GAS SORPTION TECHNIQUES FOR CHARACTERIZING CARBON FIBER COMPOSITE MOLECULAR SIEVES

E. Loren Fuller, Jr., T. D. Burchell, and M. R. Rogers
Carbon Materials Technology, Metals and Ceramics Division
Oak Ridge National Laboratory, Oak Ridge TN 37831-6088

Introduction

Carbon Fiber Composite Molecular Sieves (CFCMS) materials are useful in sorption and separations systems.[1] The Oak Ridge National Laboratory (ORNL) has and extensive program to study the preparation and the chemical and physical characterization of these materials.[2]

Experimental

The experimental equipment and techniques are described elswhere.[2] The CFCMS sample used in the study was prepared by steam activation at ORNL.[1] and nitrogen sorption at 77K indicated an apparent surface area of 610 m^2gm^{-1}. Carbon dioxide and methane isotherms were acquired at 0, 30, 60 and 100 C to evaluate reactivity for these gases.

Results and Discussion

Carbon Dioxide isotherms are presented graphically in Figure 1. A large portion of the low pressure data is obscured in the lower left portion of the figure. To aid in evaluation of the processes and the energetics the data is recast in terms of the sorption energy, E(A), where $E(A) = -RT\ln[P/P(std)]$. The standard reference pressure, P(std) is taken to be one atmosphere by the normal thermochemical convention. The higher temperature isotherm is quite linear in the transformed coordinate system as noted in Figure 2. The lower temperature (higher coverage) data shows ever increasing deviation from linearity. However the smooth trends in the data are quite well fitted by second order least squares functions ($y = \text{intercept} + ax - bx^2$) These functions serve well as three parameter equations to fit the data and serve as excellent means of predicting sorption behavior in industrial applications. The temperature variation of the derived coefficients for carbon dioxide are presented in Figure 3.

Methane sorption isotherms show similar trends as presented graphically in Figures 4 and 5. The variation of the fitting parameters (Figure 6) are markedly different for methane sorption

There are several implications inherent in these studies. (1) The steam activation process seems to produce a large amount of surface and/or porosity. (2) The activated CFCMS has an appreciable affinity for carbon dioxide and methane over the temperature range studied. (3) The uptake of carbon dioxide is nearly twice that of methane at any given pressure and temperature. The pi bonds and polar functional groups on the CFCMS surfaces form a surface electrostatic field that attracts the polarizable carbon dioxide more strongly. (4) For most applications CFCMS has comparable reactivity to granular carbons. (5) The

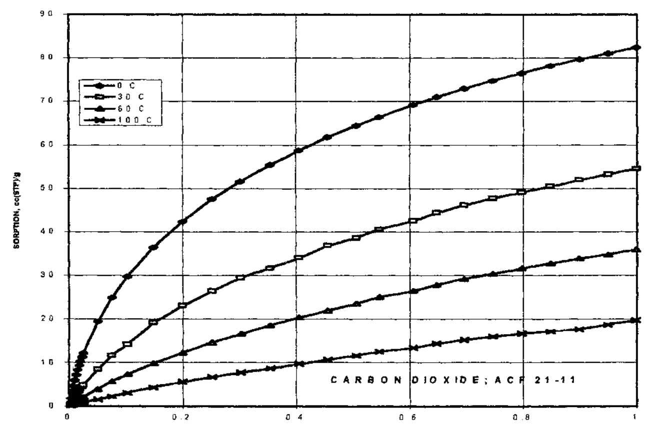

Figure 1. Carbon Dioxide on CFCMS

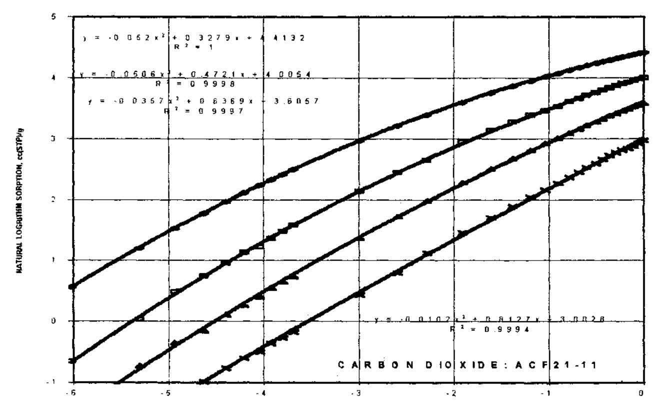

Figure 2. Exponential Plot: Carbon Dioxide.

favorable monolithic structure of CFCMS makes it better for most commercial and laboratory applications. (6) The exponential, Γ = Γ (std) exp[E(A)/RT], serves well to describe the data and provide prediction and correlation's for applications in separation and sorption applications.

separation applications. Gas phase sorption analyses are the most informative single method of obtaining the chemical and physical characteristics of porous materials. The results are valuable for determination of thermodynamics and mechanisms and for optimizing commercial processes..

