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工程热物理

燃煤烟气NO/SO2对CI/CI2形成过程的影响机制

王帅¹,高继慧¹,吴燕燕¹,汪细河²,吴少华¹

1. 哈尔滨工业大学能源科学与工程学院, 2. 武汉锅炉股份有限公司

摘要: 燃煤烟气中CI/CI2的形成过程对HgO的转化有重要影响。应用CHEMKIN软件包,在典型燃煤烟气温降速率下,通过化学动力学模拟的方法,研究了NO/SO2对CI/CI2形成过程的影响,主要得出以下结论:CI原子形成过程中OH是重要反应物,NO抑制CI原子形成的原因是由于NO会与CI原子生成反应竞争反应物OH。另外,NO与OH反应后的产物HONO会与CI原子反应生成HCI和NO2,从而进一步降低烟气中的CI原子浓度。SO2会大量消耗反应体系中的O原子,而O原子主要通过OH转化生成,O原子的大量消耗促进了OH转化为O原子,使得OH在CI原子形成过程中的作用被削弱,从而使SO2抑制了CI原子形成。CI2主要通过CI原子转化形成,因此CI原子的形成受到抑制将同时导致CI2形成过程受到抑制。

关键词: 燃煤烟气 CI/CI2 CHEMKIN 化学动力学

Effect Mechanism of NO/SO2 on CI/CI2 Formation in Coal-fired Flue Gas

WANG Shuai¹, GAO Ji-hui¹, WU Yan-yan¹, WANG Xi-he², WU Shao-hua¹

- 1. School of Energy Science and Engineering, Harbin Institute of Technology
- 2. Wuhan Boiler Co. Ltd.

Abstract: CI/CI2 formation plays a significant role in Hg0 conversion process in coal-fired flue gas. This paper presented data taken by kinetic calculations based on a packet of CHEMKIN. The calculations were executed at a typical quench rate of coal-fired flue gas. Effects of NO/SO2 on CI/CI2 formation were researched. The results showed that OH was an important reactant during CI atom formation. A part of NO react with OH, and compete with CI-atom formation reactions for OH. Thus, NO has an inhibitory effect on CI atom formation. Furthermore, the product of NO and OH, HONO, may react with CI atom to form HCI and NO2. These reactions promote the consumption of CI atom and finally cause a decrease in CI2 concentration. Reaction of SO2 and O atom promotes the formation of O atom that is obtained by the conversion of OH, and the effect of OH on CI formation is weakened. These reactions lead SO2 to inhibit the CI formation process. CI2 is formed mainly through the conversion of CI atom, so the inhibition to CI formation also causes an inhibition effect to CI2 formation.

Keywords: coal-fired flue gas CI/CI2 CHEMKIN chemical kinetics

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通讯作者: 高继慧

作者简介: 作者Email:

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