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Carbon Dioxide Removal with Tuff: experimental measurement of adsorption properties and breakthrough modeling using CFD approach

Andrea Aquino^{a*}, Emanuele Bonamente^a, Cinzia Buratti^a, Franco Cotana^a, Beatrice Castellani^a, Valerio Paolini^b, Francesco Petracchini^b.

^aCIRIAF, Interuniversity Research Centre on Pollution and Environment "Mauro Felli", University of Perugia, Via G. Duranti 67, Perugia, Italy
^bInstitute of Atmospheric Pollution Research, Italian National Research Council, V. Salaria km 29.300, Monterotondo (RM), Italy

Abstract

This work presents the study of tuff as an alternative material for CO₂ capturing and removal by pressure swing adsorption techniques. Tuff represents an economic and environmentally sustainable alternative to commonly-used synthetic zeolites. The proposed methodology includes a laboratory characterization of the CO₂ adsorption process under different operative conditions and experimental layouts. Measured data are also used to setup computational fluid dynamics simulations of the fixed-bed adsorption column. Results can be used to define optimal design parameters needed to implement and to improve different applications for biogas upgrading (CO₂/CH₄ ratio adjustment) or carbon capture and storage.

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1. Introduction

The International Panel on Climate Change (IPCC) estimates that average CO₂ concentration level may rise up to 570 ppm by year 2100 causing an increase in mean sea level height of 38 cm and the rise in mean global average temperature of about 1.9°C [1],[2]. To reduce the CO₂ concentration in the environment, several approaches are available: (i) improve the energy efficiency, (ii) reduce the CO₂ emissions by expanding renewable energy resources

* Corresponding author. Tel.: +39 075 585 37 88; fax: +39 075 585 3697.
E-mail address: aquino@crbnet.it

[3][4], (iii) capturing the CO₂ [5]. The physical adsorption of CO₂ on a solid adsorbent can be easily exploited by several applications exploiting weak, intra-molecular forces such as the universal van der Waals interactions [6]. A typical application using physical adsorption for gas mix separation is the Pressure Swing Adsorption (PSA) coupled with Vacuum Swing Adsorption (VSA). A typical PSA-unit is formed by several columns packed with adsorbent particles. Modifying the residence time in the column, PSA can be operated either in batch-mode or in continuum-mode. In batch-mode, the more strongly adsorbed components of a gas mixture are retained within the column, while in continuum-mode the less diffusive gas species is captured [7]. After the saturation, the adsorbent can be regenerated at low pressure by VSA, and reused in subsequent adsorption cycles. This technique can be easily suited for several applications aimed to CO₂ removal/capture. A common application for PSA is cleaning and upgrading of biogas [8] to produce biomethane. This final product is of great interest because can be used in substitution of natural gas for heat and power generation and as vehicle fuel [9]. In this application, the CO₂ separation process is based on different adsorption equilibrium between carbon dioxide and methane at the same operative pressure. Another interesting PSA/VSA application which involves the adsorption reaction between CO₂ and a solid medium, is the carbon capture and sequestration (CCS). The CCS technique can be used to isolate CO₂ for a long period of time in naturally occurring geological storage or mineral carbonation [10]. Several adsorbents have been proposed for carbon dioxide adsorption. Zeolites are crystalline aluminosilicates of alkali or alkali earth elements, which exhibit unique adsorption properties because of their surface chemistry: tetrahedral of silicon and aluminum (SiO₄ and AlO₄), assembled into units of different shape (cubes, hexagonal prisms, octahedral, and truncated octahedral). Their adsorptive properties are due on the ability of these open crystalline structures to enclose charged and neutral species within cavities. Although most synthetically produced zeolites, as 5A and 13X, have been successfully used for the adsorption of CO₂ [11], currently, there is an increasingly demand of natural zeolites, such as Clinoptilolite, Modernite, Erionite, Ferrierite, and Phillipsite [12]. The aim of the current work is to measure the CO₂ adsorptive properties of tuff, a low-cost mix of natural zeolites, easily available as byproduct of building industries. Thanks to the high adsorption efficiency, tuff can be considered an interesting alternative to synthetic zeolites for CO₂ adsorption via PSA. To classify tuff such as a porous adsorbent several experimental activities were performed. The mercury porosimetry was used to determine the tuff superficial pore size, their distribution and other important physical properties [13]. A small scale laboratory unit is used to measure the quantity of adsorbed CO₂ by tuff in equilibrium conditions. The measured data can be used to estimate the real process performance of tuff, expendables in industrial applications.

