Virial Equation of State for Methane and Carbon Dioxide Binary Mixture using ab initio Calculation

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Intermolecular interaction between methane (CH4) and carbon dioxide (CO2) is important for the removing process of acidic components from natural gas. We calculated the potential energy surface of CH4 and CO2 dimer for 36 orientations using ab initio method. The fourth order virial equation of state (VEOS4) was developed using the developed intermolecular potential function and the Mayer sampling Monte Carlo simulations. Pressure-density diagram for temperature 300 K was predicted using the developed VEOS4 and the values were compared with experimental data of Esper et. al.. The results showed that the VEOS4 can explain the experimental data up to about 200 bar for any binary compositions at 300 K without any adjustment.