

Simulation of water vapor sorption profiles on activated carbons in the context of nuclear industry

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S. 1 Detailed description of the employed method for numerical resolution : “the method of lines” :

This method involves the approximation of the spatial derivative by a discrete difference between two points. The axial axis is discretized in n points, and the spatial derivative for a point i can be calculated as:

$$\frac{\partial C_i}{\partial Z} = \frac{C_i - C_{i-1}}{\Delta Z}$$

The second order derivative can then be calculated by applying the last equation with the first order derivative.

The numerical resolution was accomplished using the MATLAB software, with a home-made code constructed specifically for this work. The system was discretized in the Z axis according to the parameters in Table S1.

Table S1 : Parameters of the discretization

Parameters	Value
Number of discretization points	400
Relative tolerance	1×10^{-5}
Absolute tolerance	1×10^{-5}
Integration time	7200 s

Discretization allows the simplification of the initial problem, converting it to n ordinary differential equations that can easily be integrated in relation to time. In this manner, the concentration of a point is affected by the previous one, and the solution will take form as n concentrations profiles in relation to time for each point of the column. A summary of the process is shown in Figure S1., where the resulted $C_n(t)$ is the breakthrough curve experimentally determined. Finally, the MATLAB function ODE15s was used for the integration.

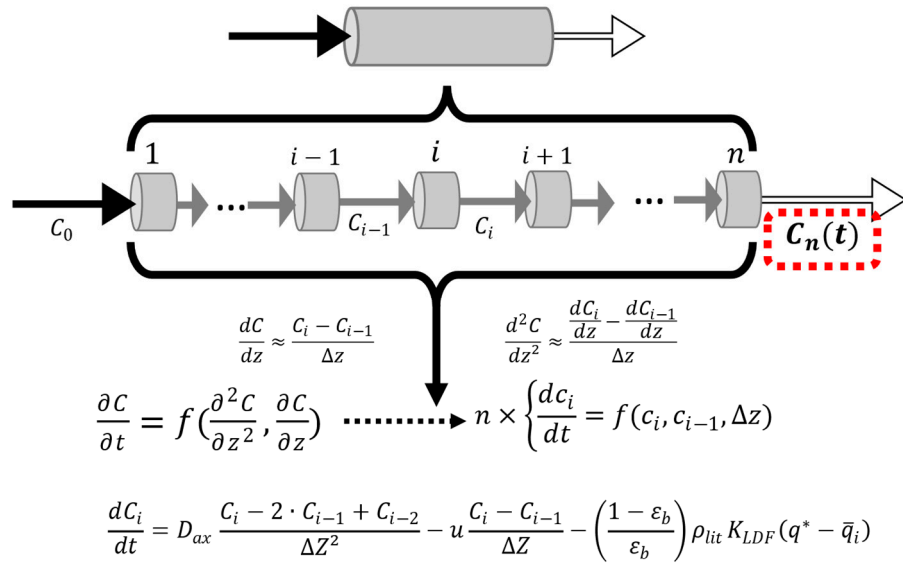
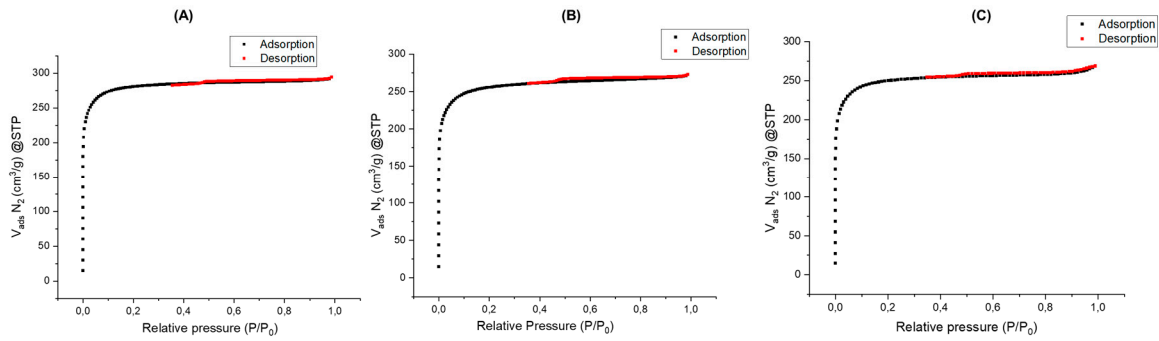


