行政院原子能委員會
委託研究計畫研究報告

非熱電漿處理柴油排氣之化學反應機制研究與模式建立

Non-Thermal Plasmas for Diesel Exhaust Treatment – Reaction Mechanism and Modeling

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受委託機關(構)：國立中央大學

計畫主持人：張木彬教授

研究參與人員：陳信良、吳義偉、林昇宏

核研所參與人員：李灝銘、陳永枝

聯絡電話：(03)4227151#34663

E-mail address: mbchang@ncuen.ncu.edu.tw

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中文摘要

本研究成功開發一個非熱電漿處理柴油引擎排氣之數值模式，本電漿化學模型包含 41 個物種、12 條電子碰撞反應及 176 條氣相反應。經比對其他研究之模擬結果，本模式之模擬結果與其趨勢相符，且結果相近，驗證本模式的適用性與正確性。

研究過程中採用敏感度分析法解析活性粒子對於 de-NO_x 效率之影響，結果顯示 N、O 和 OH 濃度與 de-NO_x 效率有密切關係，然其各自扮演不同角色，就 N 原子而言，其可藉由 $NO+N \rightarrow N_2+O$ 反應途徑還原 NO；O 原子藉 $NO+O+M \rightarrow NO_2+M$ 反應將 NO 氧化為 NO_2；OH 則將 NO 轉化為成 HNO_2 ($NO+OH+M \rightarrow HNO_2+M$)。

模擬結果顯示添加劑如 O_2 和 $H_2O_{(g)}$濃度之改變，對於 de-NO_x 效率具不同影響。當電漿反應器能量密度固定時，增加 O_2 濃度，有助於 NO 轉化成 NO_2；但增加 $H_2O_{(g)}$濃度對於 NO 和 NO_x 之去除均具負面效應。

本研究亦針對核研所實驗所得之柴油引擎尾氣組成進行案例分析，結果顯示當氣流溫度為 400 K 時，NO 可完全去除，NO_x 的去除效率約 20%；但當溫度升至 600 K 時，兩者之去除效率均為負值，亦即尾氣經處理後，會有額外的 NO 與 NO_2 生成。換言之，溫度太高時 de-NOx 效率反而下降。典型柴油引擎的尾氣溫度可達數百℃，因此電漿反應器必須放置在引擎後端適當位置（換言之，適當溫度的位置），以獲致較高之 de-NO_x 效率。

Abstract

A numerical model simulating NO_x removal from diesel engine exhausts has been successfully developed in this study. The plasma chemistry model includes 41 species involving in 12 electron-impact reactions and 176 gas-phase reactions, respectively. The results show good consistency between the simulation results reported in relevant literatures, confirming the validity of this model.

Sensitivity analysis is adopted to investigate the importance of chemically active species including N, O and OH for de-NO_x process. The concentrations of these chemically active species highly impact the de-NO_x efficiency. Simulation results indicate that nitrogen atom (N) plays the role as a reducing agent for the removal of NO. On the other hand, oxygen atom (O) can oxidize NO into NO_2. As for the hydroxyl radical (OH), it can convert NO into HNO_2.

The concentrations of O_2 and $H_2O_{(g)}$ additives show different effects for the performance of de-NO_x process. With a fixed specific energy density, increasing the O_2 content is beneficial for the oxidation of NO to NO_2; however, the increase in the $H_2O_{(g)}$ content would decrease the de-NO_x efficiency.

The simulation results show that increasing the temperature would affect 8/the de-NO_x efficiency dramatically. This result is quite important for the treatment of diesel engine exhaust because its temperature might be as high as several hundreds ^oC. A nonthermal plasma reactor should be placed at an appropriate location downstream of diesel engine to ensure its better performance.