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Gas Adsorption Equilibria

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GAS ADSORPTION EQUILIBRIA

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INTRODUCTION

Gas adsorption is a process for purification or separation of gas mixtures. Distillation is usually the first choice for bulk separations when liquefaction can be accomplished conveniently and when the relative volatilities of the materials to be separated do not approach or equal unity (azeotropy). If these conditions are not met, adsorption may offer an advantage, either by avoiding high or low temperatures or by providing higher separation factors and lower energy costs. Therefore the first step in the consideration of adsorption for a particular separation is the identification of a suitable adsorbent.

Physical structure, chemical characteristics, and polarity of the adsorbent are some of the important factors which determine its equilibrium properties. These factors are useful for making qualitative estimates of selectivity of an adsorbent with respect to the components of a gas mixture. Selectivity refers to the ratio of the separation factors of two species; for example, for component 1 relative to component 2 the definition is:

$$s_{12} = (x_1/y_1)/(x_2/y_2) \tag{1}$$

where x and y are the adsorbed and gas phase compositions, respectively. Preferential adsorption of component 1 means $s_{12} > 1$. Like vapor-liquid equilibrium, many systems form adsorption azeotropes ($s = 1$) at particular

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values of pressure and temperature, so that detailed knowledge of the equilibrium is necessary to avoid these points under actual operating conditions.

The next step is the gathering of experimental information for the specific adsorbent and gas mixture under consideration. Unfortunately, that information is usually unknown for the desired range of temperature, pressure and composition so experimental data are usually required. Sometimes predictive or correlative methods are applied to interpolate or extrapolate data when it is available. In either case, the minimum data required are the adsorption isotherms for the individual components of the mixture; mixture data can be predicted from these (see Appendix 3).

COMPILATION OF DATA FOR ADSORPTION FROM GAS MIXTURES

During the last 50 years a large amount of experimental data on adsorption has been published. Most of that data is related to adsorption of pure gases; less information is available for binary and multicomponent gas mixtures.

For binary mixtures, a comprehensive review covering the period up to 1959 was given by Young and Crowell [144]. For the period from 1960 to 1977, Hall and Müller [56] published a useful compilation of data on binary and multicomponent mixtures. This review covers the period from 1950 to the present and thus overlaps the two previous ones in order to provide an up-to-date listing in one place. We have omitted some references for which we were unable to obtain the original article, since our compilation requires more information than is customarily found in abstracts. The adsorbents are in general those used in industry, with large surface areas equal to or greater than 500 square meters per gram. However, we have included low-area graphitized carbon because of its theoretical importance as a homogeneous surface.

Our compilation of data for adsorption from gas mixtures in Appendix 1 includes, in addition to the literature reference, the commercial name of the adsorbent, with information on its surface area and pore volume. Also, Appendix 1 gives the experimental technique employed and the range of temperature and pressure covered. Since tabular data are generally more useful than figures, the method of reporting results is listed.

Adsorbent

Information about the type of adsorbent is coded as follows:

SG	Silica Gel
AC	Activated Carbon
CMS	Carbon Molecular Sieve
GC	Graphitized Carbon
Z	Zeolite

The adsorbents are listed in the above order. Additional information about the brand, if available, is included in brackets, using the following abbreviations:

CO	Columbia
CE	Compania Espanola de Carbones Activos
DC	Davison Chemical Company
FS	Fisher Scientific Co.
PC	Pittsburgh Chemical Company
SS	Sutcliffe and Speakman

Experimental Technique

Experimental methods for measuring equilibrium data are divided into static (S) and flow (F), with subdivisions as follows:

STATIC (S)	
G	Gravimetric, using a McBain spring balance or electrobalance
V	Volumetric
C	Combination of volumetric and gravimetric techniques [12,57]
FLOW (F)	
C	Chromatographic
N	Non-chromatographic methods using external analysis

A summary of experimental techniques was reported by Hall and Müller [56].

Type of Data

The method of presenting data is encoded as follows:

T	Tabular
G	Graphical

The superscript SE means that only an average selectivity is published, and superscript BT means only breakthrough curves are reported.

Adsorbates

The data in Table 1 are grouped according to the type of adsorbent, in the order silica gel (SG), activated carbon (AC), carbon molecular sieves (CMS), graphitized carbon (GC) and zeolites (Z). Each of these adsorbents is subdivided according to the type of adsorbate mixture in the following order:

hydrocarbon + hydrocarbon
hydrocarbon + organic
organic + organic
organic + inorganic
inorganic + inorganic

The compilation of data in Appendix 2 for adsorption of ternary gas mixtures uses the same abbreviations as Appendix 1.

ADSORPTION DATA BANK

In both theoretical and applied research on adsorption, considerable effort has been devoted to the collection of data. These data are widely dispersed in journals published in many different countries, and of course in several languages. Often the data are incomplete; for example, mixture data without measurements of the pure gas isotherms. Thermodynamic consistency tests are rare, so that judgments on the quality of the data are difficult to make.

Similar problems in vapor–liquid equilibrium have been partially overcome by the implementation of data banks of available information such as that of Gmehling and Onken [51]. We are developing a similar data bank of adsorption equilibrium properties at the University of Pennsylvania (see note at end of article). Standard procedures of statistical analysis, uniform pro–

cedures for optimizing model parameters, and the determination of standard properties (adsorption second virial coefficients, heats of adsorption, saturation capacity, etc.) provide a sound basis for interpolation, correlation, and prediction of equilibrium properties. For example, Figure 1 shows the file of an isotherm for adsorption of ethylene on silica gel.

There are some difficulties related to the development of a data bank of this type for adsorption. Variables are not always specified; adsorbents are often poorly characterized; experimental techniques are sometimes inadequately described; and different methods of reporting data are used by different laboratories. Data are often published in graphical form for concise reporting, but tabular data are more useful for making thermodynamic consistency tests and comparisons with theories.

The adsorption data bank has been written in FORTRAN using the structure described below.

Data Files

The system contains four data files:

SINGLE	- Data on adsorption of pure gases
CHEMICALS	- Properties of pure substances (adsorbates)
GBINARY	- Data on adsorption from binary gas mixtures
LBINARY	- Data on adsorption from binary liquid mixtures

These are random access files stored on secondary memory in the computer. Each file is divided into records containing fields for identification, parameters, experimental data and a set of pointers. The identification field contains the names of the adsorbates and adsorbent and the reference. The parameter field contains constants of mathematical models or certain physical properties. For example, SINGLE files contain values for temperature, vapor pressure, and constants for various adsorption isotherms in this field, as well as thermodynamic properties such as the Gibbs free energy of immersion, the adsorption second virial coefficient, and the isosteric heat of adsorption.

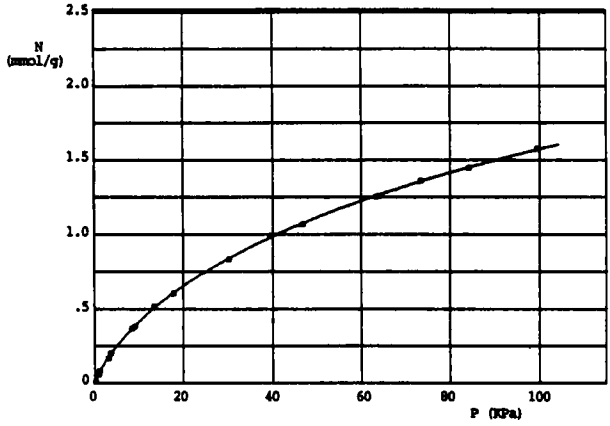
The field assigned for storage of experimental data is a very flexible one designed to accomodate different numbers of experimental points and dif-

```
ETHYLENE
--------------------------------------------------------------------------------
SILICA GEL
--------------------------------------------------------------------------------
ADSORBENT : 14/20 MESH  REF. GRADE  DAVISON CHEMICAL Co of BALTIMORE
ADSORBATE : PURITY 99.5 (mol %)
EXP.      : VOLUMETRIC METHOD;STATIC EQUILIBRIUM TECH
REF.      : LEWIS, W. K.;GILLILAND, E. R.;CHERTOW, B.;DAREIS, D.

                TEMP   (K)=   273.15
                PSAT (kPa)=  4106.78

BFUNCT.                     TOTH                        UNILAN
A  =     2.1852             B  =     5.7359   kPa      C  =  3013.2000   kPa
B  =    11.3262             M  =     .4126             S  =     5.4288
D  =     .0000              NI =     7.0687   mmol/g    M  =     7.8471   mmol/g
M  =    3.4319   mmol/g     DG =   -32.3854   J/g       DG =   -29.6980   J/g
DG =   -29.0997   J/g        BIS= .23268+000   1/g       BIS= .12412+000   1/g
BIS= .18324+000   1/g        QIS=    29.4125   kJ/g      QIS=    25.3664   kJ/g
QIS=    29.2797   kJ/mol

 P (kPa)     N (mmol/g)
    .253         .012
   1.013         .060
   1.120         .083
   3.120         .171
   3.640         .206
   8.320         .370
   9.053         .384
  13.350         .516
  17.770         .604
  30.190         .834
  39.410         .993
  46.720        1.068
  63.480        1.256
  73.270        1.360
  84.210        1.449
  99.400        1.576
```




```
 P (kPa)        DN BFUNCT.     DN  TOTH       DN UNILAN
    .253           .007          .009          .002
   1.013           .007          .010          -.006
   1.120          -.009          -.006         -.024
   3.120           .001          .005          -.018
   3.640          -.011          -.008         -.030
   8.320          -.006          -.004         -.017
   9.053           .002          .004          -.007
  13.350          -.011          -.011         -.012
  17.770           .006          .005          .012
  30.190           .011          .008          .025
  39.410          -.010          -.013         .005
  46.720           .011          .008          .024
  63.480           .009          .007          .014
  73.270          -.002          -.003         -.003
  84.210           .002          .003          -.006
  99.400          -.011          -.006         -.028
  SUM OF
(NCAL-NEXP)**2    .0011          .0009         .0047

                DN=(NCAL-NEXP)

END OF FILE
->
```

FIGURE 1. Output from database file for isotherm of ethylene adsorbed on silica gel at 273.15 K [81]. Three columns at top give parameters of various adsorption equations, and four columns at bottom show errors for these equations.

ferent loci of measurements (constant pressure, constant vapor composition, etc.).

The pointer field provides connections between different files to simplify the recovery of information. For example, the pointer field of a record in the GBINARY file contains the addresses for the corresponding pure-component adsorption isotherms stored in the SINGLE file.

Data Management Package

This is a set of subroutines for the storage and retrieval of information in the data files based on an exploratory algorithm called HASHING [74]. It uses key words stored in the identification field of the records. In addition, these subroutines regulate the flow of information between the data files and other elements of the system. For example, for the testing of a model for predicting binary gas adsorption, these subroutines supply the experimental mixture data from GBINARY, pure component isotherm parameters from SINGLE and properties of the adsorbate such as vapor pressure from CHEMICAL.