Nomenclature

V_s	Volume of adsorption equilibrium unit containing the sample (m ³);
V_r	Volume of adsorption equilibrium unit for the measurement of the initial CO ₂ amount (m ³);
V_{eq}	Total volume of adsorption equilibrium unit (m ³);
P_{air}	Equilibrium pressure of the residual atmospheric air inside the adsorption equilibrium unit (MPa);
P_0	Equilibrium pressure of the initial CO ₂ amount inside V_r , the adsorption equilibrium unit (MPa);
P_{eq}	Equilibrium pressure of the unadsorbed CO ₂ inside V_{eq} (MPa);
R	Gas constant (J·K ⁻¹ ·mol ⁻¹);
n_0	Initial CO ₂ amount (mol);
n_f	Residual CO ₂ amount (mol);
n_{ads}	Adsorbed CO ₂ amount (mol);
B	Langmuir B constant (MPa ⁻¹);
q_m	Langmuir maximum adsorption capacity (kg _{CO2} /kg _{Tuff});
$\dot{q}_{ads}(x)$	CO ₂ adsorption rate (kg _{CO2} /s);
$\dot{q}_{ads}(0)$	Initial CO ₂ adsorption rate (kg _{CO2} /s);
q_{ads}	Cumulative CO ₂ adsorbed amount (kg _{CO2});
q_{ads}^{max}	Maximum CO ₂ adsorbable amount (kg _{CO2});
$Y(x)$	Adsorption rate $\in [0,1]$ (-);
x	Saturation level $\in [0,1]$ (-);
a	Saturation parameter (-).

2. Experimental layouts

The tuff sample, according to previous analysis [14], presents the following chemical composition: chabazite ($65\% \pm 5\%$), phillipsite ($3\% \pm 2\%$), K-feldspate ($10\% \pm 3\%$), augite ($2\% \pm 1\%$), mica ($5\% \pm 2\%$) and volcanic glass ($15\% \pm 4\%$). The gas used to directly measure the adsorption performance is carbon dioxide. Nitrogen is used as purge and desorption gas because its adsorbed amount is negligible. Totally, three samples of about 0.5 kg each are collected from the same stock. Before each experimental activity, a pre-treatment phase is implemented to ensure the optimal activation of zeolites and to avoid irreversible changes in their structure [15]. The tuff samples are firstly washed up with de-mineralized water, and then heated at 220°C for 12 hours.

Each sample is analyzed in sequence by two porosimeters (mod. Pascal 140 & mod. Pascal 240 Thermoscientific™) at different operative pressure. The low pressure porosimeter operates to a maximum pressure of 400 kPa, while the high pressure porosimeter can operate to a maximum pressure of 200 MPa. The minimum measurable pore diameter is between $0.0074\ \mu\text{m}$ and $15\ \mu\text{m}$. As it will be shown in section 3., the measured physical properties of tuff are affected by a high grade of variability. This characteristic is due to the high heterogeneity of tuff geometry and chemical composition [14], and the low capacity of porosimeters, which can characterize only small samples (few grams) for each analysis.

Saturation curves, necessary to study the adsorption process in transient condition and to validate the model implemented for the CFD simulations, are obtained with a custom device: a breakthrough unit is implemented to measure the saturation level of the collected samples, each one analyzed under a specific set of operative conditions [16]. The layout of the breakthrough unit (Fig. 1) consists of a gas mixer, a flow rate meter, a cylindrical adsorption column cartridge, a vent, and an infrared gas analyzer [17]. At the beginning of each analysis the column bed is purged with nitrogen flow, until zero concentration of CO_2 is measured at the outlet. Afterwards, a gas mixture of CO_2 and N_2 is flowed through the column, and the gas composition at the outlet is recorded every 5 seconds. The saturation of the sample is achieved when the outflow gas composition (CO_2 and N_2 concentration) is equal to the inlet composition. After each analysis, the column is refilled with new pre-treated adsorbent. Exhausted adsorbent are regenerated, before reuse in following analysis.

