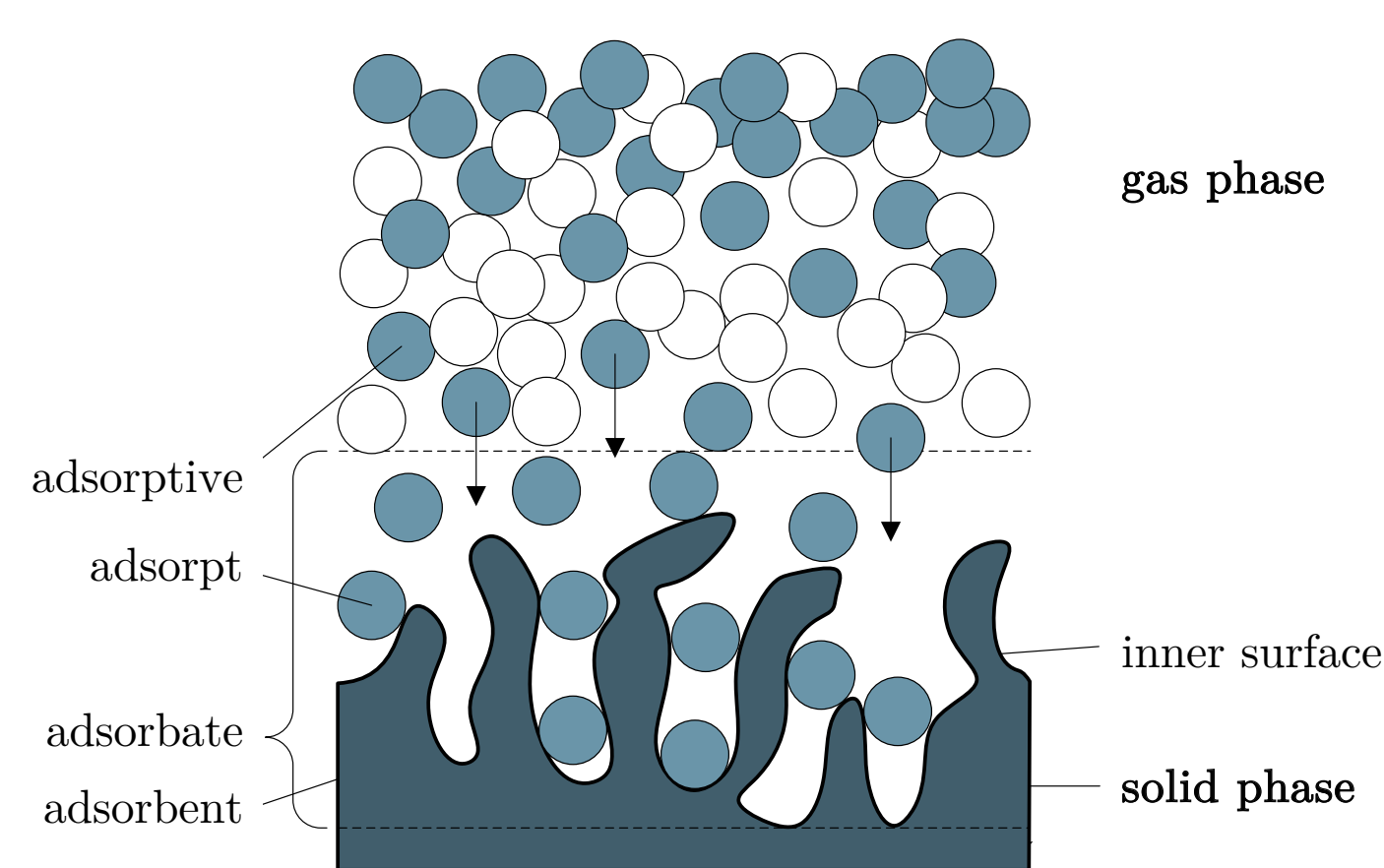


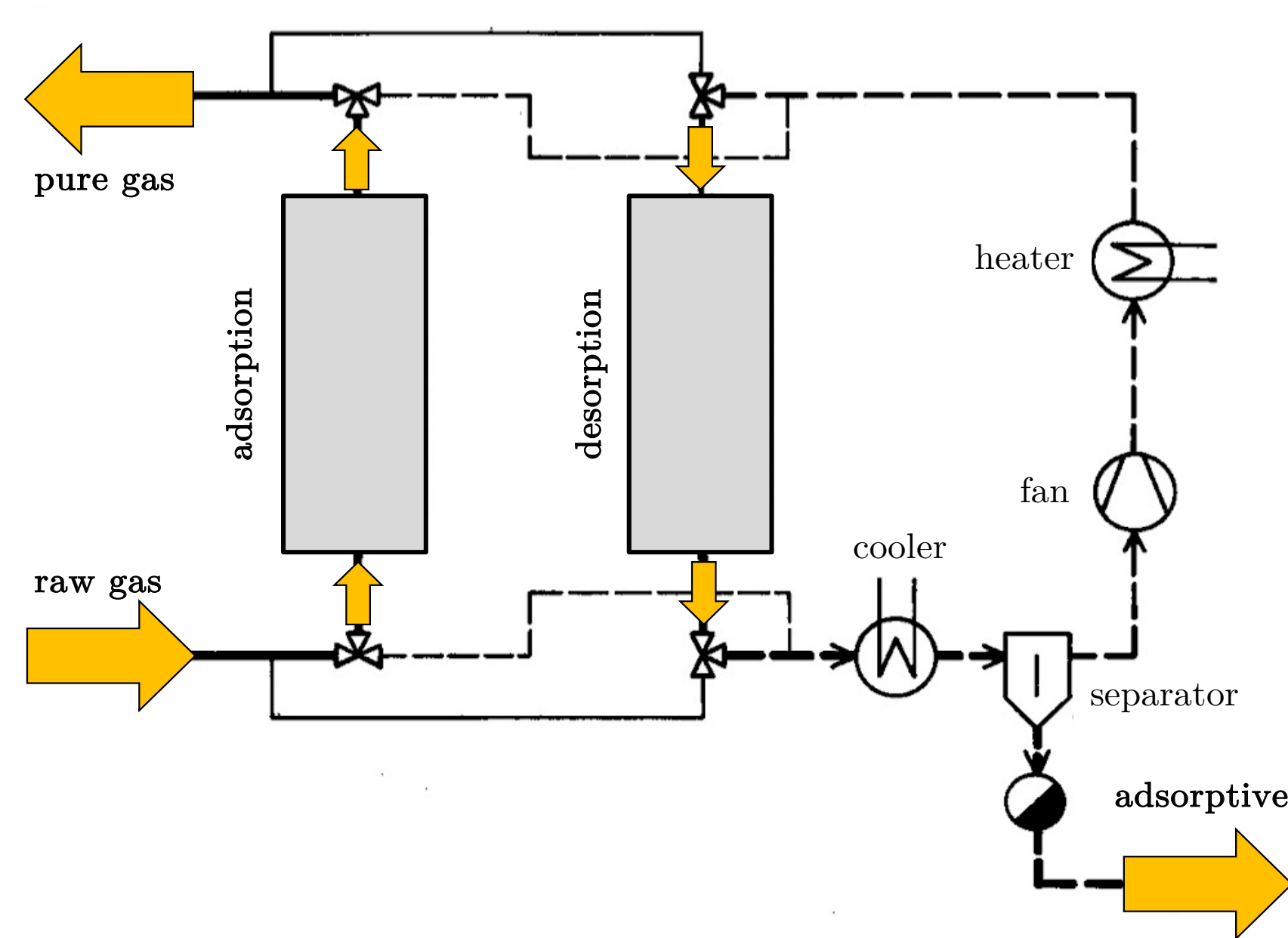
Master-Thesis Engineering, Specialisation Energy and Environment