Thermodynamic Package

This portion of the data base contains subroutines for correlating and predicting physical and thermodynamic properties of pure fluids and their mixtures. For example, for volumetric properties of gases, options are provided for the use of the virial equation truncated after the second virial coefficient at low pressure, and the Peng-Robinson equation [108] at higher pressure.

Volumetric properties of liquids are calculated by well-established empirical methods [26,113,143]. Perfect-gas heat capacities [118], the Watson equation [138], and PVT equations of state provide energetic properties such as enthalpy.

Saturation vapor pressures for vapor-liquid equilibrium calculations are obtained from the Antoine equation [2], the Harlacher-Braun correlation [58] or, if necessary, by the Lee-Kesler corresponding states method [80].

Activity coefficients in the bulk liquid phase are determined by either the Wilson equation [140] or the UNIQUAC equation [1].

Subroutines for calculating thermodynamic properties of the adsorbed phase, such as spreading pressure, two-dimensional compressibility factor, or Gibbs free energy of immersion are included in the thermodynamic package.

Programs

This portion of the system contains interactive programs for access to the system. There are three kinds of programs:

INPUT/OUTPUT. Stores and recovers information from the data files. Gives indices to indicate which information is available and provides standardised output of that information. Figure 1 shows sample output for data from SINGLE.

OPTIMIZATION. A set of programs designed to generate optimised sets of parameters for the various equations employed to fit pure-gas adsorption isotherms. The Complex [18] algorithm is used for this purpose.

CALCULATION. Programs to generate properties such as isosteric heat of adsorption, spreading pressure, adsorption second virial coefficients, and programs to compare predictive methods with experimental data for adsorption of mixtures. Figure 2 shows, for example, results for predictions by IAS theory [96] with experimental data.

ADSORBENT CHARACTERISTICS AND THEIR INFLUENCE UPON ADSORPTION

The physical structure and chemical characteristics of solids determine their use as adsorbents. The primary considerations in industrial applications are the adsorptive capacity and the selectivity. The pore distribution may have a significant effect on the preference of the adsorbent for molecules of different size and shape. Polarity and chemical composition

(1) ETHANE

(2) ETHYLENE

ACTIVATED CARBON

ADSORBENT : BPL 6/16 MESH , PITTSBURGH CHEMICAL COMPANY
ADSORBATE : PURITY (1) > 99.96 (mol%) (2) > 99.96 (mol%)
EXP : VOLUMETRIC METHOD , STATIC EQUILIBRIUM TECHNIQUE
REF : REICH,R.;ZIEGLER,W.T.;ROGERS,K.A. IND ENG CHEM. PROCESS DES. DEV. 1980,19,336-344

TEMP = 301.40 (K)
Y1 = .2400

P (KPa)	X1	X1(cal)	N(mmol/g)	N(cal)	Sexp	Scalc
137.894	.2810	.3159	2.9880	2.8533	1.2376	1.462
308.193	.2900	.3137	3.8490	3.7003	1.2934	1.447
737.043	.2860	.3092	4.7190	4.5506	1.2684	1.417
1341.020	.2750	.3046	5.3780	5.0556	1.2011	1.387
1981.540	.2720	.3011	5.9380	5.3439	1.1832	1.364

TEMP = 301.40 (K)
Y1 = .4720

P (KPa)	X1	X1(cal)	N(mmol/g)	N(cal)	Sexp	Scalc
217.873	.5590	.5651	3.5930	3.4209	1.4180	1.453
549.508	.5330	.5604	4.5820	4.3291	1.2767	1.426
1132.800	.5330	.5544	5.3800	4.9384	1.2767	1.392

TEMP = 301.40 (K)
Y1 = .6820

P (KPa)	X1	X1(cal)	N(mmol/g)	N(cal)	Sexp	Scalc
144.099	.7620	.7578	3.2670	3.0639	1.4929	1.459
346.114	.7480	.7553	4.0760	3.9448	1.3840	1.439
692.917	.7460	.7519	4.8700	4.5680	1.3695	1.413
1367.910	.7270	.7473	5.6060	5.0844	1.2417	1.379

TEMP = 212.70 (K)
Y1 = .2400

P (KPa)	X1	X1(cal)	N(mmol/g)	N(cal)	Sexp	Scalc
139.962	.3460	.3137	6.7320	6.6675	1.6753	1.447
224.078	.3330	.3099	7.0940	7.0386	1.5810	1.422
405.408	.3250	.3031	7.7840	7.4694	1.5247	1.377

TEMP = 212.70 (K)
Y1 = .6820

P (KPa)	X1	X1(cal)	N(mmol/g)	N(cal)	Sexp	Scalc
137.205	.7900	.7555	6.6750	6.6771	1.7541	1.441
240.625	.7790	.7514	7.1880	7.0456	1.6436	1.409
343.356	.7740	.7474	7.5140	7.2574	1.5969	1.379

FIGURE 2. Output from database program for predicting binary gas adsorption from IAS theory. Comparison with experimental data [117] for adsorption of ethane and ethylene on activated carbon.

of the surface determine the ability of the adsorbent to separate molecules of different polarity or hydrocarbons with different degrees of saturation.

Properties of commercial adsorbents are described in several reviews. [120,135]. Adsorptive properties of activated carbons were reviewed by Dubinin [36]. Properties of carbon molecular sieves were described by Mahajan and Walker [86]. The structure of carbon blacks and graphitized carbon blacks was reviewed by Avgul and Kiselev [5]. Details of the preparation and structure of silica gel were presented by Iler [65]. Zeolite structure and properties have been extensively reviewed by Breck [20] and by Reed et al. [115,116]. A summary of key characteristics of industrial adsorbents, with examples of particular applications, follows.

Silica Gel

The basic structure of silica gel consists of approximately spherical particles of polymeric orthosilicic acid H_4SiO_4 in the form of chains and nets. These particles agglomerate with bond formation between adjacent particles by elimination of water between neighboring hydroxyl groups. The final structure is a physically-robust porous material. The pore size for adsorption depends on the particle size, which ranges from 2 to 20 nm. Silica gels have a narrow and unimodal pore size distribution. The physical properties of two typical silica gels are given in Table 1.

The surface hydroxyl groups impart a degree of polarity which is evident in the preference of silica gel for polar molecules and unsaturated hydrocarbons. Silica gel has a strong preference for aromatic π bonds and it is highly hydrophilic. An example of this effect, which is counterbalanced by the preference of the adsorbent for molecules of greater molecular weight, can be observed in the data of Lewis et al. [82] in Table 2. Shen et al. [121] found that benzene is preferentially adsorbed from mixtures of benzene and n-hexane.

Activated Carbon

The basic structure of activated carbon is elementary microcrystallites of graphite stacked together in random orientation to form a porous structure. The arbitrary but useful classification of pore sizes by Dubinin [37]

Table 1. Typical physical properties of silica gel.

	High Area	Low Area
Specific Pore Volume, cm^3/g	0.43	0.9
Average Pore Diameter, nm	2	14
Specific Surface Area, m^2/g	830	380
Reference	[121]	[14]

Table 2. Selectivities of hydrocarbon mixtures adsorbed on silica gel. T = 298 K, P = 101 kPa, x_1 = 0.5 [82].

Component #1	Component #2	s_{12}
$CH{\equiv}CH$	$CH_2{=}CH_2$	3.0
$CH_2{=}CH_2$	$CH_3{-}CH_3$	2.7
$CH_2{=}CH{-}CH_3$	$CH_3{-}CH_2{-}CH_3$	3.1
$CH_2{=}CH{-}CH_2{-}CH_3$	$CH_3{-}CH(CH_3){-}CH_3$	3.1
$CH_2{=}CH_2$	CH_4	19.0
$CH_2{=}CH{-}CH_3$	$CH_2{=}CH_2$	6.6
$CH_3{-}CH_2{-}CH_3$	$CH_3{-}CH_3$	4.8
$CH_3{-}CH_2{-}CH_3$	$CH_2{=}CH_2$	2.1

is in wide use: Pores of width below 2 nm are described as micropores and those above 20 nm are called macropores. The transitional pore sizes from 2 to 20 nm are called mesopores. This classification is associated with a characteristic adsorptive behavior that has been studied by Gregg and Sing [55].

Because of its predominantly nonpolar surface, activated carbon is hydrophobic and organophilic. These characteristics make activated carbon useful for the recovery of organic substances from aqueous media. Recovery of organic substances from humid air is another application. When the humidity is high, capillary condensation of water vapor hinders the adsorption of solvents [102].

Unlike silica gel, activated carbon does not have a preference for unsaturated hydrocarbons because of the nonpolar character of the carbon surface. This property is illustrated in Table 3, which indicates that the

Table 3. Selectivities of hydrocarbon mixtures adsorbed on activated carbon. T = 298 K, P = 101 kPa [127].

Component #1	Component #2	s_{12}
$CH_2=CH_2$	CH_4	13.3
CH_3-CH_3	CH_4	18.4
CH_3-CH_3	$CH_2=CH_2$	1.5
$CH_3-CH_2-CH_3$	CH_3-CH_3	6.8
$CH_2=CH-CH_3$	$CH_2=CH_2$	12.0
$CH_3-CH_2-CH_3$	$CH_2=CH-CH_3$	1.1
$CH_3-CH_2-CH_2-CH_3$	$CH_3-CH_2-CH_3$	3.4

increase of selectivity with molecular weight is the most important effect. Another characteristic of activated carbon is a pronounced decay of the selectivity with increasing pressure [117].

Carbon Molecular Sieves

With the use of special activation procedures [68,131], it is possible to prepare activated carbons which possess a narrow distribution of pore sizes and therefore are capable of excluding large molecules from the active surface area. Carbon molecular sieves with apertures ranging from 0.4 to 0.9 nm have been prepared. Although these adsorbents have less adsorptive capacity than conventional activated carbons, they provide higher values of selectivity for molecules of different size.

Carbon molecular sieves provide an alternative to zeolites in the case of adsorption from acidic solutions because of their higher stability and less hydrophilic character compared to zeolites [137]. Details of the sieving action are given by Eguchi [42]. Benzene is adsorbed preferentially to cyclohexane [101]. Nakahara et al. [98,99,100] recently reported data for mixtures of ethylene + ethane, ethylene + propylene, and ethane + propane. Since these adsorbates have an effective diameter smaller than the average pore diameter, no sieving effect was observed for their mixtures.

Carbon Blacks

Carbon black consists of spherically shaped solid particles containing small crystallites of graphite with intrusion of amorphous carbon. Depending on

its origin and mode of preparation, carbon blacks are classified as: channel, acetylene, furnace, lamp and thermal. Typical values of particle size and surface area are given in Table 4.

Carbon blacks contain hydrogen and oxygen impurities; hydrogen from the hydrocarbon source of the black, and oxygen from oxidative processes. For example, channel carbon black has the following elementary composition [73]: C (94.8%), H (0.75%), and O (4.45%). Functional groups containing hydrogen and oxygen such as hydroxyl, carboxyl, peroxide, etc. are present on the particles, either bound directly to the surface by chemisorption or contained in molecules which are physically adsorbed to the surface.