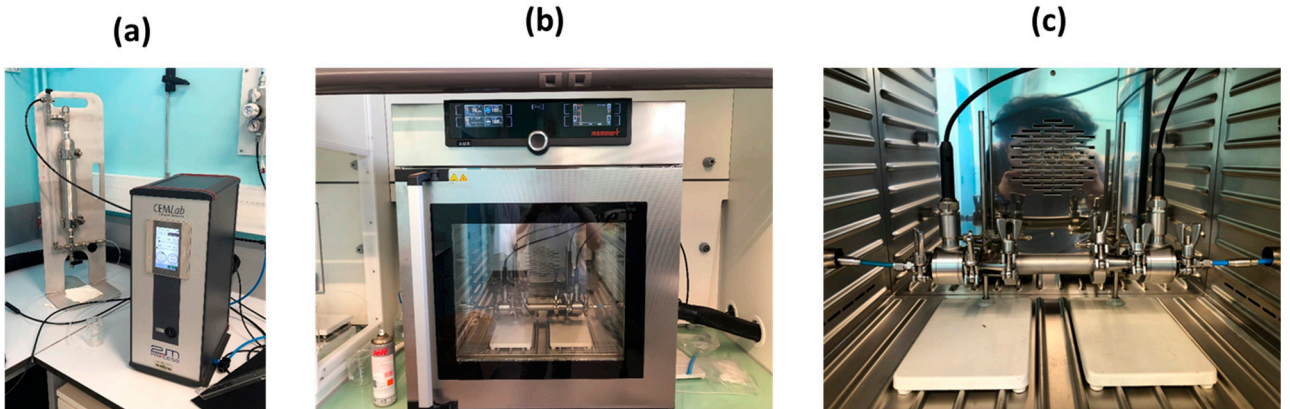
Figure S1 : Diagram of the discretization and numerical resolution

The code was structured in a modular way, allowing the inclusion of more elements to describe the adsorption kinetics, and to use of any model for the adsorption isotherm.

S2. N₂ adsorption/desorption isotherms at 77 K of the tested activated carbons: (A) AC nI and (B) AC 5KI, (C) AC Nuclear.



S3. Photos of the experimental apparatus



(a) Generation of water vapor;

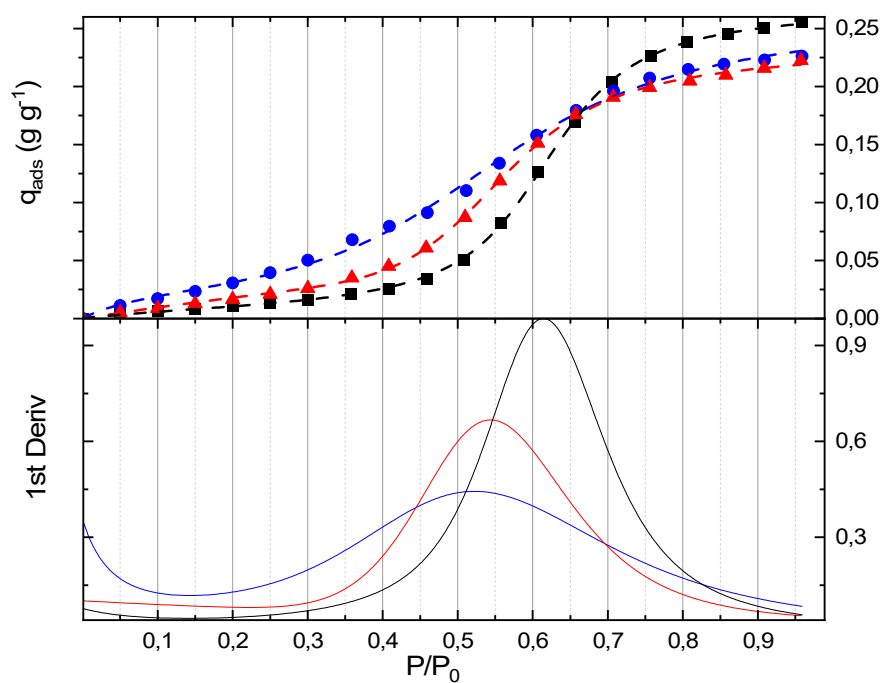
(b) Incubator allowing the temperature control;