# Design, simulation and analysis of multi-component gas adsorption processes in fixed bed columns

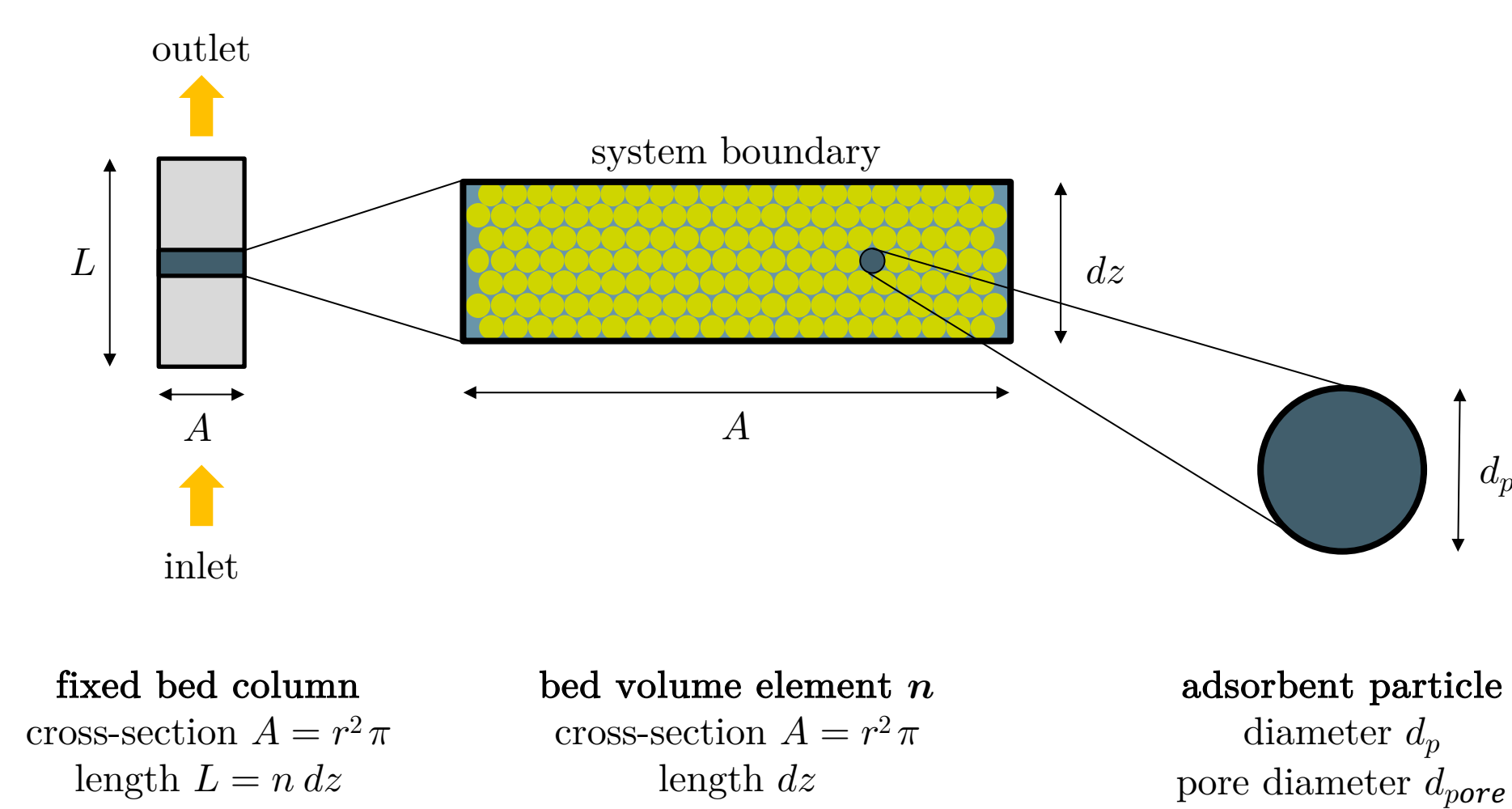
Basic concept of adsorption



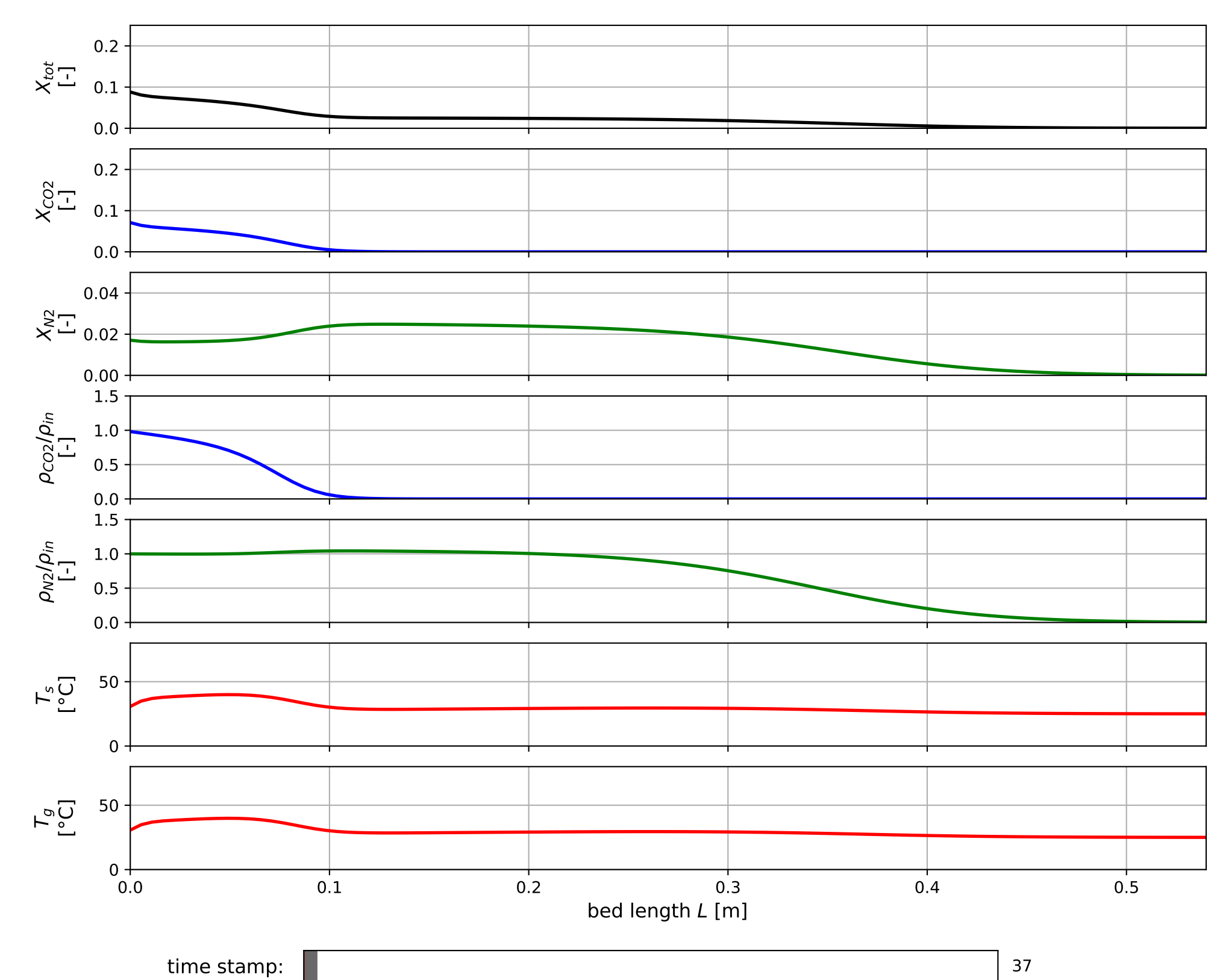
Flow diagram of an adsorption plant



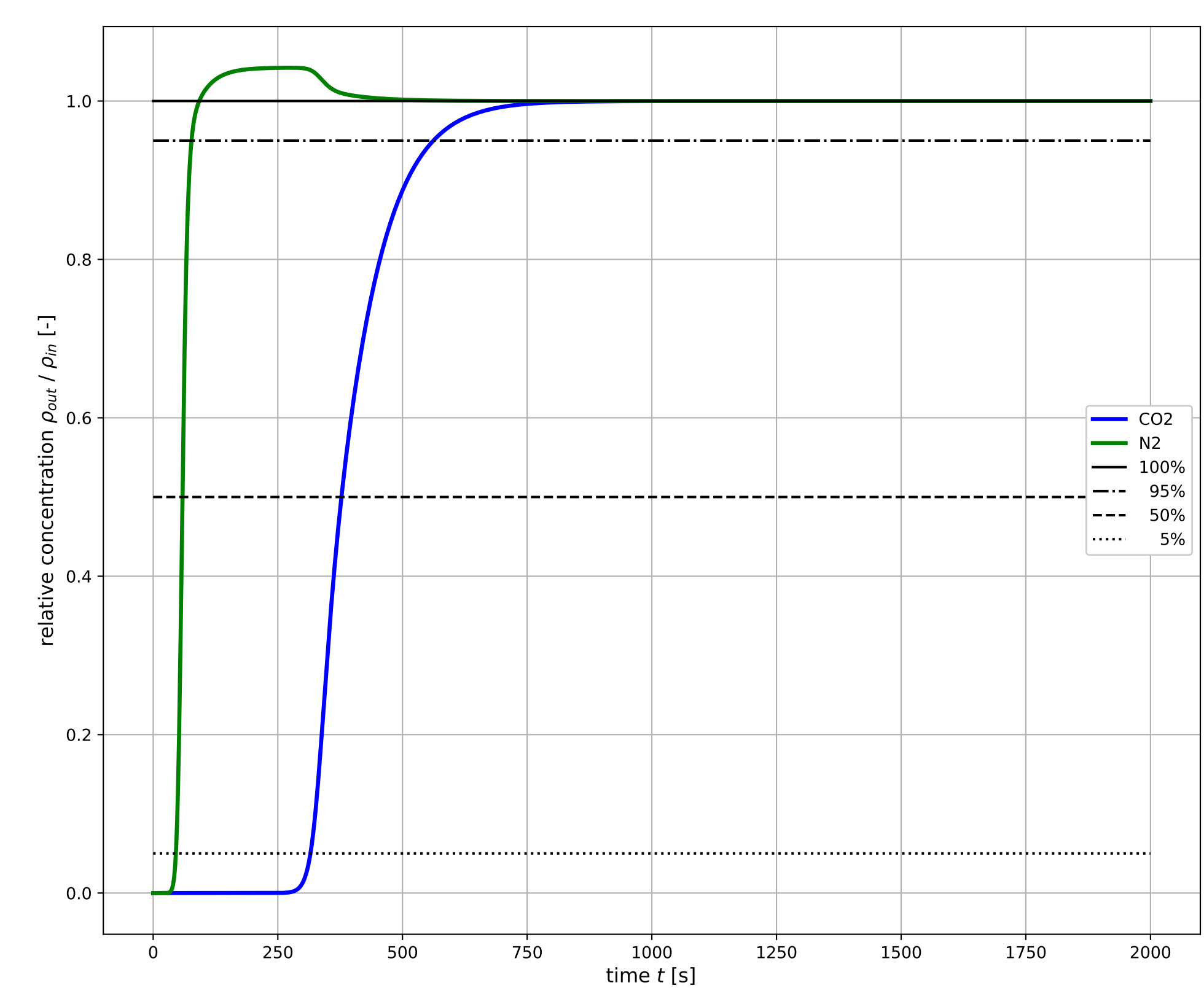
Balance area of adsorber bed volume element



Axial adsorptive concentrations, adsorbent loadings and temperature profiles through adsorption column



Breakthrough curves of investigated adsorptives at outlet of adsorption column



**Background**

Adsorption processes are among the most important process engineering methods for large scale gas separation and purification tasks in industry. Recent developments in separation technology have included new process designs and new adsorbents which offer attractive characteristics regarding energy demand, throughput, regeneration of the adsorbent and purity of the product.

