CALCULATION OF BINARY ADSORPTION EQUILIBRIA:
HYDROCARBONS AND CARBON DIOXIDE ON ACTIVATED CARBON

L. Marcussen and A.E.W. Krøll
Department of Chemical Engineering
Technical University of Denmark, Building 229
DK-2800 Lyngby, Denmark

Introduction

The calculations are based on pure component and multicomponent models for adsorption equilibria which have been derived in details elsewhere [1],[2].

The pure component model was derived on the basis of Vacancy Solution Theory (VST) [3], [4] and the Non-Random-Two-Liquid (NRTL) model [5]. The NRTL equation is capable of describing equilibria in immiscible liquid systems; consequently, it is expected to be able to describe strongly non-ideal adsorbates.

The multicomponent model was derived by combining the pure component model with Adsorbate Solution Theory (AST) [6] thus yielding a model for non-ideal multicomponent adsorption equilibria.
In this work activity coefficients in the adsorbate phase are calculated by means of the Spreading-Pressure-Dependency (SPD) model [7].

Parameter estimation has been performed in two steps::
1. The five parameters of the pure component model were estimated for each adsorbate using experimental pure component data. The five parameters are (subscript i refers to adsorbate and v to vacancies):
a_{iv}, the nonrandomness constant
and the temperature dependent parameters
$Q_i^{\infty}(T)$, the amount of adsorbed i at saturation
$b_i(T)$, Henry's law constant
$\tau_{iv}(T)$, $\tau_{vi}(T)$, parameters in the NRTL equation.
2. The shape factors s_1, s_2 and the cross-lateral interaction parameter β_{ij} in the SPD model were estimated using experimental data for binary adsorption.

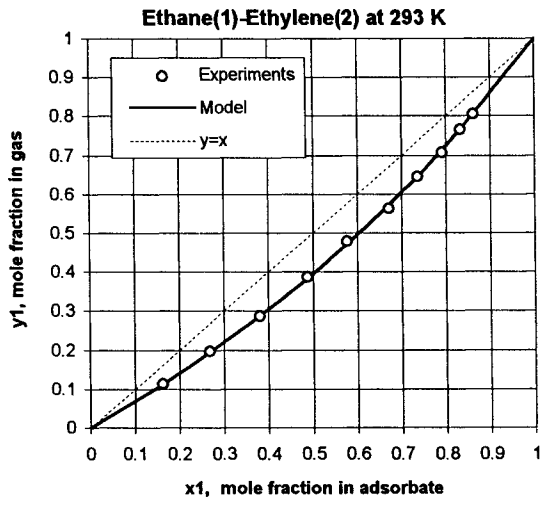
Results and Discussion

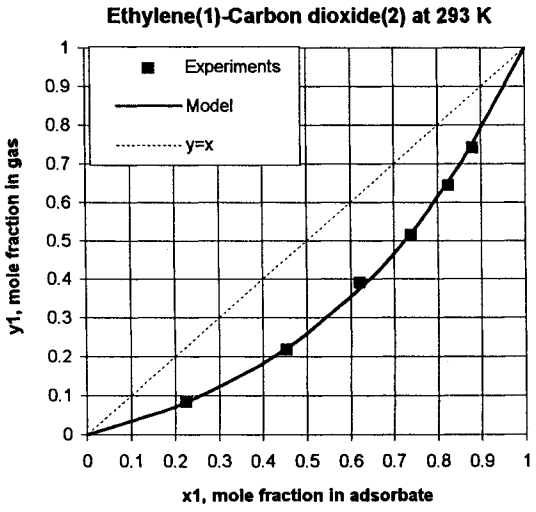
In this work the multicomponent model is compared to experimental data for binary adsorption of hydrocarbons and carbon dioxide on Nuxit-AL active carbon. The experimental data are from [8], [9] and [10].

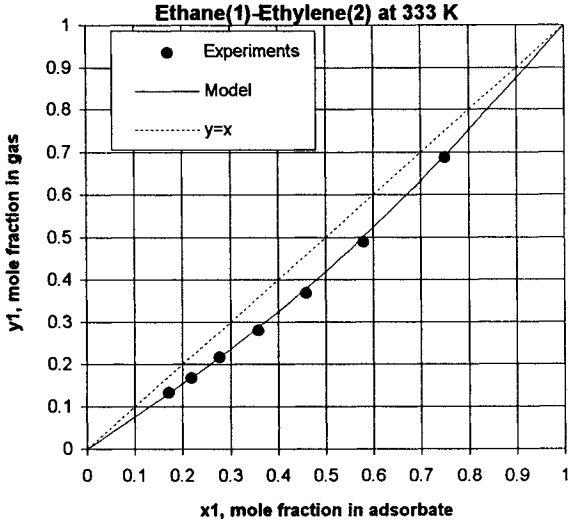
Good agreement between model and experiments is obtained for the binary mixtures of ethane-ethylene at 293 and 333 K, ethylene-carbon monoxide at 293 K and propane-propylene at 293 K (shown graphically on the next page).

