



Thermodynamics of thermally-driven adsorption compression



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ABSTRACT

Adsorption compressors are an emerging technology used to compress a gas stream with low grade heat which is of interest for the next long term extra-planetary bases. An analysis of thermodynamics of multicomponent gas/vapour mixtures compression with a thermally-driven adsorption bed is reported. In this unit a multicomponent stream is firstly adsorbed and secondly compressed by heating a bed at closed volume. The analysis is based on adsorbed solution theory applied to closed vessels where the composition and pressure of the bulk gas phase depends on temperature and volume of the whole system, leading to an isochoric-isothermal flash problem. Analysis of both an ideal and non-ideal adsorption compressor shows that the ideal approach is conservative, resulting in lower compression ratios at higher energy consumption.

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1. Introduction

The recent development of highly selective adsorption materials have enabled their integration in a number of traditional technologies, resulting in advanced processes demanding a sensibly lower energy consumption delivered at lower temperatures than their traditional counterparts [1–3]. A partial list of cases is included in Table 1. All these new technologies include a fundamental component that is the adsorption bed, which can be structured in numerous different shapes depending on the regeneration strategy [4–7].

Adsorption beds are often operated as open systems where a single or multicomponent feed flows through the unit. However, some emerging technologies need to operate adsorption beds as closed systems. This is the case of the carbon dioxide removal and compression system, currently operating on the International Space Station and still under development to serve the next long term Mars or lunar bases [16–18].

Adsorption is the favourite method to produce a compressed gas in space applications because it does not have moving parts, requiring virtually no maintenance, and does not generate vibrations. The carbon dioxide removal system is the upstream process of the Sabatier reaction, which will be used in extra-terrestrial bases for the production of water. As demonstrated elsewhere [19,20], the standard operating conditions to drive the Sabatier reaction towards higher CO₂ conversion are temperature ranging between 250 and 400 °C and pressure of reagents >130 kPa. So, compression of CO₂ from 20 kPa (Mars atmosphere) to

130 kPa (Sabatier reaction pressure) is required, resulting in a minimum compression ratio of 6.5.

In this technology, compression is performed through a change in the bed temperature at closed volume. The operational steps of an adsorption compressor can be scheduled as:

- 1) Adsorption step: the adsorption bed is kept isothermal and is fed with the inlet stream at constant pressure and temperature.
- 2) Heating step: the bed is heated at constant volume. The new equilibrium state after heating results in a partition of the components between bulk gas phase and adsorbed phase at a bulk gas phase pressure higher than the initial pressure during the feeding. The pressure increase is mainly because of the release of material from the adsorbed phase to the bulk gas phase. The composition and the level of pressure in the bulk gas phase depend on the final temperature, volume available for the bulk gas phase, mass of adsorbent and total amount of moles in the enclosure.
- 3) Supply step: the outlet valve is open with a decrease in pressure and a variable flow of material is discharged.

Thus, adsorption compressors are thermally-driven compression systems adopting adsorption materials and operating according to temperature swing adsorption processes. An early thermodynamic analysis for adsorption of pure fluids has been presented in [21,22] but no thermodynamic basis has been provided for the adsorption compression of a multicomponent mixture to date and some units such as the air revitalization module of the International Space Station (ISS) have been designed on the basis of simplifying assumptions, refining the performance in successive, trial and error steps. The air revitalization

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Table 1
Emerging adsorption technologies.

Sector	Traditional technology	Adsorptive technology	Ref.
Refrigeration & air conditioning	Electrically-driven vapour compression system	Adsorption refrigerators & heat pumps	[8–10]
Drying	Electrical dishwasher	Adsorption dishwasher	[11]
Desalination	Multi-effect distillation	Adsorption desalination	[12]
CO ₂ removal	Absorption	Temperature and/or vacuum swing adsorption	[13–15]

unit of the ISS uses zeolites 5A and 13X which adsorb significant amounts of carbon dioxide and nitrogen. This aspect has been addressed, at the design stage, by oversizing the mass of required material with a safety factor [22,23]. The present work provides a tool for consistent thermodynamic investigation of adsorption compression of multi-component gas mixtures.

The fundamental calculation for adsorption compression is the isochoric-isothermal flash (VT flash). VT flash in bulk gas/adsorbed phase equilibria has been already formulated by minimization of the Helmholtz energy of the system [24]. In this work we show that the well-known Rachford-Rice system of equations can be also applied to adsorption equilibrium after appropriate modifications.

For sake of clarity, at first an ideal ternary mixture in equilibrium with an ideal adsorbed solution [25] is evaluated. The aim is to provide the thermodynamic framework for the simple ideal case. Secondly, a non-ideal ternary mixture is considered using the Soave-Redlich-Kwong (SRK) equation of state for the description of the bulk gas phase and a Gibbs excess model for the adsorbed phase. This is aimed to show the differences between an ideal and non-ideal formulation.

