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REVIEWS

CO_2-H_2O和CO_2-H_2O-NaCl 体系的相平衡研究进展

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摘要 To study the feasibility of CO2 geological sequestration, it is needed to understand the complicated multiple-phase equilibrium and the densities of aqueous solution with CO2 and multi-ions under wide geological conditions (273.15—473.15K, 0—60MPa), which are also essential for designing separation equipments in chemical or oil-related industries. For this purpose, studies on the relevant phase equilibria and densities are reviewed and ana-lyzed and the method to improve or modify the existing model is suggested in order to obtain more reliable pre-dictions in a wide temperature and pressure range. Besides, three different models (the electrolyte non random two-liquid (ELECNRTL), the electrolyte NRTL combining with Helgeson model (ENRTL-HG), Pitzer activity co-efficient model combining with Helgeson model (PITZ-HG)) are used to calculate the vapor-liquid phase equilib-rium of CO2 -H2O and CO2-H2O-NaCl systems. For CO2-H2O system, the calculation results agree with the
experi-mental data very well at low and medium pressure (0—20MPa), but there are great discrepancies above 20MPa. For the water content at 473.15K, the calculated results agree with the experimental data quite well. For the CO2-H2O-NaCl system, the PITZ-HG model show
better results than ELECNRTL and ENRTL-HG models at the NaCl concentration of 0.52mol•L−1.
Bur for the NaCl concentration of 3.997mol•L−1, using the ELECNRTL and ENRTL-HG models
gives better results than using the PITZ-HG model. It is shown that available experimental data and the thermodynamic calculations can satisfy the needs of the calculation of the sequestration capacity in the temperature and pressure range for disposal of CO2 in deep saline aquifers. More experimental data and more accu-rate thermodynamic calculations are needed in high temperature and pressure ranges (above 398.15K and 31.5MPa).

关键词 CO_2-H_2O CO_2-H_2O-NaCl high temperature high pressure phase equilibrium density
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Progress in the study on the phase equilibria of the CO_2-H_2O and CO_2-H_2O-NaCl systems

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Abstract To study the feasibility of CO2 geological sequestration, it is needed to understand the complicated multiple-phase equilibrium and the densities of aqueous solution with CO2 and multi-ions under wide geological conditions (273.15—473.15K, 0—60MPa), which are also essential for designing separation equipments in chemical or oil-related industries. For this purpose, studies on the relevant phase equilibria and densities are reviewed and ana-lyzed and the method to improve or modify the existing model is suggested in order to obtain more reliable pre-dictions in a wide temperature and pressure range. Besides, three different models (the electrolyte non random two-liquid (ELECNRTL), the electrolyte NRTL

combining with Helgeson model (ENRTL-HG), Pitzer activity co-efficient model combining with Helgeson model (PITZ-HG)) are used to calculate the vapor-liquid phase equilib-rium of CO2 -H2O and CO2-H2O-NaCl systems. For CO2-H2O system, the calculation results agree with the experi-mental data very well at low and medium pressure (0—20MPa), but there are great discrepancies above 20MPa. For the water content at 473.15K, the calculated results agree with the experimental data quite well. For the CO2-H2O-NaCl system, the PITZ-HG model show better results than ELECNRTL and ENRTL-HG models at the NaCl concentration of 0.52mol•L－1. Bur for the NaCl concentration of 3.997mol•L－1, using the ELECNRTL and ENRTL-HG models gives better results than using the PITZ-HG model. It is shown that available experimental data and the thermodynamic calculations can satisfy the needs of the calculation of the sequestration capacity in the temperature and pressure range for disposal of CO2 in deep saline aquifers. More experimental data and more accu-rate thermodynamic calculations are needed in high temperature and pressure ranges (above 398.15K and 31.5MPa).

Key words CO_2-H_2O; CO_2-H_2O-NaCl; high temperature high pressure; phase equilibrium; density

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