(c) Zoom on the adsorbent bed and relative humidity captors downstream and upstream.

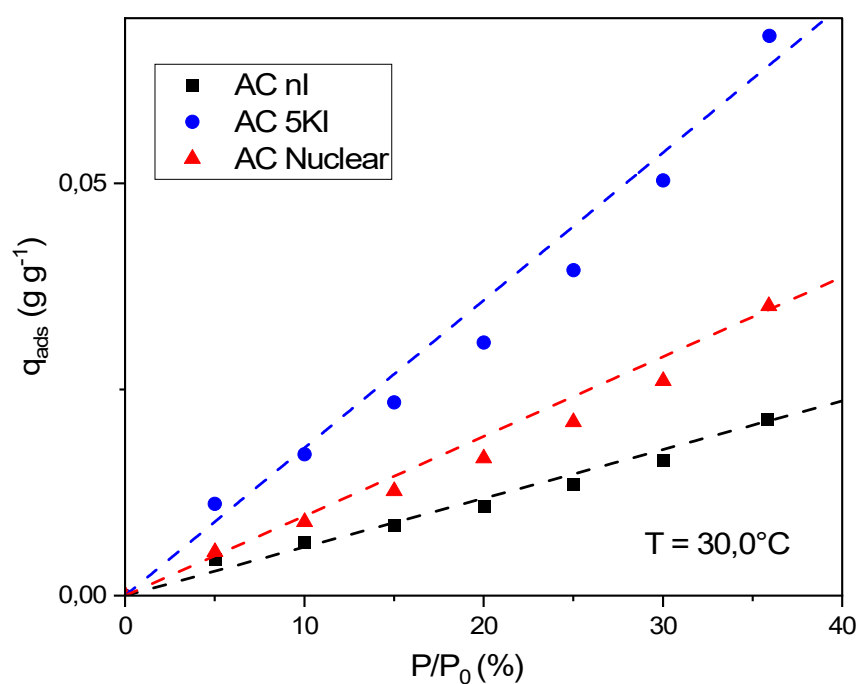


Sorption Microbalance

S4. First derivative of the adsorption isotherms



S5. Adsorption isotherms modeled with henry's model



S6. correlation coefficient (R^2), breakthrough time ($t_{5\%}$), saturation time ($t_{95\%}$) and prediction errors for the gas flow of 1.5 and 6.5 L.min⁻¹ (NTP) and program versions

Q = 1.5 L.min ⁻¹ (NTP)					
Version	R^2	$t_{5\% \text{ model}}$ (min)	Error (%)*	$t_{95\% \text{ model}}$ (min)	Error (%)
1	0.8501	6.5	80	17.5	61
2	0.9746	5.7	55	40	11
Q = 6.5 L.min ⁻¹ (NTP)					
Version	R^2	$t_{5\% \text{ model}}$ (min)	Error (%)*	$t_{95\% \text{ model}}$ (min)	Error (%)
1	0.8875	1.5	18	4.1	67
2	0.9866	1.3	2	9.0	27