Since no experimental multicomponent equilibrium data are presently available for this problem, the thermodynamic consistency of the results is validated through the common tangent plane approach for adsorption derived in [26]. The last section of this work is devoted to the performance analysis of ideal and non-ideal compressors.

2. Ideal isothermal-isochoric flash for adsorption

The ideal case includes an ideal bulk gas phase in equilibrium with an ideal adsorbed solution. The pressure and compositions in the new equilibrium state can be calculated considering the usual method based on the Rachford-Rice equations system [27], once a number of additional conditions arising from the adsorbed solution theory are provided [28]. The resulting system of equations for NC components is:

$$\sum_i^{NC} \frac{z_i(k_i-1)}{1 + \frac{G}{F}(k_i-1)} = 0 \quad (1)$$

$$x_i = \frac{z_i}{1 + \frac{G}{F}(k_i-1)} \quad (2)$$

$$G = \frac{P_{bulk} V_{void}}{RT} \quad (3)$$

$$k_i = \frac{P_i^0}{P_{bulk}} \quad (4)$$

$$y_i P_{bulk} = P_i^0 x_i \quad (5)$$

$$\frac{m_{ads}}{N} = \sum_{i=1}^{NC} \left(\frac{x_i}{n_i} \right) \quad (6)$$

$$\psi_i = \int_0^{P_i^0} n_i d(\ln P_i) \quad i = 1, 2, \dots, NC \quad (7)$$

$$\psi_i = \psi_{eq} \quad i = 1, 2, \dots, NC \quad (8)$$

$$F - (G + N) = 0 \quad (9)$$

Eq. (1) is the original Rachford-Rice solving equation; Eq. (3) is the ideal gas equation of state for the calculation of the amount of moles in the bulk gas phase. Eqs. (4)–(8) follow the ideal adsorbed solution theory [27,28]. Eq. (9) is the overall mass balance. Assuming that the adsorbent occupies all the volume available in the vessel, the gas mixture volume is calculated by:

$$V_{void} = \frac{m_{ads}}{\rho_b} (\varepsilon_b + (1 - \varepsilon_b) \varepsilon_p) \quad (10)$$

Usually the parameters involved in Eq. (10) are omitted in equilibrium measurements. This work assumes the values reported in Table 2. Although the values of Table 2 do not perfectly correspond to the experimental equilibrium data used for single isotherm parameters regression, they lay in the average range commonly assumed for this kind of materials.

The system of Eqs. (1)–(9) can be reduced in a straightforward way to only two equations by substitution of variables, holding the final variables P_{bulk} and reduced grand potential ψ_{eq} . The equivalent two equation system includes Eqs. (1) and (9).

Eqs. (1)–(9) can be effectively solved by the Newton numerical method without any issue on the estimation of the best initial guess. That is because the system has always only one solution in the physically meaningful domain $P_{bulk} > 0$ and $\psi_{eq} > 0$. In order to show this feature for the ideal problem, the Nitrogen/Oxygen/Argon ternary system adsorption on zeolite 5A has been considered, using the Langmuir isotherm with parameters reported in Table 3.

Fig. 1 illustrates the solution of the system composed by Eqs. (1) and (9). In the physically meaningful region, the two functions intersect only in one point. The same equilibrium compositions are confirmed by the common tangent plane of Gibbs energy of mixing (Fig. 2). The presence of a common tangent plane of the Gibbs energy of mixing at the equilibrium point of Table 4 validates the thermodynamic consistency of the solution. In Table 4 it can be noted that while the bulk gas phase composition is very different from the feed, being enriched by oxygen and argon which are the less strongly adsorbed components, the adsorbed phase composition is close to the feed, being slightly richer in nitrogen over the other components.

3. The non-ideal isothermal-isochoric flash

In the non-ideal formulation fugacity and activity coefficients respectively for the bulk gas phase and the adsorbed phase are considered [33]. Based on the experimental measurement reported in [34], the ternary mixture Methane/Nitrogen/Carbon Dioxide on activated carbon Norit R1 Extra at 298 K and high pressure is analysed. Single component adsorption experimental data were fitted using the Unilan isotherms, considering the absolute adsorbed amount versus fugacity, resulting in the parameters of Table 5.

Table 2
Adsorption materials and beds properties.

	m_{ads} [kg]	ε_b	ε_p	ρ_b [kg m ⁻³]	Ref
Zeolite 5A	1	0.39	0.50	687	[29]
Activated carbon Norit R1 Extra	1	0.35	0.84	420	[30]
Zeolite 13X	1	0.37	0.60	641	[31]

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