

## 열/화학적 에너지 평형을 고려한 통합 연료 개질 시스템의 수치적 연구

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### Numerical Analysis of Integrated Fuel Processing System Considering Thermo-Chemical Energy Balance

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This paper focuses on a systematic configuration of steam reforming fuel processor, particularly designed for small and medium sized hydrogen production application. In a typical integration of the fuel processor, there exist significant temperature gradients over the entire system which has negative effect on both catalyst life-time and system performance. Also, the volumetric inefficiency should be avoided to obtain the possible compactness for the commercial purpose. In the present work, the computational analysis will be performed to gain the fundamental insight on the transport phenomena and chemical reactions in the reformer consisting of preheating, steam reforming (SR), and water gas shift (WGS) reaction beds in the flow direction. Also, the fuel processing system includes a top-fired burner providing necessary thermal energy for endothermic catalytic reactor. A fully two-dimensional numerical modeling for a integrated fuel processing system is introduced for in-depth analysis of the heat and mass transport phenomena based on surface kinetics and catalytic process. In the model, water gas shift reaction and decomposition reaction were assumed to be at equilibrium. A kinetic model was developed and then computational results were compared with the experimental data available in the literature. Finally, the case study was done by considering the key parameters, i.e. steam to carbon (S/C) ratio and temperature. The computer-aided models developed in this study can be greatly utilized for the design of advanced fast-paced compact fuel processors research.

**Key words** : Integrated Fuel Processor(통합 개질기), Steam Reforming Reaction(수증기 개질 반응), Water Gas Shift Reaction(수성가스 전이반응), Hydrogen Production(수소 생산), Computational Analysis(전산 해석)

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## 질소가 포함된 탄소나노튜브의 질소 원자를 이용한 이중 금속 촉매 제조 및 그의 수소 발생 촉매 특성 분석

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### Facile Fabrication of Bimetallic Catalysts via Selective N atoms of N-Doped Carbon Nanotubes and Their Superior Catalytic Activities for Hydrogen Generation

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One-dimensional nanostructures such as carbon nanotubes could be ideal templates for formation of metallic nanoparticles. Furthermore, bimetallic component nanoparticles have recently been interesting issues for having high catalytic activity. This work provides both a facile method to synthesize bimetallic catalysts via N atoms of carbon nanotubes and also a picture about how to design the optimal bimetallic catalyst for hydrogen generation from the hydrogen storage material. In principle, the ratio of one component to another component could be generically extended to fabricate the high-performance bimetallic catalysts on host nanostructures. Indeed, we demonstrate that the bimetallic catalyst composed of the optimum composition results in the excellent hydrogen generation property from an aqueous borane ammonia solution, thus being capable of satisfying the Depart of Energy in USA target required for many advanced applications even with the small amount of our bimetallic catalysts attached onto the N-doped carbon nanotubes. This high hydrogen generation rate is found to be attributed to the optimal distance between active Pt and cheap Ni atoms for effective hydrogen generation.

**Key words** : Bimetallic Catalyst(이중금속촉매), Carbon Nanotube(탄소나노튜브), Ammonia Borane(암모니아 보레인), Hydrogen Generation(수소발생)

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