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Modelling of krypton-xenon separation by dynamic fixed-bed adsorption on zeolite

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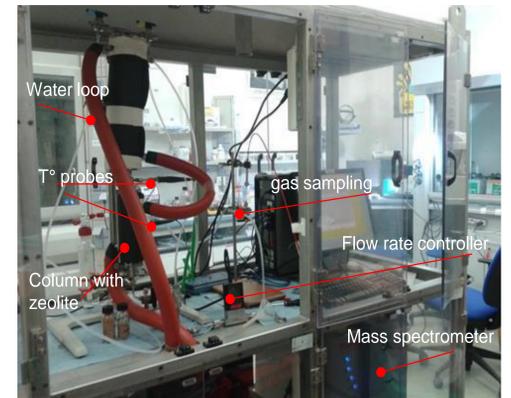
2- ProSim SA Immeuble Stratège A, 51, rue Ampère F-31670 Labège, France

Introduction

- Currently noble gases separated by cryogenic distillation \Rightarrow expensive process with safety constraints due to the cryogenic temperatures used
- Adsorptive separation (temperature/pressure swing adsorption) \Rightarrow an energy, safety and cost effective alternative method
- Different selective materials used from inorganic adsorbents based on physical adsorption to new metal-organic frameworks (MOFs) based on size and chemistry

OBJECTIVES

- Development of a Kr/Xe separation process by selective adsorption on a chabazite zeolite in a fixed bed column
- Experimental study of the Kr and Xe adsorption dynamics at different temperatures and under different operating conditions
- Modelling of the Kr/Xe adsorption separation from a gas mixture



Experimental set-up: fixed-bed adsorption column

Experimental study

Choice of the adsorbent

- A dozen of zeolites experimentally tested
- \Rightarrow selection of a synthetic chabazite AW500 of general formulae $M_x[(AlO_2)_x(SiO_2)_y]zH_2O$ due to its capture performances



Properties of the adsorbent

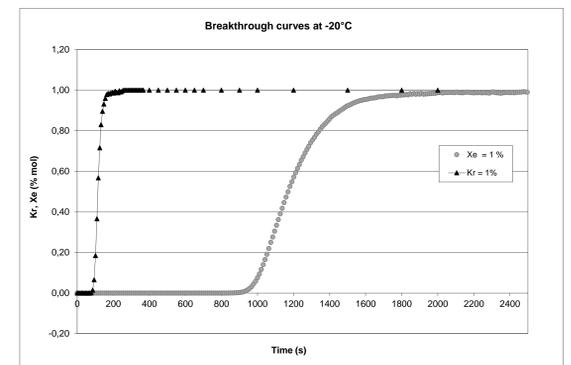
Particule diameter μm	250 – 500
Surface area (m^2/g)	327
Porosity volume (cm^3/g)	0,32
Particle density (kg/m^3)	1400
Pore diameter (nm)	11



Mass spectrometer

Fixed-bed adsorption

- Continuous acquisition of Kr/N₂ and Xe/N₂ breakthrough curves in a fixed-bed column
- Adiabatic system
- Temperatures: from -20°C to +20°C
- Initial feed concentrations: between 0 and 1%
- Gas concentrations followed by mass spectrometry
- Solid adsorbent thermally pretreated at 300°C under nitrogen

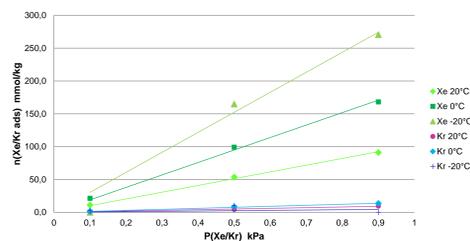


Example of breakthrough curves of Kr and Xe in N₂ at -20°C

Thermodynamic models

- linear law
- Adsorption enthalpy: -7.3 kJ.mol⁻¹

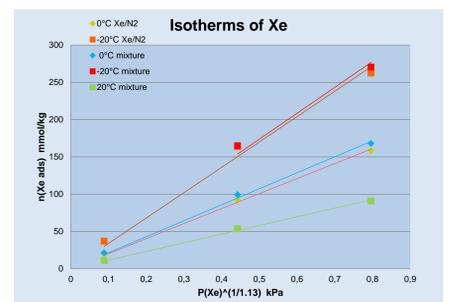
- Freundlich - Heller model
- Adsorption enthalpy: -18.8 kJ.mol⁻¹



Isotherms of Xe and Kr in N₂ at different temperatures

Gas Mixtures

- Tests on Xe/Kr/NO/NO₂/N₂ mixtures
- \Rightarrow absence of interactions between components



Comparison of the behaviour of Xe alone in N₂ and in Kr/NO/NO₂/N₂ mixtures

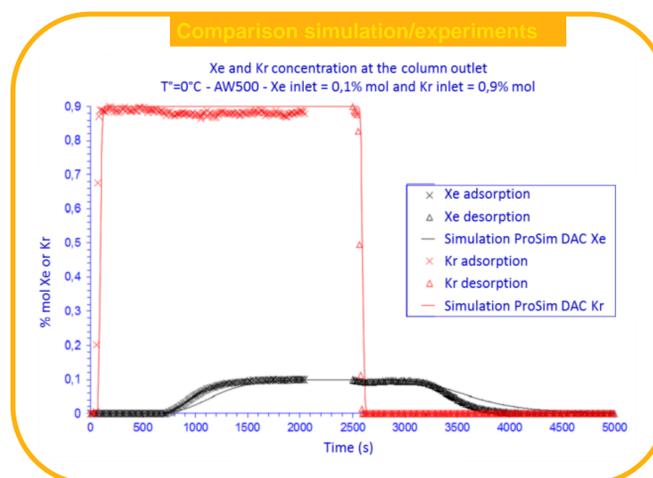
Modelling using ProSim

Dynamic simulation software ProSim DAC

- Based on the mass, energy and momentum balances
- Propagation of the gas flow described by the axially dispersed plug flow
- Mass transfer described by the Linear Driving Force Model (LDF)

Hypotheses:

- Adsorbent assumed to be thermodynamically inert
- Radial concentration gradients negligible
- Gas mixtures supposed to behave as an ideal gas



✓ Good agreement for both Kr and Xe

Application for a sensitivity analysis:

- Adsorbent characteristics \Rightarrow no impact on the adsorption and separation performances
- Process parameters: temperature, feed flow or initial concentration \Rightarrow high impacts

Conclusion

- Zeolite AW500 suitable for Xe/Kr separation process from a gas mixture flow as their breakthrough times are significantly different
- Development of an adsorption modelling using software ProSim DAC
- The model developed can be applied to design PSA/TSA cycles to separate Kr and Xe

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