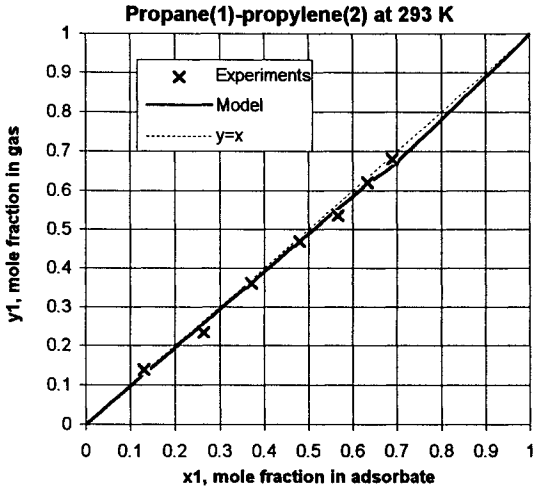
References

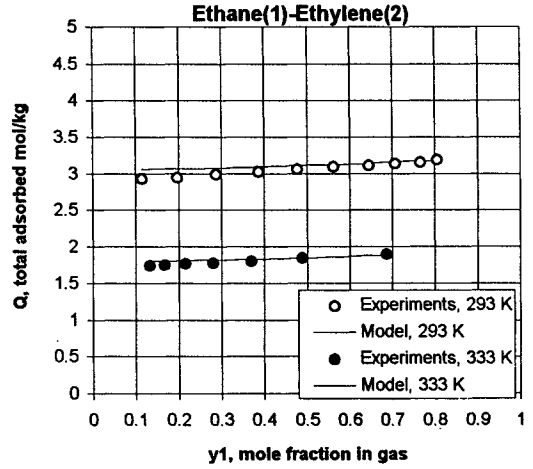
1. Marcussen L. Modelling pure component and multicomponent adsorption equilibria. Research report from the project "Heat and mass transfer in multicomponent systems". Department of Chemical Engineering, Technical University of Denmark, December 1987.
2. Aasberg-Petersen K. Modellering og beregning af multikomponent adsorptionsligevægte. M.Sci. Thesis, Department of Chemical Engineering, Technical University of Denmark, 1988.
3. Suwanayuen S and Danner RP. A Gas Adsorption Isotherm Equation Based on Vacancy Solution Theory. AIChE J. 1980;26:68.
4. Suwanayuen S and Danner RP. Vacancy Solution Theory of adsorption from gas mixtures. AIChE J. 1980;26:76.
5. Renon H and Prausnitz JM. Local compositions in thermodynamic excess functions for liquid mixtures. AICHE J. 1968;14:135.
6. Myers AL and Prausnitz JM. Thermodynamics of mixed-gas adsorption. AIChE J. 1965;11:121.
7. Talu O. Multicomponent gas adsorption equilibria of non-ideal mixtures. Ph.D. Thesis, Arizona State University, 1984.
8. Szepesy L and Illés V. Adsorption of gases and gas mixtures, I. Acta Chim. Hung. Tomus 1963;35:37.
9. Szepesy L and Illés V. Adsorption of gases and gas mixtures, II. Acta Chim. Hung. Tomus 1963;35:53.
10. Szepesy L and Illés V. Adsorption of gases and gas mixtures, III. Acta Chim. Hung. Tomus 1963;35:245.

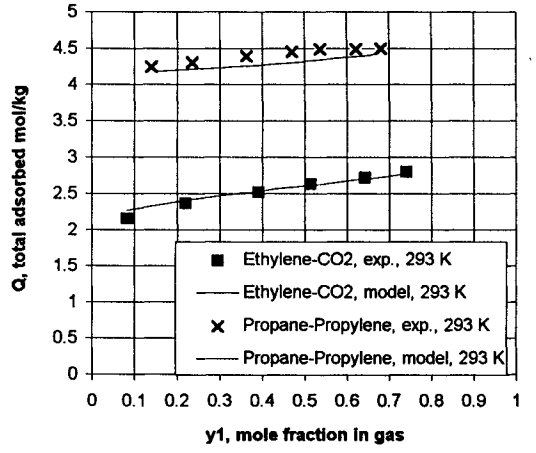

Ethane(1)-Ethylene(2) at 293 K
Experiments
Model
y=x
y1, mole fraction in gas
x1, mole fraction in adsorbate


Ethylene(1)-Carbon dioxide(2) at 293 K
Experiments
Model
y=x
y1, mole fraction in gas
x1, mole fraction in adsorbate


Ethane(1)-Ethylene(2) at 333 K
Experiments
Model
y=x
y1, mole fraction in gas
x1, mole fraction in adsorbate


Propane(1)-propylene(2) at 293 K
Experiments
Model
y=x
y1, mole fraction in gas
x1, mole fraction in adsorbate


Ethane(1)-Ethylene(2)
Experiments, 293 K
Model, 293 K
Experiments, 333 K
Model, 333 K
Q, total adsorbed mol/kg
y1, mole fraction in gas


Ethylene-CO2, exp., 293 K
Ethylene-CO2, model, 293 K
Propane-Propylene, exp., 293 K
Propane-Propylene, model, 293 K
Q, total adsorbed mol/kg
y1, mole fraction in gas