The graphitization of the carbon source material is by heat treatment in vacuum, in an inert gas or in a reducing atmosphere. Up to 1100 C, volatile substances and most of the oxygen are eliminated. Thermal cracking of chemisorbed substances occurs between 1300 to 2200 C. Finally, between 2800 and 3200 C, growth and ordering of the crystals takes place, accompanied by a change of the particle shape from spherical to polyhedral. The surface area diminishes as the crystals grow in size. Sterling FT graphitized carbon, for example, has a surface area of about 12 m^2/g [113]. At temperatures close to 3000 C, the graphitization yields polyhedral particles with all of the faces the same: the basal plane of graphite. This homogeneity of the external surface of the particles makes graphitized carbon an ideal surface for theoretical studies.

Graphitized carbon blacks are non-specific adsorbents because of the absence of functional groups on the surface. The selectivity for mixtures is similar to that for activated carbon (see Table 3), but it is fairly constant with respect to variation of composition at fixed temperature and pressure. Likewise, the selectivity of graphitized carbon varies only weakly with pressure at fixed temperature and gas-phase composition. The strong variation of the selectivity of activated carbon with both composition and pressure is therefore probably due to its surface heterogeneity.

Zeolites

Zeolites are porous crystalline aluminosilicates. The basic, repetitive structure consists of assemblages of SiO_2 and AlO_2 tetrahedra joined

Table 4. Properties of carbon blacks.

Type	Avg. Particle Diameter, μm	Surface Area, m^2/g
Channel (Spheron)	40	110
Acetylene	50	65
Lamp	140	25
Thermal (Sterling FT)	150	20

together through shared oxygen atoms to form a cell with a central cavity, into which molecules can penetrate through several window-like apertures. Stacking these units into a lattice gives a three-dimensional structure of channels which connect the cavities through their windows. Unlike silica gel and activated carbon, the micropore structure is regular as determined by the crystalline lattice, so there is no pore size distribution.

Zeolites are classified according to the crystalline structure of the cell. Although 34 species of zeolite minerals and about 100 synthetic structures have been identified or synthesized [20], only a few are used commercially for gas adsorption operations. Detailed reviews of zeolites have been given in recent years [7,20,91]. The following description summarizes the most common types of zeolites.

The cell of zeolite Type A has a cavity 1.1 nm in diameter, accessible through 6 windows. These windows are partially obstructed by cations that determine their effective aperture. For example, the aperture for the sodium form, called NaA or 4A, is 0.4 nm. The sodium cation can be exchanged. For example, if it is replaced by a divalent cation, the requirement of electroneutrality removes alternate cations and thus increases the effective aperture of the windows. For example, replacement of Na^+ by Ca^{2+} or Mg^{2+} increases the aperture to 0.5 nm so that larger molecules can penetrate to the effective surface area of the cavity. Exchange of Na^+ with the larger K^+ ion decreases the aperture size to 0.3 nm.

Zeolites Type X and Y have a similar crystalline structure with a large cell dimension of nearly 2.5 nm. These cells have very large windows with effective apertures of 0.74 nm so that molecules as large as isobutane can

penetrate the cavities. Each cell is connected through windows with four identical cells; the result is a porous structure containing about 50% void space. A cell consists of 192 $(Si,Al)O_4$ tetrahedra. X and Y zeolites differ in the Si/Al ratio, which is 1.0 to 1.5 for X zeolites and 1.5 to 3.0 for Y zeolites. The selectivity can be modifed by ion exchange [19].

THEORIES OF MIXED-GAS ADSORPTION

Reviews of mixed-gas adsorption equilibria over the past decade include those by Sircar and Myers [123], Bülow et al. [23] and Jaroniec [67]. The simplest theory for a porous adsorbent is the Langmuir [77] equation as extended to mixtures by Markham and Benton [87]:

$$n_i = mK_iPy_i(1 + \Sigma K_iPy_i)^{-1} \quad (2)$$

where K_i is the Langmuir constant for the i'th pure gas at the same temperature. The theory requires that all adsorbates have the same value of saturation capacity (m). Eqn. (2) is analytical but it incorrectly predicts that the isothermal selectivity s_{ij} is constant with respect to coverage and gas-phase composition. The Langmuir equation was extended to multilayer adsorption by Brunauer, Emmett and Teller (the BET equation [21]), and the BET equation for mixtures was derived by Hill [60,61]. The Langmuir and BET equations are still used extensively, in spite of their failure to fit data accurately over wide ranges of pressure, partly because of their simplicity and partly because they may be derived from statistical mechanics by relatively simple models [24,29,44,45,139]. Another model with a statistical basis is that of Ruthven [120] for adsorption in zeolites.

Since neither the Langmuir nor the BET equation fits the experimental data for adsorption of a pure gas on adsorbents like silica gel, activated carbon and zeolites, it is necessary to use more complicated equations which contain three or even four parameters. In Appendix 3 are compared three particular theories: ideal-adsorbed-solution theory (IAS) [96], the vacancy-solution model (VSM) [41,125,126] and the Polanyi potential theory [38,39, 40,52,54,83,112] as extended to mixtures by Grant and Manes (GM) [53]. The listing of 145 experimental points for adsorption of binary gas mixtures on silica gel, activated carbon and zeolites was chosen on the basis of avail-

ability of data for the pure-gas isotherms. Each entry indicates the gas mixture, the adsorbent, the experimental conditions of temperature, pressure and composition, and the measured selectivity. The latter is compared with the value predicted by the IAS, VSM and GM methods using the procedures described below.

Method of Grant and Manes

According to this method [52,53], the basic equation is:

$$(v_{1s})^{-1} \ln[P_{1s}x_1/Py_1] = (v_{2s})^{-1} \ln[P_{2s}x_2/Py_2] \qquad (3)$$

where v_{is} is the molar volume of i'th adsorbate in the state of saturated liquid at its normal boiling point, and P_{is} is the vapor pressure of the saturated liquid at the temperature of the adsorption isotherm. Having fixed the temperature, pressure (P) and gas-phase mole fractions $\{y_1,y_2\}$, Eqn. (3) may be solved implicitly for x_1 since $(x_1 + x_2) = 1$. Then the selectivity is calculated from Eqn. (1). The total amount adsorbed is obtained from the characteristic curves [53] of the adsorbates.

The predictions of selectivity for the GM method in Appendix 3 were calculated from Eqn. (3). For supercritical temperatures, the adsorbate vapor pressures were estimated by extrapolation. The more general form of Eqn. (3) includes corrections to the fugacity for nonidealities in the gas phase. However, in the interest of simplicity and uniformity, we have ignored gas-phase imperfections for all three methods (IAS, VSM, and GM).

Vacancy Solution Model

The adsorption isotherm for a pure gas (component #1) is [125]:

$$P = (m_1/b_1)[\theta_1/(1-\theta_1)]\Lambda_{13}[1-(1-\Lambda_{31})\theta_1][\Lambda_{13}+(1-\Lambda_{13})\theta_1]^{-1} \times$$
$$\exp\left[-\Lambda_{31}(1-\Lambda_{31})\theta_1[1-(1-\Lambda_{31})\theta_1]^{-1} - (1-\Lambda_{13})\theta_1[\Lambda_{13}+(1-\Lambda_{13})\theta_1]^{-1}\right] \qquad (4)$$

The set of four constants $\{m_1, b_1, \Lambda_{13}, \Lambda_{31}\}$ is determined from the experimental data for the adsorption of the pure gas. The following equations then describe binary gas adsorption:

$$m = x_1 m_1 + x_2 m_2 \tag{5}$$

$$\theta = n/m \tag{6}$$

$$x_1^s = x_1\theta \tag{7}$$

$$x_2^s = x_2\theta \tag{8}$$

$$x_3^s = 1 - \theta \tag{9}$$

$$\ln(\gamma_k^s) = 1 - \ln\Big[\sum_{j=1}^{3} x_j^s \Lambda_{kj}\Big] - \sum_{i=1}^{3}\Big[x_i^s \Lambda_{ik}\Big(\sum_{j=1}^{3} x_j^s \Lambda_{ij}\Big)^{-1}\Big] \qquad \{k = 1,2,3\} \tag{10}$$

$$-\Pi_i^* = [1 + (m - m_i)/n] \ln(\gamma_3^s x_3^s) \qquad \{i = 1,2\} \tag{11}$$

$$n = P\Big[\sum_{i=1}^{2} \gamma_i^s x_i m_i \Lambda_{i3} (m b_i)^{-1} \times \exp(\Lambda_{3i} - 1) \times \exp(\Pi_i^*)\Big]^{-1} \tag{12}$$

$$y_i = \gamma_i^s x_i n (m_i/m) \Lambda_{i3} (b_i P)^{-1} \times \exp(\Lambda_{3i} - 1) \times \exp(\Pi_i^*) \tag{13}$$

Given the constants for adsorption of the pure gases, and having specified the independent variables temperature (T), pressure (P) and adsorbed–phase composition (x_1,x_2), there remain 11 unknowns $\{\gamma_1^s,\gamma_2^s,\gamma_3^s,x_1^s,x_2^s,x_3^s,\Pi_1^*,\Pi_2^*,\theta,n,m\}$ in the 11 Equations (5)–(12) above. Finally, Eqn. (13) is solved for the unknown vapor composition last because it is the only equation containing this variable. The subscripts {1,2} refer to the adsorbates and subscript ≠3 refers to the lattice vacancies. Eqn. (10) is the Wilson equation for a ternary mixture. The "s" superscripts refer to the composition of the adsorbed phase treating the vacancies as an additional component. Π_i^* is the dimensionless spreading pressure of the adsorbates, θ is their fractional loading, n is the total amount adsorbed, and m is the saturation capacity for the mixture.

The algorithm used for solving these equations is as follows:

(1) Calculate m from Eqn. (5).

(2) Estimate a value for θ in the interval $0 < \theta < 1$.

(3) Calculate the compositions $\{x_i^s\}$ from Eqns. (7)–(9).

(4) Obtain n from Eqn. (6).

(5) Evaluate the activity coefficients $\{\gamma_i^s\}$ by Eqns. (10).

(6) Calculate the spreading pressures $\{\Pi_i^*\}$ from Eqns. (11).

(7) Solve Eqn. (12) for n.

(8) Recalculate θ from Eqn. (10) and compare with the previous value in step 2. Repeat to convergence of θ.

(9) Calculate the vapor compositions $\{y_i\}$ using Eqns. (13). In the binary case only y_1 need be calculated because $y_2 = 1 - y_1$.

(10) Determine the selectivity from Eqn. (1).

Selectivities calculated this way are reported in Appendix 3 in the VSM column. The constants for the pure–gas isotherms were derived from the experimental data using the optimization procedure described above.

