Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2017-0012

Vol. **23**, No. 5, pp. 1602-1625
May 2018

Numerical Implementation of the Multicomponent Potential Theory of Adsorption in Python Using the NIST Refprop Database

Raphaël Gervais Lavoie*, Mathieu Ouellet, Jean Hamelin and Pierre Bénard

Institut de recherche sur l'hydrogène, Université du Québec à Trois-Rivières; Département de chimie, biochimie et physique, Université du Québec à Trois-Rivières, Québec G9A 5H7, Canada.

Received 18 January 2017; Accepted (in revised version) 3 June 2017

Abstract. In this paper, we present a detailed numerical implementation of the multicomponent potential theory of adsorption which is among the most accurate gas mixtures adsorption models. The implementation uses the NIST Refprop database to describe fluid properties and applies to pure gases and mixtures in both subcritical and supercritical regimes. The limitations of the model and the issues encountered with its implementation are discussed. The adsorption isotherms of CH_4 / CO_2 mixture are modeled and parameterized as implementation examples.

PACS: 68.43.-h, 64.75.Cd

Key words: Adsorption, mixture adsorption, multicomponent adsorption, potential theory of adsorption, MPTA, density functional theory.

1 Introduction

Gas adsorption in porous material is relevant to a wide variety of industrial and scientific applications, ranging from gas purification and separation to gas storage in stationary or mobile applications. While adsorption experiments of pure gases can be performed readily, experiments on gas mixtures can be challenging, expensive and time-consuming [1]. This situation motivates the utilization of theoretical models to predict the behavior of gas mixtures in the presence of adsorbent.

Several approaches have been proposed to model the adsorption isotherms of both pure gases and mixtures [2–15]. In this paper, we will concentrate on the potential theory

*Corresponding author. *Email addresses:* raphael.gervaislavoie@uqtr.ca (R. Gervais Lavoie), mathieu.ouellet@uqtr.ca (M. Ouellet), Jean.hamelin@uqtr.ca (J. Hamelin), Pierre.benard@uqtr.ca (P. Bénard)

of adsorption (PTA), a two-parameter thermodynamic model developed by Shapiro and Stenby [16], based on the pore filling approach of Polanyi's theory of adsorption [17]. For gas mixtures adsorption, the PTA model generalizes into the multicomponent potential theory of adsorption (MPTA), which can deliver great performance, especially when considering disordered adsorbents such as activated carbon (an overview of mixture adsorption models is presented in Ref. [18]). For a N components gas mixture, the simplest MPTA model requires the adjustment of only $N+1$ parameters, obtained from pure components adsorption isotherms.

The objective of this paper is to present a detailed numerical implementation of the MPTA model. In this spirit, we will write down explicit lines of code, written in Python, an increasingly popular, easy to follow, non-compiled and non-proprietary programming language. We will also point out pitfalls and subtleties encountered, and show how to identify and deal with phase transitions.

Definitions and symbols used in this paper are described in Table 1.

Table 1: Variables definition.

Variables	Type	Definition
μ_B , `chem()`	function	Chemical potential of the bulk phase (J/mol)
μ_{Ad} , `chem()`	function	Chemical potential of the adsorbed phase (J/mol)
ε , `DRA()`	function	Adsorbent surface potential (J/mol)
ρ_B , `dB`	float	Fluid density in the bulk phase (mol/L)
ρ_{Ad} , `d_z`	float	Fluid density in the adsorbed phase (mol/L)
ε_0 , `eps0`	float, array	Characteristic energy of adsorption (J/mol)
z , `z`	float	Microporous volume (cm^3/g)
z_0 , `z0`	float	Limiting micropore volume (cm^3/g)
β	float	Heterogeneity parameter (fix to 2 in this work)
N_{ex} , `N_ex_`	function	Excess (Gibbs) adsorption (mol/Kg)
`d_pure(), d_mix()`	function	Fluid density functions (mol/L)
`dataP`	array	Experimental values of pressure (KPa)
`dataD`	array	Corresponding values of fluid density (mol/L)
`dataAd`	array	Experimental values of excess adsorption (mol/Kg)
x_B , `xB`	array	Bulk phase molar fraction array
x_{Ad} , `x_z`	array	Adsorbed phase molar fraction array
`x_z_A, x_z_B`	float	Adsorbed phase molar fraction of components
`d_max`	function	Maximal fluid density allowed by the Refprop (mol/L)
`d_liq`	float, array	Fluid liquid density at dew point (mol/L)
`X`	array	Array containing pure gases arrays
`d0`	float	Initial guess for fluid density (mol/L)
`x0`	array	Initial guess for mixture molar fraction array
`T`	float	Fluid temperature (K)