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反应堆工程

# 压水堆核电站锆水反应微观机理

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摘要 压水堆核电站严重事故下的氢气行为研究需建立氢气生成的动力学模型，氢气生成反应的微观机理和反应速率常数是建立动力学模型的基础。本工作采用量子化学理论，应用量子化学软件包Gaussian03，在HF/3-21G理论模型上研究了压水堆严重事故下锆水反应的微观机理，并计算了反应速率常数。计算结果表明，锆水反应是由4个基元反应组成的总包反应。第2步基元反应的正反应速率最小，是锆水反应的速控步。在微观上研究减少或控制氢气生成的措施应从第2步基元反应入手。文中的计算结果偏于保守，以该方法建立起的动力学模型模拟压水堆核电站严重事故下的氢气行为是安全的。

关键词 压水堆 严重事故 锆水反应 反应机理

分类号



# Mechanism of Zirconium-Water Reaction for Pressurized Water Reactor

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**Abstract** A kinetics model should be constructed to study the hydrogen behaviorin the severe accidents for the pressurized water reactor (PWR). The reaction mechanisms and the release rate of hydrogen are the bases of kinetics model. The quantum chemistry software Gaussian03 was used to study the reaction mechanism of zirconium-water based on the HF/3-21G theory model of quantum chemistry. The reaction rate constants were also calculated. The results show that the reaction of zirconium-water is an overall reaction, which is divided into four elementary reactions. The reaction rate of the overall reaction was determined by the second elementary reaction due to its slowest reaction rate constant. It is concluded that the second elementary reaction should be the key elementary reaction to reduce the hydrogen generation. The conservative results reveale that it is safety to study the hydrogen behavior in the severe accidents for PWR using the kinetics model constructed in this presented method.

**Key words** pressurized water reactor severe accident reaction of zirconium-water reaction mechanism

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