Ideal Adsorbed Solution Theory

IAS theory equates adsorbed– and gas–phase fugacities:

$$Py_i = P_i^\circ(\Pi)x_i \tag{14}$$

where P_i° is the pressure which, for adsorption of pure component "i", yields the same spreading pressure (Π) as that of the mixture. Spreading pressure is given by the integral:

$$(\Pi A/RT) = \int_{P=0}^{P_i^\circ} (n_i^\circ/P)dP \tag{15}$$

n_i°, a function of P_i°, is the adsorption isotherm for the i'th pure gas. Any equation which fits the experimental data may be used; we selected the Toth isotherm [129,130]:

$$n = mP(b + P^t)^{-1/t} \tag{16}$$

The three constants {m,b,t} were derived from the experimental data for adsorption of the pure gases using an optimization program. For binary adsorption equilibrium, there are 3 degrees of freedom which are normally specified in terms of temperature (T), pressure (P) and vapor composition (y_1,y_2). There are 5 unknowns: $\{x_1,x_2,P_1^\circ,P_2^\circ,\Pi\}$. Eqns. (14) and (15), plus the con–

straint ($x_1+x_2=1$) provide an equal number of equations, so that a unique solution exists. Details of the solution algorithm are available [97]. Finally, the selectivity was calculated by Eqn. (1) and the results are reported in Appendix 3 under the column IAS.

Comparison of Predictions with Experimental Data

Predicted selectivities are compared with experiment in Appendix 3 because this is a more sensitive test than either total loading or composition. We have restricted the number of points to three for each system because of space limitations. In addition to the values of selectivity, the percentage error defined by $100\times(s_{CALC}-s_{EXP})/s_{EXP}$ is reported. An asterisk means that the calculated selectivity was more than twice as large as the experimental value.

The average absolute errors for the IAS, VSM and GM methods were 35, 41 and 80 percent, respectively. In calculating the average, the asterisks were assigned values of 100.

The conclusion is that none of these theories is in good agreement with experiment for all systems. However, the IAS and VSM methods give results significantly better than that of GM. As mentioned before, the selectivity is a very sensitive parameter. The average error of 35 percent in selectivity for IAS corresponds to an average absolute error of 0.04 in mole fraction.

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NOTE

A book containing some of the information contained in the data bank described above is planned for publication in 1985. This book will contain data on adsorption of pure gases and vapors in a format similar to Fig. 1, data on the adsorption of binary gas mixtures as in Fig. 2, and data on adsorption from liquid mixtures. Additional information may be obtained by writing to the authors.

REFERENCES

1. D.S. Abrams and J.M. Prausnitz, *AIChE J.* 21, 116 (1975).
2. C. Antoine, *Compt. Rend.* 107, 681 (1888).
3. G.G. Arenkova, V.I. Lozgachev and M.L. Sazonov, *Russ. J. Phys. Chem.* 48, 219 (1974).
4. L.F. Atyaksheva, G.I. Emel'yanova and N.I. Kobozev, *Russ. J. Phys. Chem.* 46, 1490 (1972).
5. N.N. Avgul and A.V. Kiselev, in *Chemistry and Physics of Carbon, Vol. 6*, ed. P.L. Walker, Dekker, New York (1970), p. 1.
6. A.G. Aylmore and R.M. Barrer, *Proc. R. Soc. London, Ser. A* 290, 477 (1966).
7. R.M. Barrer, *Zeolites and Clay Minerals*, Academic Press, London (1978), Chap. II.
8. D. Basmadjian, *Can. J. Chem.* 38, 141 (1960).
9. L.B. Begun, V.M. Kisarov and A.I. Subbotin, *Sov. Chem. Ind.* 6, 212 (1974).
10. B.P. Bering, O.A. Likhacheva and V.V. Serpinskii, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* 509 (1961).
11. B.P. Bering, N.M. Pavlyuchenko and V.V. Serpinskii, *Vesti Akad. Nauk Belarus. SSR, Ser. Khim. Nauk* 5, 39 (1969).
12. B.P. Bering and V.V. Serpinskii, *Dokl. Akad. Nauk USSR* 90, 811 (1953).
13. B.P. Bering and V.V. Serpinskii, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* 1146 (1959).
14. B.P. Bering and V.V. Serpinskii, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* 1817 (1961).
15. B.P. Bering and V.V. Serpinskii, *Izv. Akad. Nauk USSR, Otd. Khim. Nauk*, 957 (1953).
16. B.P. Bering, V.V. Serpinskii and S.I. Surinova, *Bull. Acad. Sci. USSR, Div. Chem. Sci.*, 753 (1965).
17. B.P. Bering, V.V. Serpinskii and S.I. Surinova, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* 21, 381 (1972).
18. G.P. Box, *Ind. Eng. Chem. Fundam.* 1, 2 (1962).
19. D.W. Breck, *Zeolite Molecular Sieves*, Wiley, New York (1974), p. 95.
20. D.W. Breck, ibid., p. 72.
21. S. Brunauer, P.H. Emmett and E. Teller, *J. Am. Chem. Soc.* 60, 309 (1938).
22. S. Brunauer, *The Adsorption of Gases and Vapours, Vol. 1*, Oxford University Press, London (1943).
23. M. Bülow, A. Grossmann and W. Schirmer, *Chem. Tech.* 24, 34 (1972).
24. B.W. Bussey, *Ind. Eng. Chem. Fundam.* 5, 103 (1966).
25. D.T. Camp and L.N. Canjar, *AIChE J.* 12, 339 (1966).
26. P.L. Chueh and J.M. Prausnitz, *AIChE J.* 15, 471, (1969).

27. M.R. Cines and F.N. Ruehlen, *J. Phys. Chem.* 57, 710 (1953).
28. E. Costa, J.L. Sotelo, G. Calleja and C. Marron, *AIChE J.* 27, 5 (1981).
29. G. Damköhler, *Z. Phys. Chem.* B23, 58 (1933).
30. R.P. Danner, *Diss. Abstr. Int. B* 27, 1461 (1966).
31. R.P. Danner and E.C.F. Choi, *Ind. Eng. Chem. Fundam.* 17, 248 (1978).
32. R.P. Danner and L.A. Wenzel, *AIChE J.* 15, 515 (1969).
33. J.J. Day, *Diss. Abstr.* 26, 3791 (1966).
34. L.V. Denisova and A.M. Tolmachev, *Russ. J. Phys. Chem.* 49, 1050 (1975).
35. M.M. Dubinin, K.M. Nikolaev, N.S. Polyakov and Yu.N. Til'kunov, *Russ. J. Phys. Chem.* 50, 628 (1976).
36. M.M. Dubinin, in *Chemistry and Physics of Carbon, Vol. 2*, ed. P.L. Walker, Dekker, New York (1966), p. 51.
37. M.M. Dubinin, *Quart. Rev. Chem. Soc.* 9, 101 (1959); *Chem. Rev.* 60, 235 (1960).
38. M.M. Dubinin and D.P. Timofeev, *C.R. Acad. Sci. URSS* 54, 701 (1946).
39. M.M. Dubinin and D.P. Timofeev, *C.R. Acad. Sci. URSS* 55, 137 (1947).
40. M.M. Dubinin and L.V. Radushkevich, *C.R. Acad. Sci. URSS* 55, 327 (1947).
41. M.M. Dubinin, *New Results in Investigations of Equilibria and Kinetics of Adsorption of Gases on Zeolites*, Fourth Intl. Conf. on Molecular Sieves, Univ. Chicago, April 18–22, 1947.
42. Y. Eguchi, *J. Jap. Petrol. Inst.* 13, 2191 (1970).
43. J.M. Fernbacher and L.A. Wenzel, *Ind. Eng. Chem. Fundam.* 11, 457 (1972).
44. R.H. Fowler, *Proc. Camb. Phil. Soc.* 31, 260 (1935).
45. R.H. Fowler and E.A. Guggenheim, *Statistical Thermodynamics*, Cambridge University Press, London (1939).
46. A. Fredenslund, R.L. Jones and J.M. Prausnitz, *AIChE J.* 21, 1086 (1975).
47. R.O. Friederich and J.C. Mullins, *Ind. Eng. Chem. Fundam.* 11, 439 (1972).
48. R.G. Gerritse and J.F.K. Huber, *J. Chromatogr.* 71(2), 173 (1972).
49. H.B. Gilmer and R. Kobayashi, *AIChE J.* 11, 702 (1965).
50. A.J. Glessner and A.L. Myers, *Chem. Eng. Prog., Symp. Ser.* 65, 73 (1969).
51. J. Gmehling and U. Onken, *Vapor-Liquid Equilibrium Data Collection*, DECHEMA, Chemistry Data Series, Frankfurt, W. Germany (1977).
52. R.J. Grant and M. Manes, *Ind. Eng. Chem. Fundam.* 3, 221 (1964).
53. R.J. Grant and M. Manes, *Ind. Eng. Chem. Fundam.* 5, 490 (1966).
54. R.J. Grant, M. Manes and S.B. Smith, *AIChE J.* 8, 403 (1962).
55. S.J. Gregg and K.S.W. Sing, *Adsorption, Surface Area and Porosity*, Academic Press, New York (1982).

56. P.G. Hall and S.A. Müller, *Surface Technology* 7, 165 (1978).
57. P.G. Hall and S.A. Müller, *J. Chem. Soc. Faraday Trans. 1* 74, 948 (1978).
58. E.A. Harlacher and W.G. Braun, *Ind. Eng. Chem. Process Des. Dev.* 9, 479 (1970).
59. J.J. Haydel and R. Kobayashi, *Ind. Eng. Chem. Fundam.* 6, 546 (1967).
60. T.L. Hill, *J. Chem. Phys.* 14, 46 (1946).
61. T.L. Hill, ibid. 268 (1946).
62. H. Hoppe, F. Winkler and E. Worch, *Z. Chem.* 18, 154 (1978).
63. H. Hoppe and E. Worch, *Z. Phys. Chemie, Leipzig* 263, 1169 (1982).
64. S.H. Hyun and R.P. Danner, *J. Chem. Eng. Data* 27, 196 (1982).
65. R.K. Iler, in *Surface and Colloid Science, Vol. 6*, ed. E. Matijevic, Wiley, New York (1973), p. 1.
66. B.I. Ivchenko, V.S. Morozov, G.P. Gubanova and V.N. Pelipas, *Russ. J. Phys. Chem.* 50, 108 (1976).
67. M. Jaroniec, *Thin Solid Films* 50, 163 (1978).
68. H. Jüntgen, *Ber. Bunsenges. Physik. Chem.* 79, 747 (1975).
69. J. Kärger, M. Bülow and W. Schirmer, *Z. Phys. Chem. (Leipsig)* 256, 144 (1975).
70. K. Karpinski, H. Kowalczyk and Z. Hinz, *Rocz. Chem.* 49, 1343 (1975).
71. K. Karpinski and H. Kowalczyk, *Rocz. Chem.* 47, 1493 (1973).
72. N.V. Kel'tsev and Yu.I. Shumyatskii, *Russ. J. Phys. Chem.* 44, 743 (1970).
73. A.V. Kiselev, N.V. Kovalena and A.Y. Korolev, *Kolloid Zh.* 23, 582 (1961).
74. D.E. Knuth, *The Art of Computer Programming, Vol. 3*, Addison–Wesley (1973).
75. N.I. Kobozev, G.I. Emel'yanova, E.V. Voloshanovskii and L.F. Atyaksheva, *Russ. J. Phys. Chem.* 48, 869 (1974).
76. H. Kowalczyk and K. Karpinski, *Rocz. Chem.* 48, 1049 (1974).
77. I. Langmuir, *J. Amer. Chem. Soc.* 40, 1361 (1918).
78. W.L.S. Laukhuf, *Diss. Abstr. Int. B*, 31, 1927 (1970).
79. P.B. Lederman and B. Williams, *AIChE J.* 10, 30 (1964).
80. B.I. Lee and M.G. Kesler, *AIChE J.* 21, 510 (1975).
81. W.K. Lewis, E.R. Gilliland, B. Chertow and D. Bareis, *J. Am. Chem. Soc.* 72, 1160 (1950).
82. W.K. Lewis, E.R. Gilliland, B. Chertow and W.P. Cadogan, *Ind. Eng. Chem.* 42, 1319 (1950).
83. Ibid., 1326 (1950).
84. W.K. Lewis, E.R. Gilliland, B. Chertow and W.H. Hoffman, *J. Am. Chem. Soc.* 72, 1153 (1950).
85. W.K. Lewis, E.R. Gilliland, B. Chertow and W. Milliken, *J. Am. Chem. Soc.* 72, 1157 (1950).
86. O.P. Mahajan and P.L. Walker, *J. Coll. Interface Sci.* 29, 129 (1969).