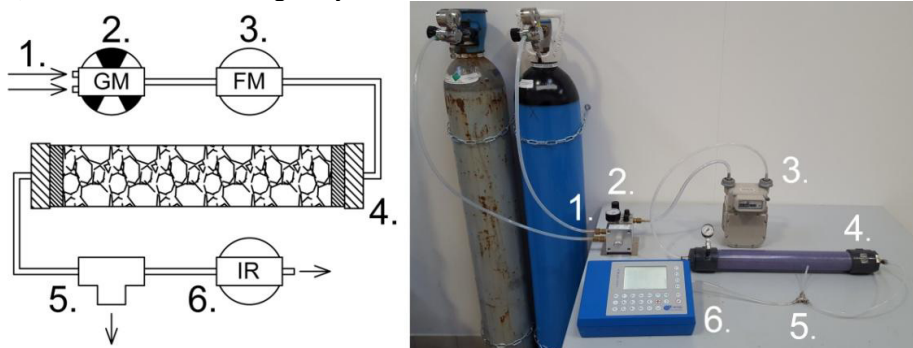


Fig. 1. Layout of the breakthrough setup: (1) feed gas inlet; (2) gas mixer; (3) flow rate meter; (4) adsorption column; (5) vent; (6) infrared gas analyzer.

The tuff adsorption efficiency (total adsorbed CO_2 per unit mass of tuff) in equilibrium conditions can be measured by volumetric methods [18][19]. This procedure is based on controlled gas expansion using the ideal gas approximation, as shown in Fig. 2. The adsorption equilibrium unit [17] uses a CO_2 feed, two expansion volumes (V_s and V_r), a vacuum pump, a digital manometer, and a switchable manifold. V_s contains the tuff sample (its volume is measured net of the sample volume). V_r is a reference volume used to measure the amount of CO_2 in the system before the adsorption process. The system is immersed in a thermostatic bath, which guarantees a constant temperature (T_b). At the beginning of the analysis, mid-vacuum is reached in the entire system (P_{air} is the residual air pressure). V_r is filled with pure CO_2 . The initial CO_2 amount (n_0) is measured following Eq. 1 subtracting P_{air} to the total measured pressure (P_0). Afterwards, the gas inside V_r expands inside V_s . The final amount of CO_2 (n_f) inside the

total volume ($V_{eq}=V_r+V_s$) at the adsorption equilibrium is measured according to Eq. 2. The total amount of adsorbed CO_2 (n_{ads}) is computed according to Eq. 3.

$$n_0 = \frac{(P_0 - P_{air}) \cdot V_r}{R \cdot T_b} \tag{1}$$

$$n_f = \frac{(P_{eq} - P_{air}) \cdot V_{eq}}{R \cdot T_b} \tag{2}$$

$$n_{ads} = n_0 - n_f \tag{3}$$

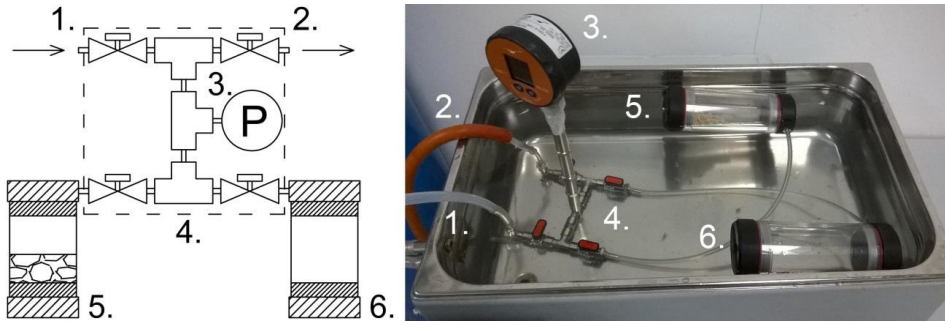


Fig. 2. Layout of the equilibrium adsorption unit: (1) feed gas inlet; (2) vacuum pump outlet; (3) manometer; (4) manifold; (5) sample volume; (6) reference volume.

