**One-way vs two-way coupling approach for predicting Brownian-Sieving Hydrodynamic Chromatography separation performance**

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**1.Introduction**

Recently, a one-way coupling approach was exploited to optimize the geometry and the operating conditions of a Brownian Sieving Microcapillary Hydrodynamic Chromatography device (BS-MHDC), an unconventional MHDC double-channel device, where a Brownian sieving mechanism acting alongside the MHDC separation drive is enforced to boost separation resolution [1-2].

The BS-MHDC consists of a two-channel coaxial annular structure, where the core and the annular channel communicate through slit openings of assigned cut-off length A. The geometry is designed so that the core and the annular channel are characterized by significantly different average velocities of the eluent. When a mixture of particles of two characteristic sizes, say d1p and d2p with d1p > A > d2p, is initially injected only within the core channel, both large and small particles flow downstream the channel under the action of the eluent pressure-driven laminar flow. Particles of diameter d2p, smaller than A, can diffuse through the openings and eventually attain a uniform distribution onto the entire accessible cross-section, so their effective velocity will be affected by the average eluent velocity in both the core and annular channel. On the contrary, particles of diameter d1p, bigger than A, are confined to the core region so that their effective velocity is influenced only by the average eluent velocity within this region.



 **Figure 1**. Schematic representation of the double-channel BS-MHDC device.

Previous approaches for quantifying the device performance hinged on the so-called one-way coupling excluded-volume approximation, in which the eluent flow is computed as a single-phase Stokes problem, and the particle-wall interactions are crudely simplified by only considering hindrance effects due to the finite size of the particle.

Bounds for the accuracy of the one-way coupling approach have been investigated in the literature only in single-channel geometries [3], where it is possible to single out a unique characteristic dimension of the cross-section which constitutes the reference length for scaling the particle size. On the contrary, the Brownian sieving device considered here possesses multiple reference lengths of the cross-section (the diameter of the core channel, the thickness of the annular channel and the slit opening A), which make the limits of validity of the one-phase approach uncertain.

The scope of this work is to explore these limits, comparing the predictions of the separation performance obtained with the one-way coupling approach with those obtained from a fully three-dimensional two-way coupling approach. Brenner's macro-transport theory [3-4] is used in both cases for obtaining the effective transport parameters, namely the effective particle velocity and the dispersion coefficient.

**References**

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