Modeling the adsorption of pure gases on coals with the SLD model


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Abstract

The simplified local density/Peng–Robinson model (SLD-PR) was modified to improve its predictive capability when dealing with near-critical and supercritical adsorption systems of the type encountered in coalbed methane recovery and CO₂ sequestration. The goal was to develop efficient equation-of-state (EOS) computational frameworks for representing adsorption behavior, as well as to improve our understanding of the phenomenon. The ability of the modified SLD-PR to correlate accurately data for supercritical adsorption systems is demonstrated using adsorption measurements on activated carbon, Illinois #6 coal, Fruitland coal, and Lower Basin Fruitland coal. The results indicate that the modified SLD-PR model, which incorporates a modified repulsive parameter “b” for the PR EOS, is capable of modeling the adsorption of pure methane, nitrogen, and CO₂ at coalbed conditions. Inclusion of a slit geometry in the adsorbent matrix yields results superior to our previous two-dimensional EOS models for the adsorbates considered. The results also indicate that accounting for the adsorption surface structure within the SLD-EOS framework is effective in improving modeling capability for high-pressure adsorption phenomena. An explanation is offered as to why the adsorbed-phase densities are close to the EOS reciprocal co-volumes. Further, the model (a) generates direct estimates for the adsorbed-phase densities (which facilitate reliable prediction of absolute gas adsorption) and (b) readily describes the observed maximum in Gibbs-adsorption isotherms of CO₂ at the temperatures and pressures encountered in coalbeds.

Author Keywords: A. Coal; Activated carbon; B. High pressure; C. Adsorption properties; D. Gas storage

\[ A \]  
Surface area

\[ a \]  
Peng–Robinson attractive parameter

\[ a_{\text{ads}} \]  
Local Peng–Robinson attractive parameter for adsorbed phase
AAD  
Average absolute deviation

\( b \)  
Peng–Robinson covolume

\( b_{ads} \)  
Modified Peng–Robinson covolume for adsorbed phase

\( f \)  
Fugacity

\( i \)  
Dummy index

\( k \)  
Boltzmann constant

\( L \)  
Slit width; defined as the normal distance between the carbon planes

\( N \)  
Number of points in regression

\( N_A \)  
Avogadro’s number

\( n \)  
Amount in moles

\( n_{Gibbs} \)  
The Gibbs excess adsorption

\( P \)  
Pressure

\( R \)  
Universal gas constant

\( T \)  
Temperature

\( V_a \)  
Adsorbed-phase volume

\( V_{void} \)  
Void volume (system volume minus adsorbent volume determined by helium)

\( v \)  
Specific volume of fluid

WAAD  
Weighted average absolute deviation

WRMS  
Weighted root mean square deviation

\( z \)  
Normal position between carbon planes; zero at one plane

\( z' \)  
Dummy position variable: \( z' = z + \sigma_{ff}/2 \)

\( Z \)  
Compressibility factor

Subscripts
a  Adsorbed-phase property
b  Bulk property
c  Critical condition
ff  Fluid–fluid interaction
fs  Fluid–solid interaction
ss  Solid–solid interaction

*Greeks*

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\alpha$</td>
<td>Temperature dependent function for Peng–Robinson EOS</td>
</tr>
<tr>
<td>$\xi_{fs}$</td>
<td>Fluid–solid interaction parameter</td>
</tr>
<tr>
<td>$A_b$</td>
<td>Modification parameter to Peng–Robinson covolume</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Defined by Eq. (19)</td>
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<tr>
<td>$\mu$</td>
<td>Chemical potential</td>
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<tr>
<td>$\rho$</td>
<td>Density</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Particle diameter</td>
</tr>
<tr>
<td>$\sigma_{exp}$</td>
<td>Expected experimental uncertainty</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Fluid–solid potential function</td>
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