3. Material properties

The physical properties of tuff, obtained with mercury intrusion porosimetry, are the total porosity, the bulk density, the average pore size, and the pore size distribution. Tuff physical properties are reported and compared with synthetic zeolites 13X in Table 1. According to the classification of porous solids [18] [20], with an average pore diameter of $4.2 \cdot 10^{-6} \pm 1.9 \cdot 10^{-6}$ m, tuff is a macroporous material. The tuff pore size distribution reports a specific volume of $1.31 \cdot 10^{-4}$ m³/kg for macropores with a diameter between $4 \cdot 10^{-6}$ m and $2 \cdot 10^{-6}$ m (porosimeters reference diameters range). To investigate smaller pore diameters range (mesopores and micropores distributions), different techniques are needed.

The breakthrough point is defined as the maximum CO_2 that the system can adsorb before the outlet CO_2 concentration exceeds some reference value [16]. In Fig. 3, the outlet CO_2 percentage is plotted as a function of the inlet CO_2 amount per unit mass of tuff (kg_{CO_2}/kg_{Tuff}) for each analyzed sample. In the present work, considering the biomethane quality requirements as in national technical regulations [21], the breakthrough point is set to an outlet CO_2 concentration of 3%. According to the results shown in Fig. 3, the maximum adsorbable CO_2 before the breakthrough point is reached between 0.028 and 0.036 kg_{CO_2}/kg_{Tuff} .

The adsorption efficiency of tuff for CO_2 adsorption is measured at increasing operative pressures up to approx. 0.35 MPa and an operative temperature of 25°C. Experimental data are reported and compared with similar literature data of 13X zeolites in Table 2. The adsorption isotherm is obtained fitting the Langmuir analytical model [23] to the experimental, data as shown in Table 3.

Table 1. Physical properties of tuff vs. synthetic zeolites 13X

Physical Properties	Tuff	Zeolite 13X [11]
Total porosity (%)	35 ± 5	54
Skeletal density (kg/m ³)	2300 ± 200	2456
Particle density (kg/m ³)	1480 ± 80	1130
Average pore diameter (m)	$(4.2 \pm 1.9) \cdot 10^{-6}$	$3.22 \cdot 10^{-7}$

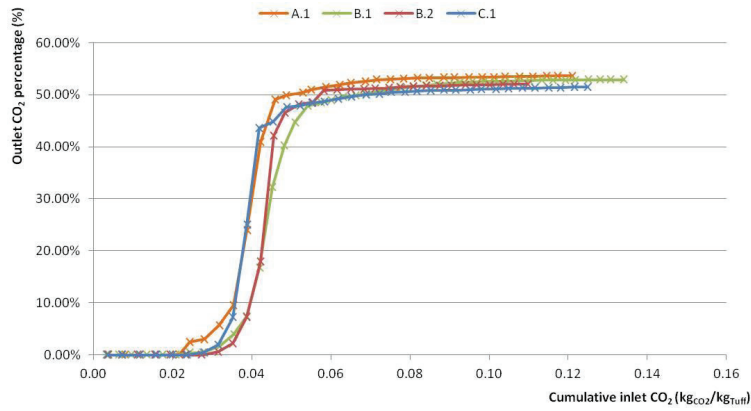
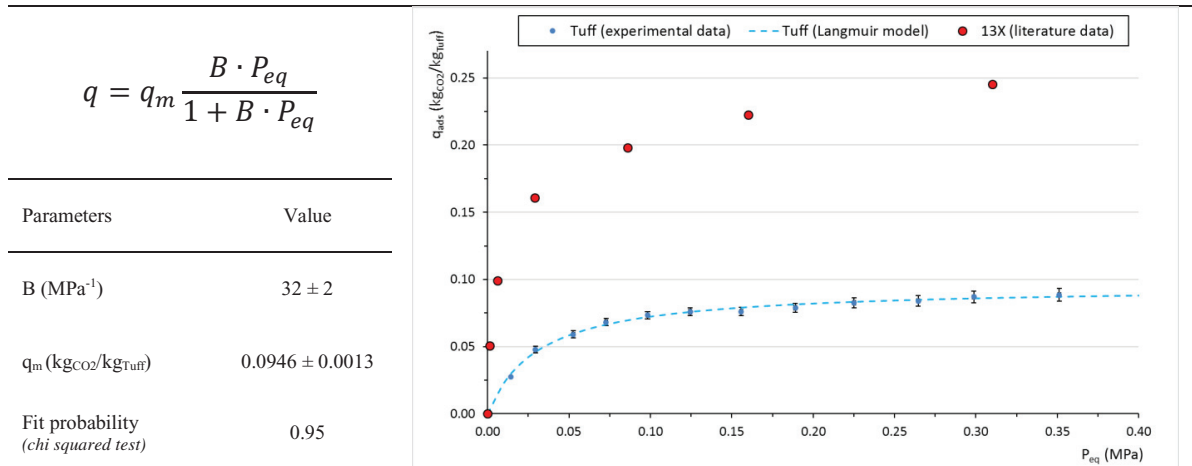