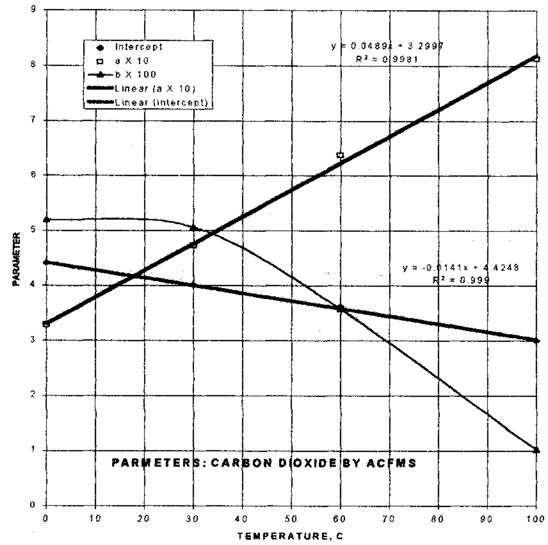

Figure 3. Fitting Parameters CO_2

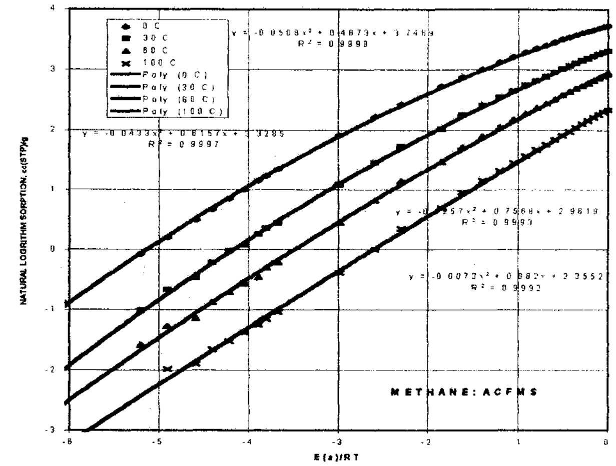

Figure 5. Exponential Plot: Methane

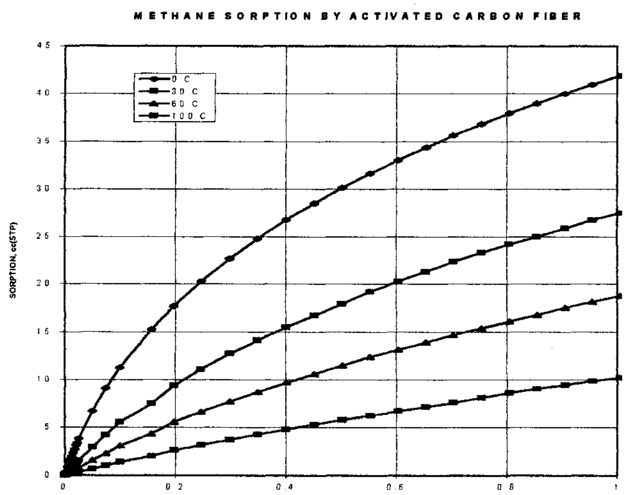

Figure 4. Methane Sorption on CFCMS

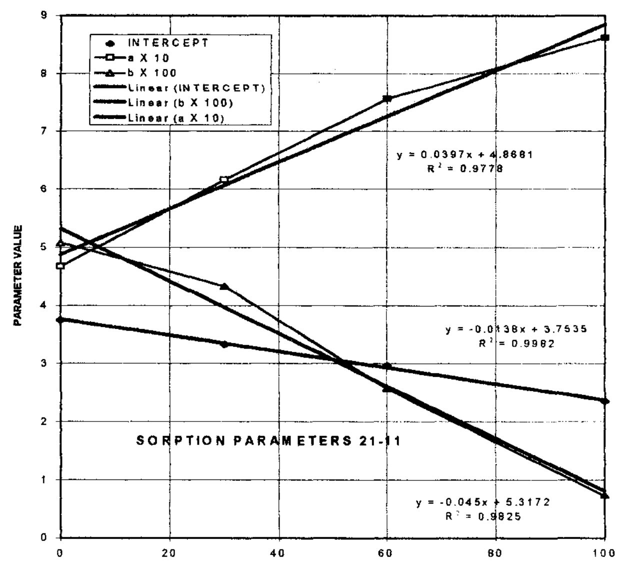

Figure 6. Fitting Parameters: CH_4

Conclusions

Carbon fiber composite molecular sieves are excellent sources of porous carbon materials with high reactivity and specificity require for most applications, with a structure that allows free passage of gas phases and does not physically deteriorate in long term sorption and

References

1. T. D Burchell and R. R. Judkins, Energy Conservation Management 37, 6 (1996)

2. E. L. Fuller, T. D. Burchell, M. R. Rogers, Carbon (in press) (1997)