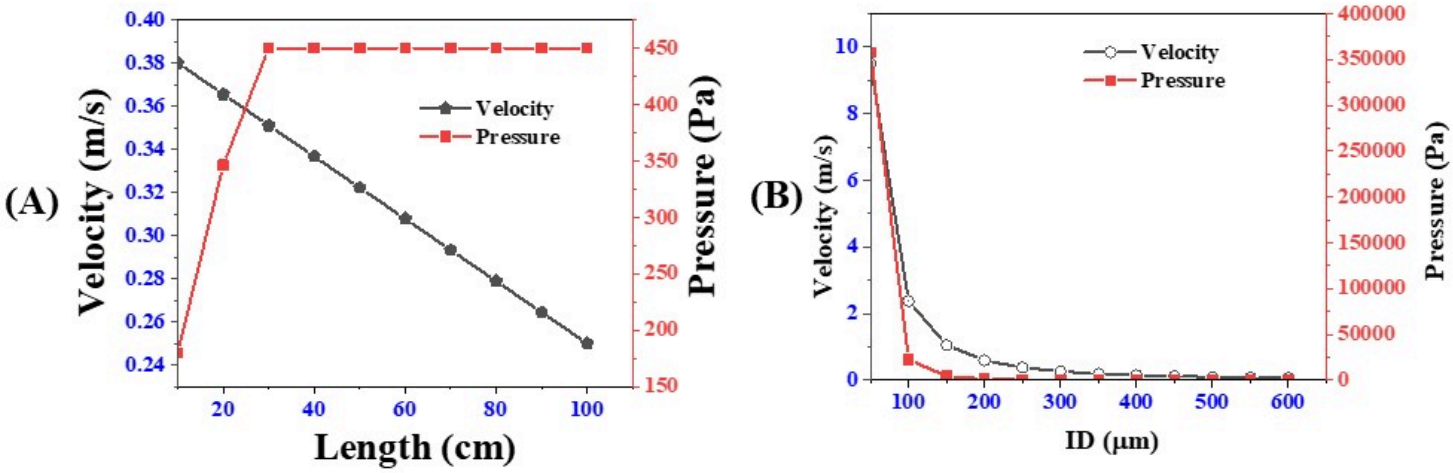


Figure 6

Parametric analysis of helium flow in a circular serpentine microcolumn showing the effects of (A) column length and (B) internal diameter on velocity and pressure characteristics.

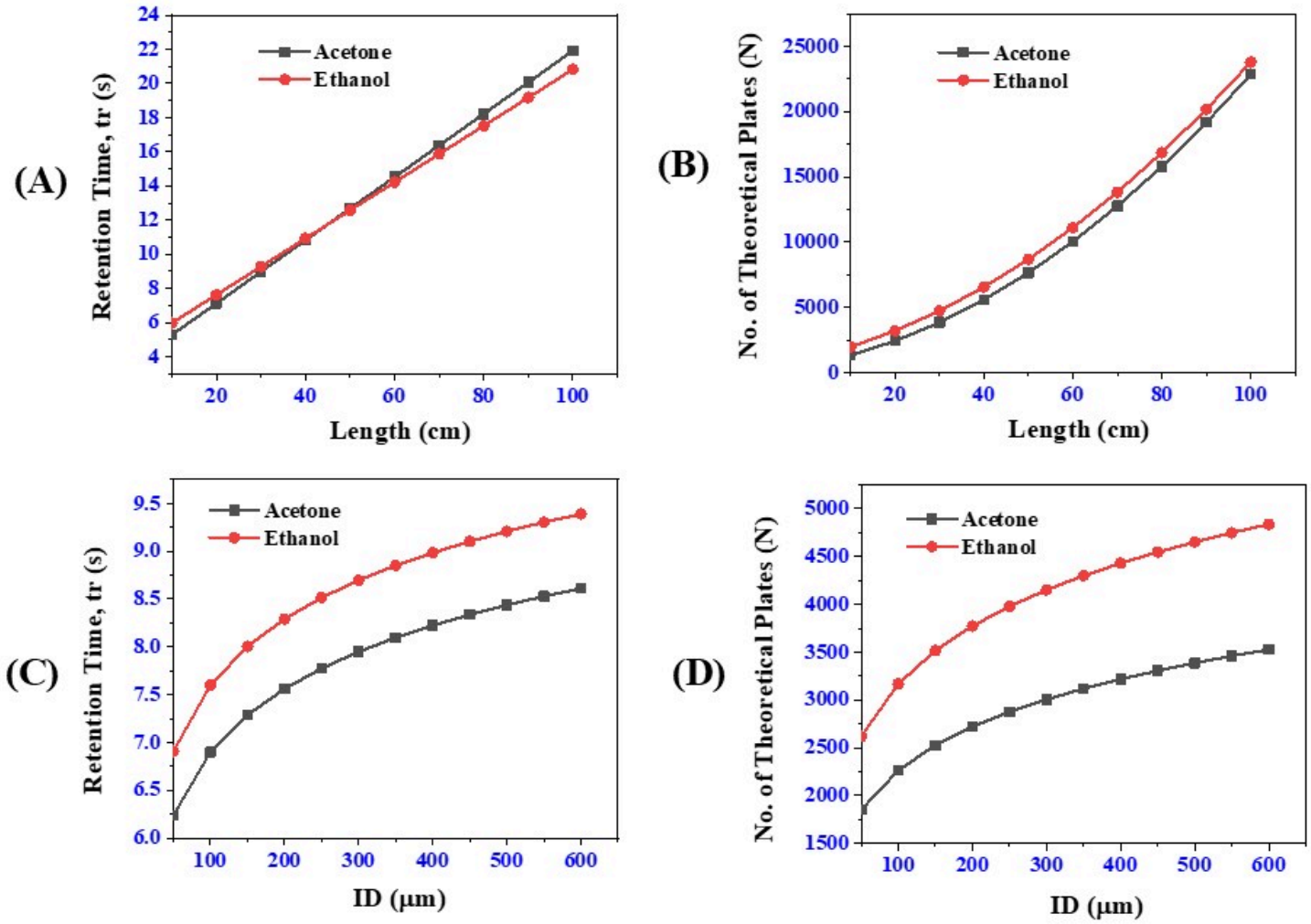


Figure 7

Effect of serpentine microcolumn dimensions on separation performance of acetone and ethanol: (A) retention time and (B) number of theoretical plates as a function of column length, and (C) retention time and (D) number of theoretical plates as a function of internal diameter.