Fig. 3. Outlet CO₂ percentage vs cumulative inlet CO₂ (experimental data)

Table 2. Adsorption efficiency vs equilibrium pressure (tuff experimental data vs 13X zeolites literature data [11])

Tuff Equilibrium Pressure	0.0144 ± 0.0008	0.0294 ± 0.0008	0.0526 ± 0.0008	0.0728 ± 0.0008	0.0983 ± 0.0008	0.1245 ± 0.0008	0.1558 ± 0.0008	0.1891 ± 0.0008	0.2251 ± 0.0008	0.2645 ± 0.0008	0.2987 ± 0.0008	0.3512 ± 0.0008
Tuff Adsorption Efficiency	0.027 ± 0.002	0.048 ± 0.003	0.059 ± 0.003	0.068 ± 0.003	0.073 ± 0.003	0.076 ± 0.003	0.076 ± 0.003	0.079 ± 0.003	0.083 ± 0.004	0.084 ± 0.004	0.087 ± 0.004	0.089 ± 0.005
13X Equilibrium Pressure	0.00118		0.00610		0.02905		0.08610		0.160		0.310	
13X Adsorption Efficiency	0.05048		0.09899		0.16103		0.19804		0.222		0.245	

Table 3. Langmuir fit parameters



4. CFD simulations

4.1. Model setup

In this section the CFD analysis of the CO₂ adsorption by tuff is presented. The process was modeled as a mixed fluid, composed by two chemical species (CO₂ and N₂), flowing through a cylindrical adsorption column packed with a porous material (tuff). The analysis, developed with Ansys Fluent 16.2 [22], aimed at studying the CO₂ adsorption process as a function of operative parameters. As a first step, the geometrical domain was developed using the same dimensions of the breakthrough unit. The parameters of the 3D model are: radius 0.057 m, length 0.45 m, volume 0.0015 m³, bed porosity 0.51-0.57. For all simulated cases the energy equation, the k-ε model, and the mixed species transport are used in order to consider the binary species mixing and transport processes in a turbulent regime. The compressible ideal gas model was also used. The diffusivity of the mix is computed with the multi-component law [18]. The porous media is assumed to be isotropic and the related pressure losses are quantified by the Ergun equation [24]. All the cases are simulated in transient regime with 1 second time step.