87. E.C. Markham and A.F. Benton, *J. Am. Chem. Soc.* 53, 497 (1931).
88. F.D. Maslan, M. Altman and E.R. Aberth, *J. Phys. Chem.* 57, 106 (1953).
89. J.P. Mason and C.E. Cooke, Jr., *AIChE J.* 12, 1097 (1966).
90. S. Masukawa and R. Kobayashi, *J. Chem. Eng. Data*, 13, 197 (1968).
91. W. Meier, in *Molecular Sieves, Proceedings of the First Intl. Conf. on Zeolites*, Society of Chemical Industry, London (1968), p. 10.
92. V.S. Morozov, B.I. Ivchenko, G.P. Gubanova and L.V. Fartushnaya, *Russ. J. Phys. Chem.* 46, 1662 (1972).
93. V.S. Morozov, B.I. Ivchenko, G.P. Gubanova and L.V. Fartushnaya, *Russ. J. Phys. Chem.* 48, 568 (1974).
94. V.S. Morozov, B.I. Ivchenko, G.P. Gubanova, L.V. Fartushnaya and V.N. Pelinas, *Russ. J. Phys. Chem.* 50, 599 (1976).
95. A.L. Myers, C. Minka and D.Y. Ou, *AIChE J.* 28, 97 (1982).
96. A.L. Myers and J.M. Prausnitz, *AIChE J.* 11, 121 (1965).
97. A.L. Myers, in *Fundamentals of Adsorption*, ed. by A.L. Myers and G. Belfort, Amer. Institute of Chemical Engineers, New York (1984).
98. T. Nakahara, M. Hirata, G. Amagasa and T. Ogura, *J. Chem. Eng. Data* 29 202 (1984).
99. T. Nakahara, M. Hirata and S. Komatsu, *J. Chem. Eng. Data* 26, 161 (1981).
100. T. Nakahara, M. Hirata and H. Mori, *J. Chem. Eng. Data* 27, 317 (1982).
101. T. Nakahara, M. Hirata and T. Omori, *J. Chem. Eng. Data* 19, 310 (1974).
102. M. Okazaki, H. Tamon and R. Toei, *J. Chem. Eng. Japan* 11, 209 (1978).
103. V.S. Parbuzin and Yu.N. Kuryakov, *Russ. J. Phys. Chem.* 49, 1057 (1975).
104. V.S. Parbuzin, G.M. Panchenkov, B.Kh. Rakhmukov and G.V. Sandul, *Russ. J. Phys. Chem.* 41, 97 (1967).
105. V.S. Parbuzin, V.A. Yakovlev and G.M. Panchenkov, *Russ. J. Phys. Chem.* 48, 1515 (1974).
106. N.M. Pavlyuchenko, *Russ. J. Phys. Chem.* 44, 152 (1970).
107. H.K. Payne, G.A. Sturdevant and T.W. Leland, *Ind. Eng. Chem. Fundam.* 7, 363 (1968).
108. D. Peng and D.B. Robinson, *Ind. Eng. Chem. Fundam.* 15, 59 (1976).
109. D.L. Peterson and O. Redlich, *J. Chem. Eng. Data*, 7, 570 (1962).
110. T.G. Plachenov, A.A. Seballo and A.N. Shiryaev, *Zh. Prikl. Khim. (Leningrad)* 45(6), 1265 (1972).
111. M. Polanyi, *Trans. Faraday Soc.* 28, 316 (1932).
112. M. Polanyi, *Verh. Dtsch. Phys. Ges.* 16, 1012 (1914).

113. H.G. Rackett, *J. Chem. Eng. Data* 15, 514 (1970).
114. J. Rabbeneau, A.F. Fillatre and M. Yvare, *Rev. Gen. Caoutchouc*, 41, 394 (1964).
115. T.B. Reed and D.W. Breck, *J. Am. Chem. Soc.* 78, 5972 (1956).
116. T.B. Reed, W.G. Eversole, R.M. Milton, T.B. Reed and T.L. Thomas, *J. Am. Chem. Soc.* 78, 5963 (1956).
117. R. Reich, W.T. Ziegler and K.A. Rogers, *Ind. Eng. Chem. Process Des. Dev.* 19, 336 (1980).
118. R.C. Reid, J.M. Prausnitz and T.K. Sherwood, *The Properties of Gases and Liquids, 3rd Ed.*, McGraw-Hill, New York (1977).
119. K.A. Rogers, *Diss. Abstr. Int. B* 34, 1495 (1973).
120. D.M. Ruthven, *AIChE J.* 22, 753 (1976).
121. J. Shen and J.M. Smith, *Ind. Eng. Chem. Fundam.* 7, 100 (1968).
122. Ibid., 106 (1968).
123. S. Sircar and A.L. Myers, *Chem. Eng. Sci.* 28, 489 (1973).
124. E.D. Sloan, Jr. and J.C. Mullins, *Ind. Eng. Chem. Fundam.* 14, 347 (1975).
125. S. Suwanayuen and R.P. Danner, *AIChE J.* 26, 68 (1980).
126. Ibid., 76 (1980).
127. L. Szepesy and V. Illes, *Acta Chim. Hung.* 35, 245 (1963).
128. W.J. Thomas and J.L. Lombardi, *Trans. Inst. Chem. Eng.*, 49, 240 (1971).
129. J. Toth, *Acta Chim. Acad. Sci. Hung.* 30, 1 (1962).
130. J. Toth, *Acta Chim. (Budapest)* 69, 311 (1971).
131. D.L. Trimm, *Carbon* 15, 273 (1977).
132. E. Van der Vlist and Jo. Van der Meijden, *J. Chromatogr.* 79 1 (1973).
133. H.C. Van Ness, *Ind. Eng. Chem. Fundam.* 8, 464 (1969).
134. L.A. Vashchenko and V.V. Serpinskii, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* 2547 (1975).
135. T. Vermeulen, G. Klein and N.K. Hiester, *Chemical Engineers' Handbook, Fifth Ed.*, McGraw-Hill, New York (1973), sect. 16.
136. M.-C. Veyssiere and A. Cointot, *Bull. Soc. Chim. Fr.* 5-6, 1071 (1975).
137. P.L. Walter, Jr., L.G. Austin and S.P. Nandi, *Chemistry and Physics of Carbon, Vol. 2*, ed. Marcel Dekker, New York (1966), p. 260.
138. K.M. Watson, *Ind. Eng. Chem.* 35, 398 (1943).
139. F.J. Wilkins, *Nature, Lond.* 141, 1054 (1938).
140. G.M. Wilson, *J. Amer. Chem. Soc.* 86, 127, 133 (1964).
141. R.J. Wilson and R.P. Danner, *J. Chem. Eng. Data* 28, 14 (1983).
142. E. Worch, *Chem. Techn.* 34, 474 (1982).
143. T. Yamada and R.D. Gunn, *J. Chem. Eng. Data* 18, 234 (1973).
144. D.M. Young and A.D. Crowell, *Physical Adsorption of Gases*, Butterworths, London, 1962, Chap. 11.
145. Z.A. Zhukova and N.V. Kel'tsev, *Russ. J. Phys. Chem.* 44, 1172 (1970).

