Topic: Chemical sensors

IMCS25_78 - Design of low-cost 3D printed micro-gas chromatography (μ-GC) column for fast VOC analysis

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Summary

This paper presents the design and simulation of a spiral-shaped μ-GC column using FE analysis to identify airborne VOCs. The column's performance was optimized by adjusting channel length and stationary phase (SP) thickness. Efficiency is defined by the number of theoretical plates (N) and separation resolution (R_S). Our best simulation gave an R_S of 12 for ethanol and toluene. Results, as expected, indicate that increasing channel length and decreasing SP thickness significantly enhance μ-GC performance. Our 2D modelling approach is a fast and simple method for optimization, which can be applied to develop basic low-cost 3D printed plastic columns.

Contents

A 2D spiral-shaped μ-GC model was developed in COMSOL by combining the transport of diluted species and fluid flow physics. Four different models have been studied by varying the channel length (*l*) and polydimethylsiloxane (PDMS) stationary phase (SP) thickness (*t*), while maintaining a constant column width of 0.3 mm. The models were; 1 (*l* = 0.4 m, *t* = 10 μm), 2 (*l* = 0.4 m, t = 3 μm), 3 (*l* = 1.2 m, *t* = 10 μm), and 4 (*l* = 1.2 m, *t* = 3 μm). The model domain is initialized with zero velocity, no-slip conditions, an inlet velocity of 0.2 m/s, and an outlet pressure of 0 Pa.

For the transport of diluted species, the molecules undergo convection, diffusion, and partitioning between the carrier gas and SP. The domain is initialized with zero chemical concentration, and injection is modelled by a Gaussian concentration profile at the inlet, peaking at 1 s with a full width at half maximum ($FWHM$) of 0.5 s and a concentration of 4.4×10^{-5} mol/m. Figure 1 shows the illustration of 2D model used to evaluate the column efficiency.

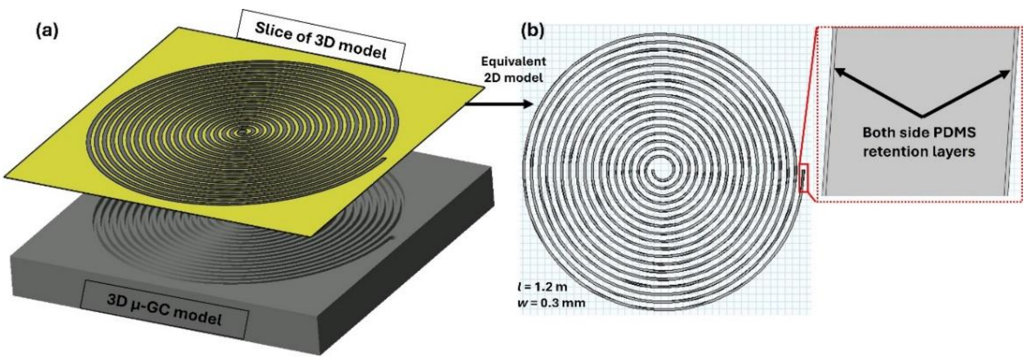

Figure 1: Developed μ-GC model in COMSOL for Multiphysics simulation.

Figure 2(a) illustrates the velocity profile of the carrier gas at the inlet and outlet of the channel, showing an average inlet velocity of 0.2 m/s, peaking at the centre and tapering to zero near the walls. Figure 2(b) depicts the simulated concentration profiles of the three chemical species in the optimal model (Model 4). The column performance in term of N and R_S, were calculated using the retention time t_R:

$$N = 5.54\left(\frac{t_R}{FWHM}\right)^2 \qquad (1)$$

$$R_S = 2\frac{t_{R(toulene)} - t_{R(EtOH)}}{FWHM_{toulene} - FWHM_{EtOH}} \qquad (2)$$

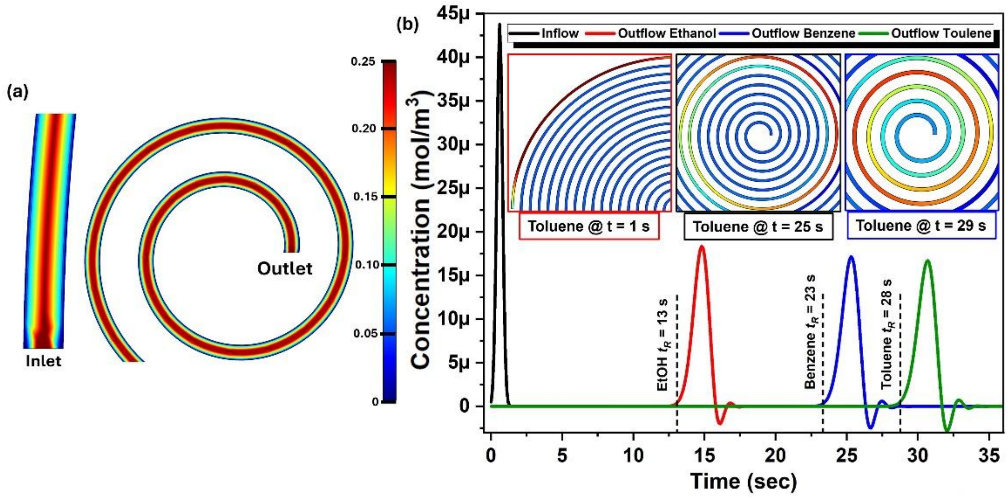

Figure 2: (a) carrier gas velocity profile, (b) model 4 inlet/outlet concentration profile, inset shows toluene profile at different time intervals.

Model 4 achieved the highest performance in N and R_S across all three chemical species which can be attributed to the thinner SP and longer channel length (see Table 1). Notably, increasing the channel length significantly improved retention time t_R, while SP thickness facilitate in enhancing $FWHM$ and R_S (Table 1). Since this analysis is based on a 2D slice of a 3D structure, it is expected that maximum separation resolution could be achieved when the optimal structure is analysed in 3D, potentially yielding much higher N and improved R_S. It should be noted that the objective here is not to replicate high performance gas chromatographs but to design basic low-cost plastic µGC columns to enhance the performance of existing e-noses.

Table 1: Performance comparison among simulated models.

Models	Species	N	R_S
1	Ethanol	62	
	Benzene	236	[a]E/B=2.11
	Toluene	295	[b]E/T=2.83; [c]B/T=0.8
2	Ethanol	178	
	Benzene	555	[a]E/B=4.74
	Toluene	845	[b]E/T=7.26; [c]B/T=2.48
3	Ethanol	197	
	Benzene	671	[a]E/B=3.44
	Toluene	798	[b]E/T=4.34; [c]B/T=1
4	Ethanol	650.77	
	Benzene	1735.68	[a]E/B=8
	Toluene	2495	[b]E/T=12; [c]B/T=4

[a]Ethanol to benzene, [b]Ethanol to toluene, and [c]Benzene to toluene.