To simulate the CO₂ adsorption process, a source term is included in the mass balance equation. User-defined functions are used to model the source term as a mass sink characterized by a decreasing adsorption rate as a function of the saturation level. The cell saturation level (eq. 4) is defined by the ratio of the cumulative adsorbed CO₂ and the maximum adsorbable amount. At the beginning of the process x is 0, and it becomes 1 for fully-saturated cells. The cell adsorption rate (kg_{CO2}/s) depends on the saturation level, and it is maximum for $x = 0$ and zero for $x = 1$.

$$x = \frac{q_{ads}}{q_{ads}^{max}} \tag{4}$$

The adsorption rate as a function of the saturation level was modeled according to eqs. 5 and 6:

$$\dot{q}_{ads}(x) = \dot{q}_{ads}(0) \cdot Y(x) \tag{5}$$

$$Y(x) = \frac{e^{-ax} - e}{1 - e} \tag{6}$$

The saturation parameter (a) is obtained with a fit using observed data as shown in Fig. 4. The total adsorbed CO₂ of the model (red) equals the observed value (green) and the behavior around the breakthrough point is well reproduced.

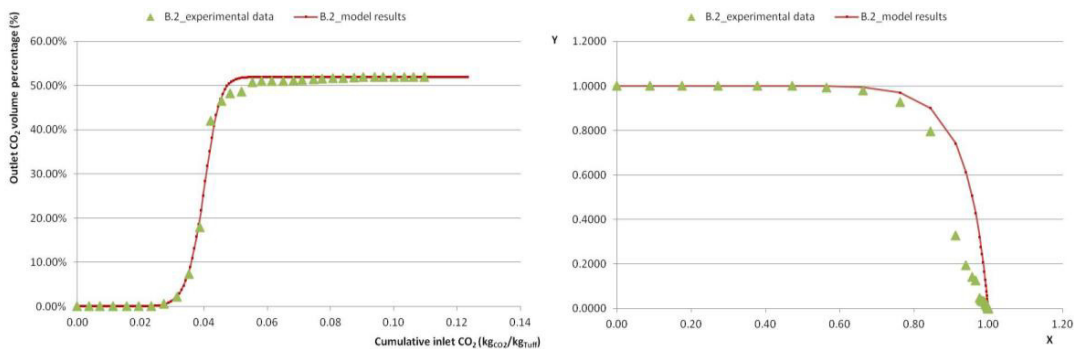


Fig. 4. Fit for saturation parameter evaluation (B.2 sample)

4.2. Model validation

The validation procedure is based on the comparison between simulated and experimental data. The boundary conditions adopted for each sample and the related simulation case are summarized in Table 4. The validation results are shown in Figs. 6-9.

Table 4. Boundary conditions

Validation case	Sample weight (kg)	Inlet Mass flow rate (kg/s)	CO ₂ volume fraction (-)	CO ₂ mass fraction (-)	q_{ads}^{max} – max adsorbable CO ₂ (kg _{CO2})	a – exponential parameter (-)
A.1	0.52266	$0.5849 \cdot 10^{-3}$	0.5360	0.6447	16.8746	7
B.1	0.59419	$0.5907 \cdot 10^{-3}$	0.5290	0.6382	23.1599	7
B.2	0.54326	$0.5912 \cdot 10^{-3}$	0.5200	0.6298	19.0113	11
C.1	0.51935	$0.5786 \cdot 10^{-3}$	0.5150	0.6552	17.0776	8

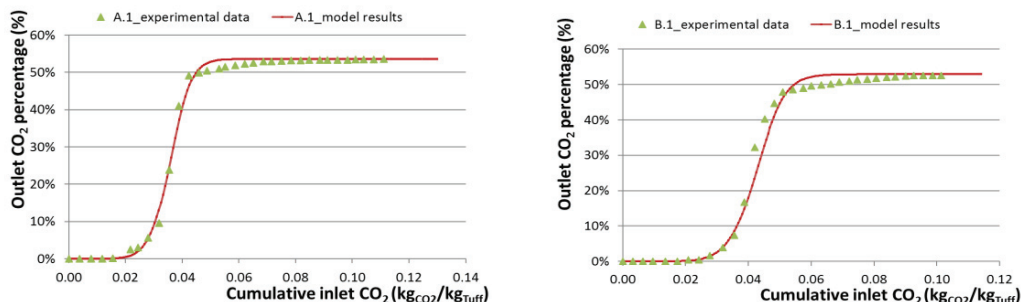


Fig. 5. A.1 (left) and B.1 (right) sample-model (red) vs. experimental data (green)