In order to predict the performance of adsorptive separation systems and to optimise the design and operation of those plants, mathematical-physical models are increasingly required. Commercial simulation software are widely used, but usually not straightforward in handling. In industrial development of adsorption processes, nevertheless, shortcut and scale-/numbering-up methods are more commonly preferred over simulations.

**Results of work**

An open-source based application was developed for the design, simulation and analysis of multi-component gas adsorption processes in fixed bed columns. The tool capabilities are placed in between commercial simulation software and common short cut methods, i.e. it is a trade-off among fast and precise execution of process design.

The specially developed adsorption model was successfully validated using a measured reference case for the separation of CO2 and N2 from He on activated carbon. The model combines mass, energy and momentum balances with a linear driving force approach for mass and heat transport. The equilibrium loadings are modelled with the extended Langmuir equation and the loading dependent enthalpies of adsorption are calculated via the isosteric method.

Based on a created concept, the user software with graphical user interfaces was implemented in Python. The current functional framework of the software basically allows the input of all defined parameters and measurement data, the modelling of adsorption equilibria, the simulation execution of designed adsorption process as well as the graphical evaluation of simulation results based on mass transfer zones and breakthrough curves.

Methodology pursued:

1. Requirements specification
2. Literature research
3. Modelling of adsorption processes
4. Conceptual design of user software
5. Software realisation in Python

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