MASS TRANSFER IN INVERSE GAS CHROMATOGRAPHY

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In order to produce polymers of desired qualities, a study of reaction kinetics is highly desired and heat and mass transfer phenomena are an important part of such kinetics. Information about the mass transfer of gases into polymer particles, or gas diffusivities, can be obtained using inverse gas chromatography (iGC). The main part of the iGC measuring device is a column packed with a stationary phase, for which the properties are to be obtained. There is a constant flow of a carrier gas. At the beginning of each measurement, a short pulse of tracer gas is injected into the column. The detector at the end of the column tells us when and how much of the tracer gas leaves the system. The obtained peak is then processed according to a theory, commonly referred to as van Deemter theory[1]. Based on the retention time and the shape of the peak, a height equivalent to the column's theoretical plate (HETP) can be calculated. After evaluating HETP for various flowrates, the diffusion coefficient can be evaluated from such data.

The van Deemter theory was derived under three assumptions: (i) linear chromatography, (ii) linear adsorption isotherms, and (iii) one characteristic diffusion time in porous particles. To examine these assumptions, we compare experimental measurements and mathematical simulations of mass transfer phenomena in the iGC column. Furthermore, through the means of simulation, we also look closer on how the morphology of the particles influences the final shape of the peak measured by the iGC device. Such study is important to deepen the understanding of the iGC measuring method and to determine, whether current theories can accurately describe all the processes occurring in the device, or whether an extended theory is needed.

Results are complementary to alternative methods of mass transport measurement in porous polyolefin particles, such as gravimetrical measurements in sorption cells or pressure-decay measurements. We explain differences and applicability of various types of measurements including iGC. The transport characteristics are independently validated by means of micro-CT images of porous polyolefin particles.

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[1] Van Deemter, J. J.; Zuiderweg, F. J.; Klinkenberg, A.: Longitudinal diffusion and resistance to mass transfer as causes of nonideality in chromatography, Chemical Engineering Science, 1956, 5, 271–289.