LABORATORY FOR CHEMICAL TECHNOLOGY
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Coach	Supervisor(s)	Funding
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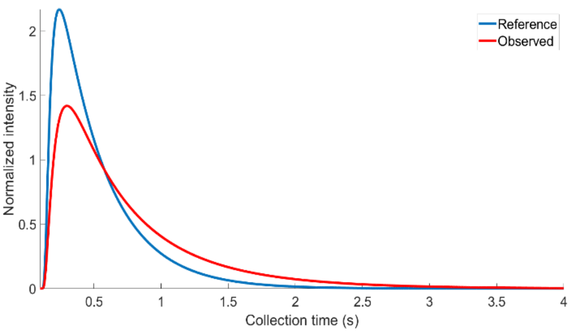
Pseudo-spectral deconvolution of parallel mass transport phenomena from transient diffusion experiments in porous materials

Aim

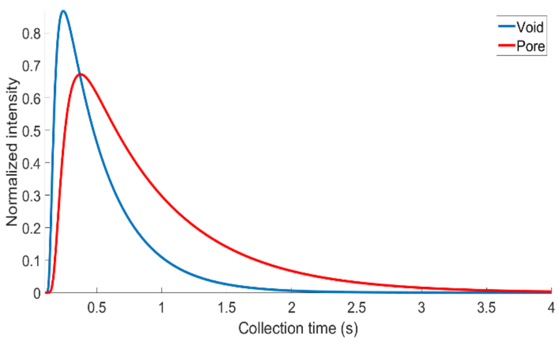
To develop a numerical method, based on spectral and pseudo-spectral techniques, capable of deconvoluting the pulse response obtained from diffusion experiments with porous materials (e.g. zeolites) in the Temporal Analysis of Products (TAP) reactor.

Justification

Porous materials, such as zeolites, constitute some of the most important types of catalysts or supports in the chemical industry. Due to their prominence, the study of diffusion mechanisms within porous materials and the determination of material characteristic parameters that control these processes hold a significant importance for academic and industrial purposes. An adequate characterization of these properties is key in the development and implementation of chemical process technology, such as sorption separation and heterogeneous catalysis.



Non-equilibrium experimental techniques can be employed for analyzing transport within solid, porous materials. TAP experiments have the potential to become a valid alternative for studying diffusion inside certain porous materials due to their experimental simplicity compared to traditional methods. The main limitation is the lack of algorithms that can reliably extract material intrinsic properties such as pore fractions, tortuosities and pore sizes from TAP diffusion experiments.



Program

- Comprehensive literature review on differential equation theory, spectral and pseudo-spectral methods for numerical analysis, TAP theory, diffusion mechanisms within porous materials and methods for the determination and measurement of transport properties.
- Development of a Chebyshev-based pseudo-spectral method for solving systems of partial differential equations (MATLAB, Python or other).
- Mathematical modeling of a TAP experiment with parallel diffusion phenomena under transient conditions. Coupling with the aforementioned spectral method for the determination of unknown values/coefficients based on a non-linear regression method from experimental/simulated data.
- Exploration of several case studies with various degrees of ideality: from basic to more complex, realistic scenarios.
- Validation of the method by contrasting its results with those reported by direct measurement techniques for various materials.

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