APPENDIX 1

Experimental Measurements of Adsorption of Binary Gas Mixtures

Adsorbates	Adsorbent	Surf. Area m^2/g	Pore Vol. cm^3/g	Temp. K	Pressure kPa	Exp. Tech.	Data Type	Ref.
$CH_4 + C_2H_4$	SG (DC,Refrig. grade)	751		298	101	S–V	T^{SE}	82
$CH_4 + C_2H_6$	SG (MSM)			298		F–C	G	3
$CH_4 + C_2H_6$	SG (DC,grade 15)	803		278–308	0–9,700	F–C	G	90
$CH_4 + C_3H_8$	SG	530		293	700–6,900	F–C	G	49
$CH_4 + C_3H_8$	SG (DC,grade 15)	803		273–313	700–6,900	F–C	T	59
$CH_4 + n\text{–}C_4H_{10}$	SG			314				33
$CH_4 + n\text{–}C_4H_{10}$	SG (DC,Refrig grade 03)	807		314	6,900	F–N	G	89
$CH_4 + n\text{–}C_6H_{12}$	SG			314				33
$CH_4 + n\text{–}C_6H_{12}$	SG (DC,Refrig grade 03)	807		314	6,900	F–N	G	89
$CH_4 + n\text{–}C_6H_{14}$	SG			314				33
$CH_4 + n\text{–}C_6H_{14}$	SG (DC,Refrig grade 03)	807		314	6,900	F–N	G	89
$C_2H_2 + C_2H_4$	SG (DC,Refrig grade)	751		298	101	S–V	T	85
$C_2H_4 + C_2H_6$	SG (DC,Refrig grade)	751		298	33–1,940	S–V	G	82
$C_2H_4 + C_3H_6$	SG (DC,Refrig grade)	751		273–313	101	S–V	T	81
$C_2H_4 + C_3H_8$	SG (DC,Refrig grade)	751		273–313	101	S–V	T	81
$C_2H_6 + C_3H_8$	SG (DC,Refrig grade)	751		298	101	S–V	T	82
$C_3H_6 + C_3H_8$	SG (DC,Refrig grade)	751		298	101	S–V	T	84
$C_3H_6 + C_3H_8$	SG (DC,Refrig grade)	751		298	33–790	S–V	T^{SE}	82
$i\text{–}C_4H_8 + i\text{–}C_4H_{10}$	SG (DC,Refrig grade)	751		298	101	S–V	G	82
$C_6H_6 + n\text{–}C_6H_{14}$	SG (DC)	832	0.43	343–403	101	F–N	G	121
$C_6H_6 + n\text{–}C_6H_{14}$	SG (DC)	832	0.43	343–403	101	F–N	G^{BT}	122
C_6H_6 + 2,4–dimethylpentane	SG (DC,#08–08–237)			339	7–67	S–G	G	27
C_6H_6 + 2,4–dimethylpentane	SG (Mallinckrodt)			339	7–67	S–G	G	27
$CH_4 + N_2$	SG (MSM)			298		F–C	G	3
$C_2H_6 + N_2$	SG (MSM)			298		F–C	G	3
$n\text{–}C_7H_{16} + H_2O$	SG (KSK)	380	0.9	348		S–C	G	14
$Ar + N_2$	SG (DC,Grade 08G)			195	101	F–N	G^{BT}	25
$CO_2 + H_2$	SG (KSM,6P)	510		120–180	253–10,000	F–N	T	92
CO_2 + He	SG			140–160				93
$CO_2 + N_2$	SG (KSM,6P)	510		100–180	250–9,000	F–N	T	94
$CO_2 + N_2$	SG			140–160				93
$D_2 + H_2$	SG (FS)	750		75–90	27–100	F–N	G	8
H_2 + Xe	SG (KSM,6P)	510		100–180	253–10,100	F–N	T	66
He + Xe	SG (KSM,6P)	510		100–180	253–10,100	F–N	T	66
$O_2 + O_3$	SG (KSS)	365	0.83	156–273	0.06–16	F–N	G	75
$O_2 + O_3$	SG (KSS)	365	0.83	156–293	0.06–16	F–N	G	4
$CH_4 + C_2H_4$	AC (PC,BPL)	990		213–301	138–2,100	S–V	T	117
$CH_4 + C_2H_4$	AC (CE, 40)	700		293	1–107	F–N	T	28
$CH_4 + C_2H_4$	AC (Nuxit,AL)			293	100	S–V	T	127
$CH_4 + C_2H_4$	AC (CO,G)			298	101	S–V	T^{SE}	82
$CH_4 + C_2H_6$	AC (PC,BPL)	990		213–301	140–2,000	S–V	T	117
$CH_4 + C_2H_6$	AC (Nuxit,AL)			293	100	S–V	T	127
$CH_4 + C_2H_6$	AC (CE, 40)	700		293	1–107	F–N	T	28
$CH_4 + C_3H_8$	AC (CO,G)	1157		303	345–73,000	S–V	T	107
$CH_4 + C_3H_8$	AC (PC,BPL)	1040		298	0–7,000	F–N	T	53
$CH_4 + n\text{–}C_4H_{10}$	AC (PC,BPL)	1040		298	0–5,300	F–N	T	53
$CH_4 + n\text{–}C_4H_{10}$	AC (CO,G)	1157		313–343	14–13,700	S–V	T	107
$CH_4 + n\text{–}C_6H_{14}$	AC (PC,BPL)	1040		298	0–7,000	F–N	T	53

APPENDIX 1 (Cont'd)

Experimental Measurements of Adsorption of Binary Gas Mixtures

Adsorbates	Adsorbent	Surf. Area m^2/g	Pore Vol. cm^3/g	Temp. K	Pressure kPa	Exp. Tech.	Data Type	Ref.
$C_2H_2 + C_2H_4$	AC (PC,EY-51-C)	805		298	101	S-V	T	85
$C_2H_4 + C_2H_6$	AC (CO,G)			298	101	S-V	G	82
$C_2H_4 + C_2H_6$	AC (PC,BPL)	990		213-301	140-2,100	S-V	T	117
$C_2H_4 + C_2H_6$	AC (CE, 40)	700		293	1-107	F-N	T	28
$C_2H_4 + C_2H_6$	AC (Nuxit,AL)			293-333	100	S-V	T	127
$C_2H_4 + C_3H_6$	AC (Nuxit,AL)			293	100	S-V	T	127
$C_2H_4 + C_3H_8$	AC (CO,G)			298	101	S-V	T	82
$C_2H_4 + C_3H_6$	AC (CE, 40)	700		293	1-107	F-N	T	28
$C_2H_4 + C_3H_8$	AC (PC, EY-51-C)	805		298	101	S-V	T^{SE}	82
$C_2H_4 + C_3H_8$	AC (CO, G)			298	101-790	S-V	T^{SE}	82
$C_2H_6 + C_3H_6$	AC			303-323				78
$C_2H_6 + C_3H_6$	AC (CE, 40)			293	1-107	F-N	T	28
$C_2H_6 + C_3H_8$	AC (Nuxit,AL)			293-333	100	S-V	T	127
$C_2H_6 + C_3H_8$	AC (PC,EY-51-C)	805		298	101	S-V	T	82
$C_3H_6 + C_3H_8$	AC (CO,G)			298	101	S-V	T^{SE}	82
$C_3H_6 + C_3H_8$	AC (CC,Black Pearls II)	705		298	101	S-V	T	84
$C_3H_6 + C_3H_8$	AC (Nuxit,AL)			293	100	S-V	T	127
$C_3H_8 + n\text{-}C_4H_{10}$	AC (Nuxit,AL)			293	100	S-V	T	127
$1\text{-}C_4H_8 + i\text{-}C_4H_{10}$	AC (PC,EY-51-C)	805		298	101	S-V	G	82
C_6H_6 + cyclohexane	AC (Calgon Filtra. 400)	1100	0.95	303	0.01-15	S-G	G	95
$C_6H_6 + n\text{-}C_6H_{14}$	AC			303-323				142
C_6H_6 + toluene	AC (B4)			303			G	62
$C_6H_6 + C_7H_8$	AC (SS-208C)	1038	0.44	423		F-N	G	128
C_6H_6 + 1,3,5-triethylbenzene	AC (ART-2,PAU)			393		F-C	G^{BT}	35
$C_6H_6 + C_2H_5OH$	AC (AR-3)			283-323	0.3-1.3		G	9
$C_6H_6 + i\text{-}C_3H_7OH$	AC (B4)	1230	0.48	303	1.8-4.0		T	63
$C_6H_6 + i\text{-}C_3H_7OH$	AC (AR-3)			283-323	0.3-1.3		G	9
$C_6H_6 + 1\text{-}C_4H_9OH$	AC (AR-3)			303	0.3-1.3		G	9
toluene + C_2H_5OH	AC (AR-3)			303	0.3-1.3		T	9
toluene + $i\text{-}C_3H_7OH$	AC (SKT)			283-303	0.3-1.3		T	9
toluene + $1\text{-}C_4H_9OH$	AC (AR-3)			303	0.3-1.3		G	9
p-xylene + C_2H_5OH	AC (SKT,AR-3)			303	0.3-1.3		T	9
p-xylene + $i\text{-}C_3H_7OH$	AC (SKT,AR-3)			303	0.3-1.3		G	9
p-xylene + $1\text{-}C_4H_9OH$	AC (AR-3)			303	0.3-1.3		G	9
$CHCl_3 + (C_2H_5)_2O$	AC			333		S-C	G	16
$C_2H_5Cl + (C_2H_5)_2O$	AC			323-344		S-C	G	16
$CH_4 + CO$	AC (PC,BPL)	1053		298	345	S-V	T	141
$CH_4 + CO_2$	AC			212-310				119
$CH_4 + CO_2$	AC (PC,BPL)	1053		298	345	S-V	T	141
$CH_4 + CO_2$	AC (AR-3)			298		F-C	G	3
$CH_4 + N_2$	AC (AR-3)			298		F-C	G	3
$CH_3OH + H_2O$	AC (HGI-780)	724	0.85	303	4-7	S-G	T	102
$CH_3OH + H_2O$	AC (Shirasagi,S)	972	0.9	303	4-7	S-G	T	102
$C_2H_4 + CO_2$	AC (Nuxit,AL)			293	100	S-V	T	127
$C_2H_5Cl + H_2O$	AC			348				13
$(CH_3)_2CO + H_2O$	AC (Shirasagi,S)	972	0.9	303	3-5	S-G	T	102
$(CH_3)_2CO + H_2O$	AC (HGI-780)	724	0.85	303	3-5	S-G	T	102
$C_6H_6 + H_2O$	AC (Shirasagi,S)	972	0.9	303		S-G	T	102

APPENDIX 1 (Cont'd)

