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硕士学位论文

基于 ASPEN PLUS 的煤气化模拟与有效能分析

Simulation and Exergy Analysis of Coal Gasification Using ASPEN PLUS

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摘 要

我国是以煤炭为主要能源的国家，随着中国能源安全问题日益严峻，煤化工已成为社会关注的热点并得到快速发展。近年来人们环保意识的强化要求企业大力开发煤炭清洁有效利用工艺。煤气化是煤化工清洁生产的核心工艺，寻求合适的煤气化工艺是解决我国能源问题的有效手段之一。为此，本文以煤气化工艺为对象，对其工艺流程模拟、系统能量衡算和有效能分析等问题进行了研究，构建煤气化工艺流程系统分析和设计的基本框架。

首先，针对固定床煤气化过程反应温度相对较低、反应产物复杂的特点，采用带 FORTRAN 气化动力学子程序的串联全混流反应器来代替 Gibbs 反应器，建立了基于 ASPEN PLUS 的固定床煤气化模型，结果表明该模型的模拟结果与实际固定床煤气化的运行数据吻合较好。并在该模型的基础上研究了串联釜数对碳转化率及出口温度的影响，研究得出随着釜数的增加，碳转化率和出口温度均更加接近于实际数据；在保证模拟精度的前提下，较少的釜数有利于减少计算量。

然后，在基于 Gibbs 自由能最小化平衡模型的基础上增加平衡温距，用于实现煤气化气流床工艺流程的模拟。并将两种典型的气流床气化炉——Texaco 水煤浆气化炉和 Shell 煤粉气化炉的工业数据对修正的平衡模型进行验证，结果表明该模型的模拟结果与实际工业数据吻合较好。并利用该模型考察了不同气化炉平衡温度选取对模拟结果的影响，以及重要操作参数——如氧气煤比和蒸汽煤比（水煤浆浓度）对气化炉出口温度和出口煤气组成的影响。

最后，针对不同煤气化工艺在 ASPEN PLUS 平台上的模拟结果，对各气化工艺进行系统能量衡算和有效能分析，识别各气化工艺系统中能量和有效能损失最大的环节及其原因，对比不同煤气化工艺流程的能量损失和有效能效率。结果表明固定床气化炉的有效能效率最高，Shell 粉煤气化炉次之，Texaco 水煤浆气化炉最低。

关键词：煤气化　ASPEN PLUS　能量衡算　有效能分析

Abstract

Chinese energy structure is coal dependent. With the energy crisis highlights, coal-chemical industry has become a hot topic and developed quickly. In recent years, for the strengthening of the environmental protection consciousness, it is necessary to develop the clean and effective utilization technology of coal. Coal gasification is the core technology for the clean production of coal-chemical industry. Suitable coal gasification process is an effective way to solve our energy problems. Therefore, in this thesis the process simulation, systematic energy balance and exergy analysis for coal gasification process are investigated, and then the basic framework of systematic analysis and design of coal gasification process are discussed.

Firstly, the fixed bed process of coal gasification is simulated. Because the reaction temperature of the fixed bed process is lower and the product is rather complex than other coal gasification process. The reaction kinetics of the gasification process is expressed by FORTRAN subroutine in RCSTRs, and then the RSCTRs in series are used to substitute the Gibbs reactor in the simulation. ASPEN PLUS is used as a platform to simulate the fixed bed for coal gasification process and the results of the simulation are in agreement with the actual fixed bed of the coal gasification process. The proposed model is applied to investigate the effect of the number of RCSTRs on carbon conversion and outlet temperature. The results show that carbon conversion and outlet temperature are closer to the actual data with the increase of number of RCSTRs. However, less number of RCSTRs helps to reduce the computation time. To keep the accuracy of the simulation results and less computation time of the simulation for coal gasification, it is suitable to use 6 RCSTRs in series to describe the fixed bed according to the results of the simulation.

Secondly, the entrained bed of coal gasification process is modeled by a balance model, which is based on the Gibbs principle of minimum free energy. To overcome the drawback of the balance model, the balance model is improved by the equilibrium temperature interval. Then the improved model is verified by the industrial data of two typical entrained bed gasifiers (Texaco gasifier and Shell gasifier). The results of the simulation are in agreement with the industrial entrained bed of the coal gasification process. The proposed improved model is applied to discuss the effects of equilibrium temperature for the simulation of different gasifiers. The effects of two important operating parameters such as the ratio of oxygen to coal and steam to coal

(CWS concentration) on the outlet temperature and gas composition of different gasifiers are considered.

Finally, with the ASPEN PLUS simulation results of different coal gasification process, systematic energy balance and exergy analysis are used for thermodynamic analysis of the coal gasification process. Energy loss and exergy destruction of the biggest segment and the reasons are analyzed. The energy loss and exergy efficiency of the different coal gasification process are also compared. The results show that the highest exergy efficiency is the fixed bed gasifier, the second is the Shell pulverized coal gasifier, and the worst is the Texaco CWS gasifier.

Key Words: coal gasification; ASPEN PLUS; energy balance; exergy analysis.

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