

能源和环境工程

## 水汽在燃煤PM<sub>2.5</sub>表面异质核化特性数值预测

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摘要

根据Fletcher经典异质核化理论建立数值实验平台, 将水汽在不可溶微粒表面异质核化临界过饱和度模拟结果与文献中实验结果进行了对比, 二者符合较好。在此基础上, 结合燃煤PM<sub>2.5</sub>物化性质及实测的表面张力与接触角数据, 数值预测了水汽及润湿剂溶液蒸气在燃煤PM<sub>2.5</sub>表面异质核化晶核形成自由能、临界晶核半径、成核速率、临界饱和度。结果表明, 添加润湿剂能降低临界晶核形成自由能, 减小临界晶核半径, 使成核速率急剧增加, 成核临界饱和度显著降低, 极大地改善了水汽的核化凝结能力, 但不同润湿剂的作用效果不同, 所选用的5种润湿剂中, 以SDS与Silanol w22效果最佳。

关键词 [燃煤PM<sub>2.5</sub>](#) [润湿剂](#) [Fletcher异质核化理论](#) [核化特性](#)

分类号

## Numerical prediction of water vapor nucleation behavior on PM<sub>2.5</sub> from coal combustion

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### Abstract

A numerical experiment platform was established according to Fletcher [DK]'s classical heterogeneous nucleation theory, and the critical saturation of water vapor nucleation on fine particles was simulated. The simulation results were compared with experiment results from literature. It was found that the simulated critical saturation agreed well with experiments. Based on the above calculation, the free energy of embryo formation, critical embryo radius, nucleation rate, and the critical saturation of water vapor (with and without wetting agent vapor) nucleation on PM<sub>2.5</sub> from coal combustion were numerically predicted, combined with the physical and chemical characteristics of PM<sub>2.5</sub> from coal combustion as well as the values of contact angle and surface tension tested by experiments. The results showed that the presence of wetting agent in water vapor could lead to lower free energy of embryo formation and smaller critical embryo radius, and cause the magnitude of nucleation rate to increase dramatically and the critical saturation of water vapor to decrease remarkably. Thus, with wetting agent in water vapor, the nucleation and condensation capabilities of water vapor were greatly enhanced, but the effects of the five wetting agents used were different, among them SDS and Silanol w22 were desirable choices.

**Key words** [PM<sub>2.5</sub> from coal combustion](#) [wetting agent](#) [Fletcher heterogeneous nucleation theory](#) [nucleation behavior](#)

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