

***Computational fluid dynamics study on the decomposition of ammonia in a selective porous membrane***

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The development of alternative technologies for the removal of gas pollutants at the integrated gasification combined cycle is considered as an important aspect for the environmental friendliness of energy production. During coal gasification, N<sub>2</sub> contained in coal is converted to NH<sub>3</sub>. As much as 50% of the ammonia in the fuel gas can be converted to nitrogen oxides in the gas turbine when the gas is combusted to produce power. The temperatures encountered in these power generation systems are far above the temperature range for conventional chemical or physical absorption systems. Water based NH<sub>3</sub> removal, for example, involves cooling the gas to about 120°C. To meet emission standards while maintaining the thermal efficiency of the process, the fuel gas should be cleaned at high temperature and pressure. At these conditions, decomposition seems to be the only solution for NH<sub>3</sub> removal. The application of a high temperature catalytic membrane reactor process integrally linked with the gasification process appears to offer a unique route toward an efficient and cost effective method of removing the NH<sub>3</sub> from coal gasification gas streams. This is because membrane based separation systems possess low energy consumption, reduced environmental impact, low costs of maintenance, space and weight efficiency and are relatively easy to install and operate. Chemical conversion and product purification take place in the same device. By the selective permeation of H<sub>2</sub> through the membrane, it is possible to achieve significant enhancement of NH<sub>3</sub> conversion. However due to the nature of the process the performing of precise experimental measurements at the direct vicinity of the selective membrane is relatively difficult and, thus, in order to investigate thoroughly the behaviour of such selective membranes, numerical methods can be used. Especially for axis-symmetric flows these methods are usually following a 1-D approach. The present work, proceeds one step further by examining the operation of a selective membrane, used for the decomposition of NH<sub>3</sub>, under a 2-D axisymmetric CFD approach where the flow field, the chemical reactions and the selective porous membrane behaviour are being modeled and computed. The presence of the selective membrane was modeled as a porous medium with predetermined pressure drop and permeance behaviour. For this reason a structured computational grid was created and the flow field was computed as compressible, laminar and steady. At the inlet of the computational domain the mass flow was prescribed under the Hagen-Poiseuille profile and the static temperature was equal to 873K. The working fluid was a mixture of ammonia, hydrogen and nitrogen with prescribed mass fractions at the inlet of the computational domain. At the outlet the static pressure was set equal to ambient pressure. Due to the fact that the problem could be treated as axisymmetric only a cross section of the geometry was computed. The main target of this effort was to obtain a more detailed view of the flow field and the calculation of the decomposition

of ammonia in comparison with previous 1-D modeling approaches and, thus, to evaluate the advantages and disadvantages of each method.

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