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Outline of Thesis for the Degree of Doctor of Enginering

A Study on Structured Microreactor for Process Intensification of Dry Reforming of Methane

Anthony Basuni Hamzah

Dry reforming of methane (DRM) offers a potential to overcome climate crisis by realizing carbon capture and storage or biomass-based greenhouse gas utilization and storage of intermittent renewable energy in the form of hydrogen. To address the issues of DRM such as high energy requirement and coking, this thesis investigated the process intensification of DRM in terms of reactor structurization rather than catalyst material selection or process design. The catalytic wall-plate microreactor (CWPMR) was chosen as a base design, which consists of a blow-through channel and a micro catalytic packed bed on a plate to attain low pressure loss and higher catalyst loading, respectively. Novel CFD modeling approaches were proposed and utilized to design the effectively structured CWPMRs, which significantly outperformed the original CWPMR. Presented thesis is divided into 6 chapters as follows.

Chapter 1 Introduction discusses motivation as well as social, technological, and industrial relevances of the research behind this dissertation. Systematic comparisons are shown to evaluate the feasibility of process-intensified DRM to solve the problems above. In the end of this chapter, an outline is given to briefly summarize the structure of the dissertation.

Chapter 2 Computational Fluid Dynamics modeling of packed bed reactor introduces the CFD modelling of packed bed and its underlying transport phenomena theories. Implementation and validation for different continuum and particle-resolved approaches are described. Empirical correlation-based and pseudo-particle resolved (PPR) continuum CFD approaches are newly established for packed bed modeling.

Chapter 3 Implementation of CFD approaches in tubular and shaped-channel packed bed presents porosity distribution and momentum, mass and heat dispersion modelling of CFD numerical study of tubular and shaped channel packed bed. The CFD approaches proposed in Chapter 2 are compared and validated using the detailed geometry-resolved CFD approach and experimental data in the literature. It is shown that the given approaches attains sufficient accuracy. It is found that directionally-averaging technique in the PPR approach can provide robust and straightforward analysis on packed bed porosity structure.

Chapter 4 Numerical and experimental validation studies of CWPMR presents the CFD study of the original design of CWPMR, which is validated with experimental results. The procedure established in Chapter 3 is employed to elucidate internal transport phenomena and identify the root cause of the sub-optimal performance of the reactor. Notwithstanding highly-porous packed bed catalytic layer, poor diffusivity of reactant and resultant transport phenomena resistances and imbalances in this layer are found to severely impair the reaction performance.

Chapter 5 Structurization of CWPMR presents the study on the internal structurization of CWPMR to mitigate the severe flow stratification in the catalytic layer. Further, optimal configuration and flow structuring are achieved by the internal structure dimension parametrizations. It is shown that the proposed new design can attain up to 17% higher conversion than that of the original CWPMR, which is confirmed by the experimental results.

Chapter 6 Conclusion, outlook, and further direction of study summarizes the achievements in this study. Perspectives of further study in multiple aspects are also put forward.