

论文

Matlab用于氨法碳捕集化学物种模拟计算

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摘要:

为找到准确表述氨法碳捕集物种分布的方法, 阐述了氨法吸收捕集CO2的主要机理, 并根据氨水吸收CO2过程中各反应的平衡常数, 推导出氨水吸收CO2过程中产生的各主要物种的分布方程, 利用计算机软件Matlab获得了该体系的物种分布, 拟合了各主要物种分布率与pH方程, 利用该函数关系可以预测某物种浓度随pH值的变化趋势。为验证理论计算模型的准确性, 将模型计算数据与同等条件下实验数据进行比较, 计算结果与实验数据符合较好。模拟结果表明, 碳酸盐体系物种分布严重依赖于pH值的变化: pH值在7.8左右时, NH4HCO3含量最大; 而在pH=10.4时, NH2CO2NH4浓度最高; pH<6时, H2CO3占优; 而pH>12时, (NH4)2CO3则占主导地位, 可认为该计算模型是可信的。

关键词: 氨法; CO2脱除; 化学物种; 反应机理

Chemical species simulation in ammonia carbon capture by Matlab

Abstract:

In order to find the accurate expressions of ammonia carbon capture species distribution, The mechanisms of CO2 capture by using ammonia solution were introduced in this paper. The equations of the distribution of each species during carbon capture using ammonia solution were derived in accordance with the equilibrium constant of the reaction in the CO2 absorption process. Species distribution diagram was obtained using Matlab software. The chemical model of the relationship between the species distribution with pH was established. The trends of the concentration of a species with pH changing can be predicted using the simulating functions. In order to verify the accuracy of theoretical models, the model calculations and experimental data under the same conditions were compared, the calculated results are consistent with the experimental data basically. The simulated results show that the distribution of species in the carbonate system is heavily dependent on the pH changes; NH4HCO3 is the main component at pH of about 7.8, H2CO3 is dominant species at pH less than 6, NH2CO2NH4 has the highest concentration at pH=10.4; while the pH is greater than 12, (NH4)2CO3 accounts for a dominant distribution. It is considered that the calculation model is reliable.

Keywords: ammonia method; CO2 removal; chemical species; reaction mechanism

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