Experimental Measurements of Adsorption of Binary Gas Mixtures

Adsorbates	Adsorbent	Surf. Area m^2/g	Pore Vol. cm^3/g	Temp. K	Pressure kPa	Exp. Tech.	Data Type	Ref.
$C_6H_5OH + H_2O$	AC (Shirasagi,S)	972	0.9	303	3–5	S–C	T	102
$CO + CO_2$	AC (PC,BPL)	1053		298	345	S–V	T	141
$CO_2 + N_2$	AC (AR–3)			298		F–C	G	3
$D_2 + H_2$	AC (CO,G)	1250		75–90	27–100	S–V	G	8
$D_2 + H_2$	AC (FS,FCC)	1100		75–90	27–100	S–V	G	8
$He + N_2$	AC (PC,BPL)	1123		100–150	100–10,000	F–N	T	43
$C_2H_4 + C_2H_6$	CMS (5A)	650	0.56	303	3–13	S–V	T	98
$C_2H_4 + C_3H_6$	CMS (5A)	650	0.56	275–323	1–10	S–V	T	98
$C_2H_4 + C_3H_6$	CMS (5A)	650	0.56	275–323	13	S–V	T	100
$C_2H_6 + C_3H_8$	CMS (5A)	650	0.56	278–323	13	S–V	T	99
$C_2H_4 + C_2H_6$	GC (Sterling FTG–D5)	13		298	93	S–G	G	47
$C_2H_6 + C_3H_8$	GC (Sterling FTG–D5)	13		298	93	S–G	G	47
$C_3H_6 + C_3H_8$	GC (Sterling FTG–D5)	13		298	1.3–93.3	S–G	G	47
benzene + Freon–11	GC (Sterling MTFF–D7)	10		298	0.5–1.2	S–G	G	124
benzene + cyclohexane	GC (Sterling MT–D5)	10		303	0.07–0.11	S–G	G	95
$C_2H_2 + C_2H_4$	Z			298			T^{SE}	72
$C_2H_4 + C_2H_6$	Z (Linde,13X)	525	0.3	298–323	138	S–V	T	31
$C_2H_4 + C_2H_6$	Z			298			T^{SE}	72
$C_2H_4 + C_3H_6$	Z			298			T^{SE}	72
$C_2H_4 + i–C_4H_{10}$	Z (Linde,13X)	525	0.3	298–373	138	S–V	T	64
$C_2H_6 + C_3H_8$	Z (5A)		0.25	273	1–53	S–G	T	136
$C_2H_6 + n–C_4H_{10}$	Z (5A)		0.25	273	1–53	S–G	T	136
$C_2H_6 + n–C_4H_{10}$	Z (5A)			308	6	S–C	T	50
$C_2H_6 + i–C_4H_{10}$	Z (Linde,13X)	525	0.3	298–323	138	S–V	T	64
$C_3H_8 + n–C_4H_{10}$	Z (5A)		0.25	273	1–53	S–G	T	136
$C_3H_8 + n–C_4H_{10}$	Z (CaA)			293–383	40	S–V	G	34
$n–C_6H_{12} + n–C_6H_{14}$	Z (CaA)			383	40	S–V	G	34
$n–C_6H_{12} + n–C_7H_{16}$	Z (Linde,5A)			573	73	F–N		109
$C_6H_6 + n–C_6H_{14}$	Z (NaX)			358		F–C	G	69
$n–C_6H_{14} + n–C_7H_{16}$	Z (CaA)			358–413	40	S–V	G	34
$n–C_7H_{16} + n–C_8H_{18}$	Z (CaA)			383	40	S–V	G	34
$n–C_7H_{16} + n–C_{12}H_{26}$	Z (CaA)				40	S–V	T^{SE}	34
$n–C_7H_{16} + n–C_{14}H_{30}$	Z (CaA)				40	S–V	T^{SE}	34
$n–C_{10}H_{22} + n–C_{12}H_{26}$	Z (CaA)				40	S–V	T^{SE}	34
$n–C_{10}H_{22} + n–C_{14}H_{30}$	Z (CaA)				40	S–V	T^{SE}	34
$n–C_{12}H_{26} + n–C_{14}H_{30}$	Z (NaA,CaA)			523–633				23
$C_3H_8 + C_2H_5Cl$	Z (NaX)			303		S–C		17
$C_2H_5OH + n–C_3H_7OH$	Z (CaA)			358–413	40	S–V	G	34
$CH_4 + N_2$	Z (CaA)			123–295	100–10,000	S–V	G^{SE}	79
$C_2H_4 + CO$	Z			298			T^{SE}	72
$C_2H_4 + CO_2$	Z (13X)	525	0.3	298–323	138	S–V	T	64
$C_2H_4 + CO_2$	Z			298			T^{SE}	72
$C_2H_6 + CO_2$	Z (5A)			308	13	S–C	T	50
$n–C_4H_{10} + H_2S$	Z (CaA)			273–348		F–N	T	145
$Ar + N_2$	Z (NaX)			140–160	0.5–65.0	S–V	G	134
$CO + N_2$	Z (Linde,5A,10X)	600		144	101	F–N	T	32
$CO + O_2$	Z (Linde,5A,10X)	600		144	101	F–N	T	32
$D_2 + H_2$	Z (Linde,CaA)			78	0–53	S–V	G^{SE}	104

APPENDIX 1 (Cont'd)

Experimental Measurements of Adsorption of Binary Gas Mixtures

Adsorbates	Adsorbent	Surf. Area m^2/g	Pore Vol. cm^3/g	Temp. K	Pressure kPa	Exp. Tech.	Data Type	Ref.
$D_2 + H_2$	Z (NaX)			62–90	0–53	S–V	G^{SE}	104
$D_2 + H_2$	Z (Linde,NaA)			62–90	0–53	S–V	G^{SE}	104
$D_2 + H_2$	Z (Linde,4A)			55–112	1–40	S–V	T^{SE}	105
$D_2 + H_2$	Z (Linde,5A)			50–112	0.3–40.0	S–V	T^{SE}	105
$D_2 + H_2$	Z (GROZNII,NaA)			48–90	0.1–15.0	S–V	T^{SE}	105
$D_2 + H_2$	Z (VNIINP,NaX)			35–90	1–6	S–V	T^{SE}	105
$D_2 + HD$	Z (Linde,CaA)			78	0–53	S–V	G^{SE}	104
$D_2 + HD$	Z (NaX)			62–90	0–53	S–V	G^{SE}	104
$D_2 + HD$	Z (Linde,NaA)			62–90	0–53	S–V	G^{SE}	104
$D_2 + H_2O$	Z (Linde,4A,5A,13X)	700		75–90	27–100	F–N	G	8
$HD + H_2$	Z (Linde,CaA)			78	0–53	S–V	G^{SE}	104
$HD + H_2$	Z (NaX)			62–90	0–53	S–V	G^{SE}	104
$HD + H_2$	Z (Linde,NaA)			62–90	0–53	S–V	G^{SE}	104
$HD + H_2$	Z (Linde,4A)			55–112	1–40	S–V	T^{SE}	105
$HD + H_2$	Z (Linde,5A)			50–112	0.3–40.0	S–V	T^{SE}	105
$HD + H_2$	Z (GrosNII,NaA)			48–90	0.1–15.0	S–V	T^{SE}	105
$HD + H_2$	Z (VNIINP,NaX)			35–90	1–6	S–V	T^{SE}	105
$N_2 + O_2$	Z (5A)			283–323		F–C		132
$N_2 + O_2$	Z (Linde,5A,13X)	600		144	101	F–N	T	32

APPENDIX 2

Experimental Measurements of Adsorption of Ternary Gas Mixtures

Adsorbates	Adsorbent	Surf. Area m^2/g	Pore Vol. cm^3/g	Temp. K	Pressure kPa	Exp. Tech.	Data Type	Ref.
$C_2H_4 + C_3H_6 + C_3H_8$	SG (DC, refrig grade)	751		298	101	S–V	T^{SE}	82
$H_2 + CH_4 + C_2H_6$	AC (Nuxit, AL)			293	101	S–V	T	127
$H_2 + C_2H_4 + C_2H_6$	AC (Nuxit, AL)			293	101	S–V	T	127
$CH_4 + C_2H_4 + C_2H_6$	AC (CE, 40)	700		293–323	10–13	F–N	T	28
$CH_4 + C_2H_4 + C_2H_6$	AC (PC, BPL)	990		213–301	124–3000	S–V	T	117
$C_2H_4 + C_2H_6 + C_3H_6$	AC (CE, 40)	700		293–323	10–13	F–N	T	28
$C_2H_4 + C_3H_6 + C_3H_8$	AC (CO, G)			298	101	S–V	T^{SE}	82

APPENDIX 3

Comparison of Predictions of Binary Gas Adsorption

Adsorbates	Adsorbent	T, K	P kPa	Mole Fract.	Selectivity, s				Percent Error			Ref.
					Exp.	IAS	VSM	GM	IAS	VSM	GM	
C_2H_2 + C_2H_4	SG	298	101	x_1 = .931	4.33	3.84	3.64	0.82	11	16	*	85
"	"	"	"	x_1 = .542	2.95	4.09	4.21	0.83	39	43	*	85
"	"	"	"	x_1 = .136	2.16	4.29	4.87	0.84	99	*	*	85
C_3H_6 + C_2H_4	SG	273	101	x_1 = .973	1.62	2.26	1.94	21	40	20	*	81
"	"	"	"	x_1 = .495	2.12	2.14	2.10	77	1	1	*	81
"	"	"	"	x_1 = .045	2.10	2.10	2.29	120	0	9	*	81
"	"	298	101	x_1 = .953	1.79	2.19	1.80	24	22	1	*	81
"	"	"	"	x_1 = .509	2.02	2.14	2.08	94	6	3	*	81
"	"	"	"	x_1 = .081	1.79	2.13	2.58	150	19	44	*	81
"	"	313	103	x_1 = .897	1.65	1.90	1.59	40	15	4	*	81
"	"	"	"	x_1 = .506	1.89	1.84	1.79	110	5	4	*	81
"	"	"	"	x_1 = .116	1.77	1.82	2.16	166	3	22	*	81
C_3H_6 + C_2H_4	SG	273	103	x_1 = .934	8.07	6.69	2.16	14	17	73	75	81
"	"	"	"	x_1 = .459	7.89	6.61	5.33	26	16	32	*	81
"	"	"	"	x_1 = .115	11.68	6.56	5.32	31	44	54	*	81
"	"	298	103	x_1 = .963	8.61	6.80	5.27	14	21	39	61	81
"	"	"	"	x_1 = .603	6.78	6.51	6.13	25	4	10	*	81
"	"	"	"	x_1 = .193	7.23	6.55	7.65	32	9	6	*	81
"	"	313	102	x_1 = .940	7.38	6.86	6.92	18	7	6	*	81
"	"	"	"	x_1 = .529	6.46	7.97	7.52	28	23	16	*	81
"	"	"	"	x_1 = .295	6.02	8.38	7.72	33	39	28	*	81
C_3H_6 + C_3H_8	SG	298	101	x_1 = .892	2.67	2.65	1.49	0.49	1	44	*	84
"	"	"	"	x_1 = .445	1.32	2.84	3.17	0.52	*	*	*	84
"	"	"	"	x_1 = .277	1.14	2.89	3.57	0.53	*	*	*	84
C_2H_6 + CH_4	AC	213	130	y_1 = .733	30.0	33.4	31.6	33.6	11	5	12	117
"	"	"	244	"	13.6	31.1	29.7	27.6	*	*	*	117
"	"	"	353	"	11.0	29.8	28.7	24.6	*	*	*	117
"	"	"	132	y_1 = .501	30.1	34.5	32.8	37.5	14	9	25	117
"	"	"	348	"	16.8	31.3	29.6	27.6	*	77	65	117
"	"	"	132	y_1 = .255	35.5	38.5	35.4	45.8	8	0	29	117
"	"	"	436	"	23.9	32.3	31.0	31.3	35	30	31	117
"	"	"	875	"	17.5	30.3	29.0	25.0	73	65	43	117
"	"	260	125	y_1 = .255	20.5	26.3	41.9	57.1	29	*	*	117
"	"	"	412	"	14.5	21.7	30.0	39.1	50	*	*	117
"	"	"	941	"	11.5	19.2	25.5	30.0	67	*	*	117
"	"	301	130	y_1 = .733	13.6	14.0	17.4	52.3	3	28	*	117
"	"	"	685	"	4.49	12.0	13.6	31.1	*	*	*	117
"	"	"	2005	"	2.48	11.2	12.4	22.2	*	*	*	117
"	"	"	132	y_1 = .501	13.0	14.5	18.7	58.5	11	43	*	117
"	"	"	693	"	6.49	12.2	14.0	34.7	88	*	*	117
"	"	"	1385	"	3.82	11.6	13.1	27.9	*	*	*	117
"	"	"	130	y_1 = .255	14.6	15.6	21.7	72.1	7	49	*	117
"	"	"	687	"	8.86	12.8	15.2	42.4	45	71	*	117
"	"	"	1373	"	6.95	12.0	13.9	34.0	73	*	*	117
"	"	293	100	x_1 = .975	14.4	15.4	17.3	15.5	7	20	8	127
"	"	"	"	x_1 = .852	17.7	18.9	20.4	21.9	6	15	23	127
"	"	"	"	x_1 = .605	21.7	22.2	24.9	31.4	2	15	45	127
C_2H_4 + CH_4	AC	213	136	y_1 = .740	20.3	23.8	24.4	17.2	17	20	15	117
"	"	"	241	"	12.2	22.7	23.1	15.8	86	90	24	117

