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

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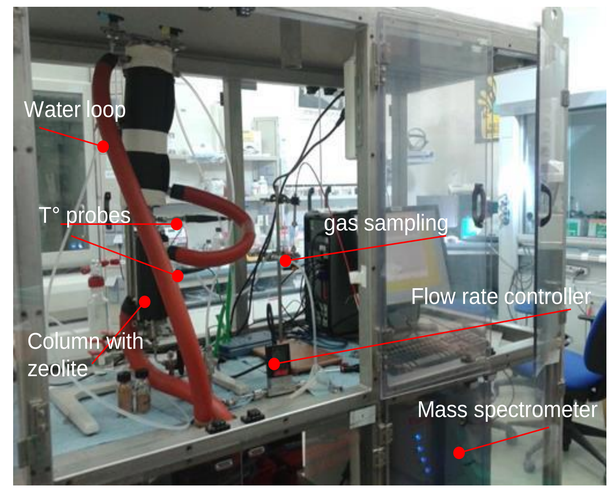
2- ProSim SA Immeuble Stratège A, 51, rue Ampère F-31670 Labège, France

Introduction

- **Currently noble gases separated by cryogenic distillation ⇨ expensive process with safety constraints due to the cryogenic temperatures used**
- **Adsorptive separation (temperature/pressure swing adsorption) ⇨ 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**
- **⇨ selection of a synthetic chabazite AW500 of general formulae $M_x[(AlO_2)_x(SiO_2)_y],zH_2O$) due to its capture performances**



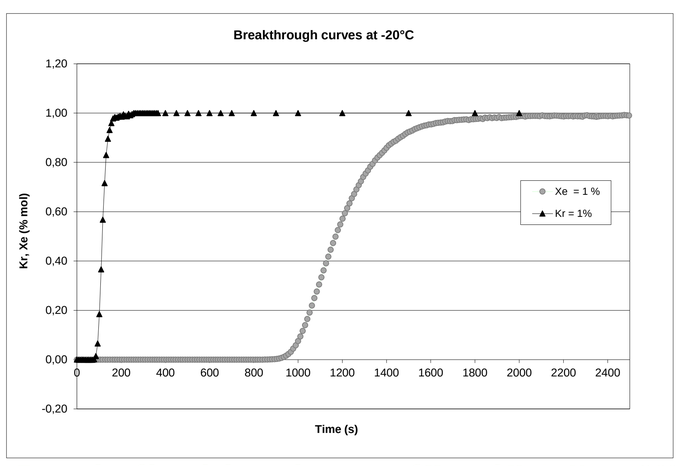
Properties of the adsorbent	
Particule diameter µm	250 – 500
Surface area (m^2/g)	327
Porosity volume (cm^3/g)	0,32
Particle density (kg/m^3)	1400
Pore diameter (nm)	11



Mass spectrometer

Fixed-bed adsorption

- **Continuous acquisition of Kr/N_2 and Xe/N_2 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 N_2 at -20°C

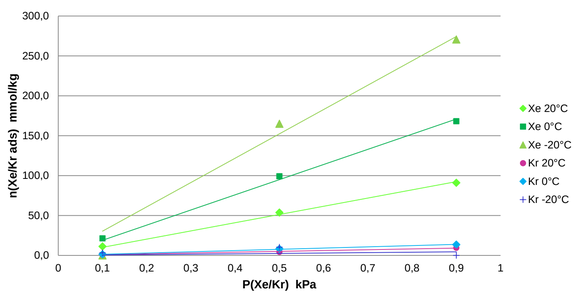
Thermodynamic models

Kr

- **linear law**
- **Adsorption enthalpy: -7.3 kJ.mol^{-1}**

Xe

- **Freundlich – Heller model**
- **Adsorption enthalpy: -18.8 kJ.mol^{-1}**

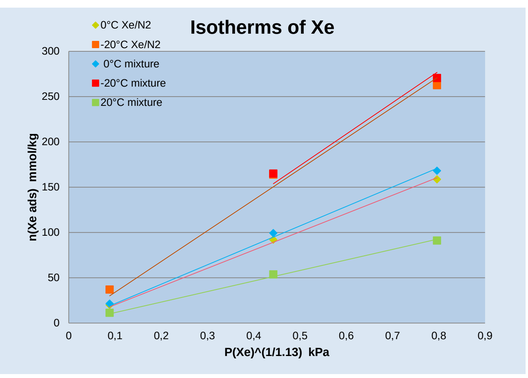


Isotherms of Xe and Xr in N_2 at different temperatures

Gas Mixtures

- **Tests on $Xe/Kr/NO/NO_2/N_2$ mixtures**

➡ **absence of interactions between components**



Comparison of the behaviour of Xe alone in N_2 and in $Kr/NO/NO_2/N_2$ mixtures

Modelling using ProSim

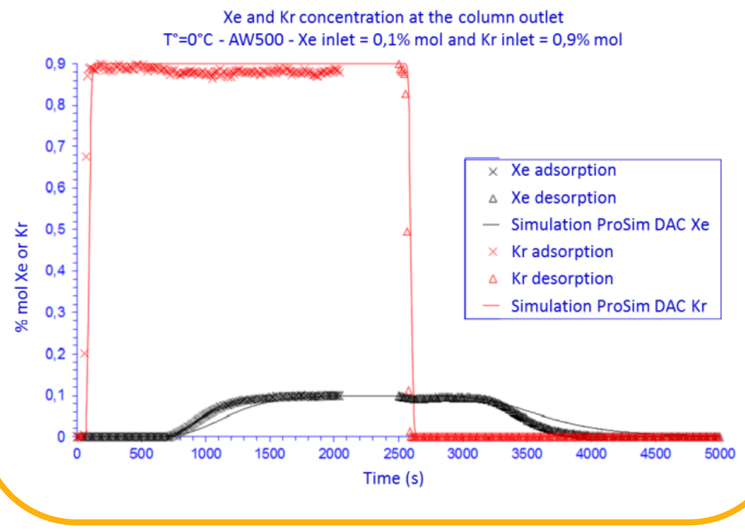
Dynamic simulation software ProSim DAC

- **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**

Comparison simulation/experiments



➡ ✓ **Good agreement for both Kr and Xe**

Application for a sensitivity analysis:

- **Adsorbent characteristics ⇨ no impact on the adsorption and separation performances**
- **Process parameters: temperature, feed flow or initial concentration ⇨ 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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