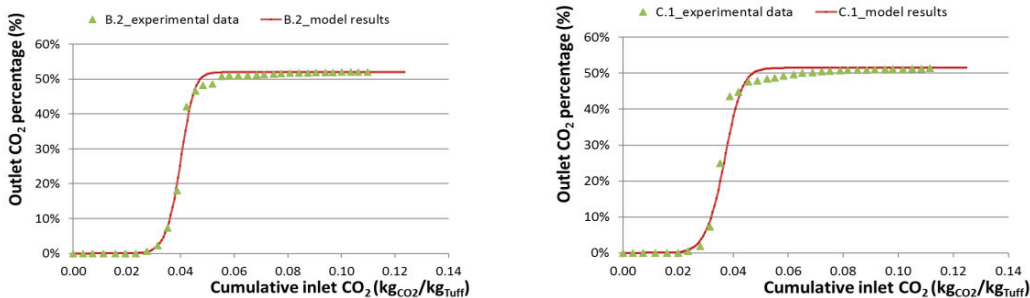


Fig. 6. B.2 (left) and C.2 (right) sample-model (red) vs. experimental data (green)

5. Conclusions

Tuff properties are characterized with laboratory measurements in order to assess its capabilities as porous adsorbent. The porous structure analysis, performed with the mercury intrusion porosimetry, describes the tuff physical structure and allows a comparison with other commonly used adsorbents. Results show a total porosity of $35 \pm 5\%$, a skeletal density of $2300 \pm 200 \text{ kg/m}^3$ corresponding to a particle density of $1480 \pm 80 \text{ kg/m}^3$, and an average pore diameter of $(4.2 \pm 1.9) \cdot 10^{-6} \text{ m}$. The measurement variability is due to the high grade of heterogeneity of the superficial and geometrical properties of tuff particles. The heterogeneity is also observed during saturation measurements, resulting in slightly different saturation curves for different samples. The evaluation of the CO₂ adsorption performance is achieved with two custom devices. The breakthrough saturation unit features a laboratory-scale adsorption column used to measure the saturation level of tuff and the adsorbable amount of CO₂ before the breakthrough point (i.e. the maximum CO₂ concentration allowed in the outlet flow) is reached. Four tuff samples were analyzed to measure the outlet CO₂ concentration as a function of adsorbed CO₂ (i.e. saturation curves). The samples weight is approx. 0.5 kg, the inlet CO₂ concentration is approx. 50% and the inflow rate is between 0.3 and 0.5 l/s. The saturation breakthrough, considering a maximum of 3% CO₂ at outlet, ranges from 0.028 to 0.036 kg_{CO2}/kg_{Tuff}. The adsorption equilibrium unit measures the tuff adsorption capacity and its dependence over operative temperature and CO₂ equilibrium pressure. Adsorption isotherms (i.e. CO₂ adsorption potential vs equilibrium pressure at a constant temperature) were obtained using this unit at 25°C and at equilibrium

pressures up to 0.35 MPa. The sample weight is approx. 0.01 kg. A reference analytical function (Langmuir) was also fitted to experimental data and the resulting maximum adsorption efficiency is found to be $0.0946 \pm 0.0013 \text{ kg}_{\text{CO}_2}/\text{kg}_{\text{Tuff}}$. A CFD model is developed with the aim of reproducing the CO_2 adsorption process inside the column and to eventually simulate the system behavior for real working conditions. Measured saturation curves for each sample are used for model validation. As a first step, an original analytic function is proposed for tuff adsorption rate (i.e. quantity of adsorbed CO_2 per unit time as a function of the saturation level). Experimental data were used to estimate the saturation parameter a . As a second step, boundary conditions from the same experimental datasets were used to perform CFD simulations in transient regime. Results show a remarkable agreement between data and simulations. CFD simulations is a useful tool to test the performance of different design approaches and to define the best configuration for industrial prototypes. The next step of this work will be the design and sizing of an adsorption column for real applications, for which it will be necessary to take into account tuff properties and their effect on the adsorption process, with a particular attention to the observed level of variability.

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