APPENDIX 3 (Cont'd)
Comparison of Predictions of Binary Gas Adsorption

Adsorbates	Adsorbent	T, K	P kPa	Mole Fract.	Selectivity, s				Percent Error			Ref.
					Exp.	IAS	VSM	GM	IAS	VSM	GM	
$C_2H_4 + CH_4$	AC	213	414	$y_1 = .740$	11.0	21.7	22.2	13.4	98	*	22	117
"	"	"	320	$y_1 = .464$	14.6	22.7	23.3	15.6	56	60	7	117
"	"	"	725	"	10.5	21.2	21.9	13.0	*	*	23	117
"	"	"	136	$y_1 = .235$	20.5	27.0	27.2	21.7	32	33	6	117
"	"	"	441	"	15.5	23.3	23.6	16.5	50	52	7	117
"	"	"	896	"	13.4	21.7	22.1	14.0	63	66	5	117
"	"	260	146	$y_1 = .235$	12.4	15.9	25.5	25.1	28	*	*	117
"	"	"	684	"	8.80	13.2	17.5	17.6	49	99	*	117
"	"	"	1411	"	6.79	12.2	15.9	14.8	80	*	*	117
"	"	301	131	$y_1 = .740$	9.41	10.0	11.0	25.5	6	17	*	117
"	"	"	683	"	4.09	8.55	9.06	17.6	*	*	*	117
"	"	"	2000	"	2.87	8.26	8.57	13.9	*	*	*	117
"	"	"	122	$y_1 = .464$	9.75	10.5	11.1	28.6	8	14	*	117
"	"	"	676	"	5.48	8.84	9.36	19.4	61	71	*	117
"	"	"	2032	"	3.52	8.26	8.68	15.2	*	*	*	117
"	"	"	129	$y_1 = .235$	10.0	11.1	13.0	32.5	11	30	*	117
"	"	"	694	"	6.43	9.17	9.85	22.1	43	53	*	117
"	"	"	1431	"	5.13	8.62	9.14	8.71	68	78	*	117
"	"	293	100	$x_1 = .971$	12.3	11.6	12.7	10.2	6	3	17	127
"	"	"	"	$x_1 = .833$	11.5	13.6	14.3	12.3	19	25	8	127
"	"	"	"	$x_1 = .634$	14.0	15.4	16.0	14.5	10	14	4	127
$C_2H_4 + C_2H_2$	AC	298	101	$x_1 = .085$	0.94	1.31	1.58	1.22	40	68	30	85
"	"	"	"	$x_1 = .428$	1.42	1.31	1.37	1.21	8	3	15	85
"	"	"	"	$x_1 = .903$	1.75	1.30	0.90	1.19	26	94	32	85
$C_2H_6 + C_2H_4$	AC	293	101	$x_1 = .162$	1.49	1.44	1.48	2.80	3	0	88	127
"	"	"	"	$x_1 = .488$	1.50	1.44	1.47	2.71	4	2	80	127
"	"	"	"	$x_1 = .863$	1.53	1.44	1.45	2.57	6	5	68	127
"	"	333	100	$x_1 = .171$	1.35	1.34	1.36	3.01	1	1	*	127
"	"	"	"	$x_1 = .459$	1.45	1.34	1.35	2.92	8	26	*	127
"	"	"	"	$x_1 = .750$	1.37	1.33	1.34	2.81	3	2	*	127
"	"	213	140	$y_1 = .240$	1.68	1.45	1.49	2.38	14	11	42	117
"	"	"	224	"	1.58	1.42	1.46	2.24	10	8	42	117
"	"	"	405	"	1.52	1.38	1.42	2.09	10	7	37	117
"	"	"	137	$y_1 = .682$	1.75	1.44	1.44	2.28	18	18	30	117
"	"	"	241	"	1.64	1.41	1.39	2.14	14	15	30	117
"	"	"	343	"	1.60	1.38	1.35	2.05	14	15	28	117
"	"	301	138	$y_1 = .240$	1.24	1.46	1.69	2.58	18	37	*	117
"	"	"	737	"	1.27	1.42	1.55	2.10	12	22	65	117
"	"	"	1981	"	1.18	1.37	1.48	1.86	15	25	57	117
"	"	"	218	$y_1 = .472$	1.42	1.45	1.63	2.37	2	15	67	117
"	"	"	550	"	1.28	1.43	1.55	2.13	12	22	67	117
"	"	"	1133	"	1.28	1.39	1.51	1.95	9	18	53	117
"	"	"	144	$y_1 = .682$	1.49	1.46	1.65	2.45	2	10	64	117
"	"	"	693	"	1.37	1.41	1.53	2.04	3	11	49	117
"	"	"	1368	"	1.24	1.37	1.48	1.88	10	8	52	117
$C_3H_6 + C_2H_4$	AC	293	101	$x_1 = .365$	12.1	13.3	13.5	28.7	10	11	*	127
"	"	"	"	$x_1 = .666$	12.3	12.3	11.4	22.6	0	7	*	127
"	"	"	"	$x_1 = .891$	12.3	10.8	8.94	16.2	12	37	32	127
$C_3H_6 + C_2H_6$	AC	293	100	$x_1 = .184$	7.25	9.48	10.0	27.1	31	38	*	127

APPENDIX 3 (Cont'd)
Comparison of Predictions of Binary Gas Adsorption

Adsorbates	Adsorbent	T, K	P kPa	Mole Fract.	Selectivity, s				Percent Error			Ref.
					Exp.	IAS	VSM	GM	IAS	VSM	GM	
$C_3H_8 + C_2H_6$	AC	293	100	$x_1 = .615$	7.80	8.51	7.92	19.0	9	2	*	127
"	"	"	"	$x_1 = .968$	4.71	6.88	5.40	10.2	46	15	*	127
"	"	333	100	$x_1 = .534$	6.92	7.79	6.78	28.1	13	2	*	127
"	"	"	"	$x_1 = .722$	6.61	7.38	6.14	22.3	12	7	*	127
"	"	"	"	$x_1 = .950$	4.69	6.62	5.08	13.6	41	8	*	127
$C_3H_8 + C_3H_6$	AC	298	101	$x_1 = .099$	0.89	1.32	1.13	2.03	49	27	*	84
"	"	"	"	$x_1 = .482$	0.86	1.31	0.99	1.94	52	15	*	84
"	"	"	"	$x_1 = .952$	0.98	1.29	0.90	1.82	32	8	87	84
"	"	293	100	$x_1 = .311$	0.96	1.00	0.96	1.94	4	0	*	127
"	"	"	"	$x_1 = .520$	0.95	0.95	0.95	1.90	0	0	99	127
"	"	"	"	$x_1 = .870$	1.08	0.95	0.94	1.81	12	13	68	127
$n-C_4H_{10} + C_3H_8$	AC	293	100	$x_1 = .132$	2.89	1.99	2.78	5.93	31	4	*	127
"	"	"	"	$x_1 = .563$	3.40	1.93	2.34	5.38	43	31	58	127
"	"	"	"	$x_1 = .737$	2.75	1.91	2.10	5.09	31	24	85	127
$C_2H_4 + CO_2$	AC	293	100	$x_1 = .881$	2.59	2.93	2.60	0.46	13	0	*	127
"	"	"	"	$x_1 = .454$	2.96	3.40	3.04	0.48	15	3	*	127
"	"	"	"	$x_1 = .224$	3.16	3.62	3.25	0.50	14	3	*	127
$i-C_4H_{10} + C_2H_4$	Z	298	138	$x_1 = .122$	2.96	1.82	6.23	1519	38	*	*	64
"	"	"	"	$x_1 = .516$	2.22	1.66	2.40	772	25	8	*	64
"	"	"	"	$x_1 = .822$	0.66	1.50	0.82	252	*	23	*	64
"	"	323	138	$x_1 = .186$	2.72	2.22	11.0	1894	18	*	*	64
"	"	"	"	$x_1 = .641$	1.36	1.80	2.30	744	33	69	*	64
"	"	"	"	$x_1 = .918$	0.60	1.65	0.59	149	77	1	*	64
"	"	373	138	$x_1 = .102$	3.24	3.43	5.67	2383	10	75	*	64
"	"	"	"	$x_1 = .662$	2.46	2.69	1.54	781	9	38	*	64
"	"	"	"	$x_1 = .983$	2.33	2.28	0.05	55.8	2	*	*	64
$n-C_4H_{10} + C_2H_6$	Z (5A)	308	6.4	$x_1 = .725$	1315	226	271	1333	*	*	*	50
"	"	"	"	$x_1 = .690$	183	230	312	1466	26	70	*	50
"	"	"	"	$x_1 = .344$	34	291	975	2710	*	*	*	50
$CO_2 + C_2H_4$	Z	323	138	$x_1 = .166$	1.80	1.71	2.09	1.98	5	16	10	64
"	"	"	"	$x_1 = .527$	1.68	1.77	1.74	1.92	6	4	14	64
"	"	"	"	$x_1 = .913$	1.10	1.87	1.51	1.84	72	36	67	64
$CO_2 + C_2H_6$	Z (5A)	308	13	$x_1 = .811$	23.2	20.0	20.2	0.78	14	13	*	50
"	"	"	"	$x_1 = .528$	41.9	19.5	21.2	0.78	53	49	*	50
"	"	"	"	$x_1 = .248$	40.9	19.8	22.0	0.77	52	46	*	50
$CO + N_2$	Z (10X)	144	101	$x_1 = .933$	5.15	5.05	5.37	11.0	2	4	*	32
"	"	"	"	$x_1 = .697$	7.92	5.18	5.35	21.9	35	32	*	32
"	"	"	"	$x_1 = .243$	15.0	5.27	5.32	44.9	65	64	*	32
$CO + O_2$	Z (10X)	144	101	$x_1 = .981$	6.32	20.7	17.7	1.32	*	*	79	32
"	"	"	"	$x_1 = .770$	10.7	25.4	28.2	1.34	*	*	88	32
"	"	"	"	$x_1 = .530$	33.0	32.6	36.7	1.36	1	11	96	32
$N_2 + O_2$	Z (5A)	144	101	$x_1 = .974$	3.61	6.01	5.90	0.05	66	63	*	32
"	"	"	"	$x_1 = .673$	6.66	6.82	7.98	0.06	2	20	*	32
"	"	"	"	$x_1 = .352$	21.2	7.58	9.80	0.08	64	54	*	32
"	Z (10X)	144	101	$x_1 = .960$	2.32	4.66	3.98	0.05	*	72	*	32
"	"	"	"	$x_1 = .686$	3.61	5.73	5.63	0.06	59	56	*	32
"	"	"	"	$x_1 = .223$	11.2	7.91	8.77	0.10	29	22	*	32
					Average Percent Error				35	41	80	