Karlstad Applied Analysis Seminar (2024)

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3 Dec 2024

Mathematical modeling of the adsorption of environmental contaminants

Abstract

It is well-documented that it is now virtually impossible to reach internationally agreed-upon energy and climate goals without active removal of environmental contaminants, combined with substantial emission reductions across all sectors. Whilst the solution can only come through a number of technologies, one of the most common and versatile methods for the capture of contaminants from a fluid is via column adsorption.

Adsorption columns are employed in the removal of greenhouse gases, volatile organic compounds, emerging contaminants and PFAs, also in water treatment, biogas cleansing and the purification of biopharmaceutical products. They are relatively easy to introduce into an industrial chain and may be applied to both liquids and gases. Consequently, they are a key tool for environmental remediation.

In this talk I will discuss recent work of the Environmental Mathematics group in Barcelona. The EM group specialises in the development and analysis of mathematical models of physical processes related to environmental issues. Mathematical solutions are particularly important since they provide explicit relations for system parameters and so lead to an understanding of the physical process not possible through purely numerical studies. After giving a brief overview of our work I will focus on our current main project, the model development and analysis of a variety of column adsorption processes.

The basic mathematical model of an adsorption column involves a coupled system of an advection-diffusion equation, describing the evolution of

the contaminant concentration as it passes through the column and a kinetic equation to account for the reaction process where contaminant attaches to an adsorbent material within the column. I will demonstrate how simple mathematical techniques can lead to solutions which accurately match experimental data. Along the way I will demonstrate how previous, long-accepted solutions contain errors and can be highly inaccurate, hopefully proving the power of applied mathematics!