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Guozhao Ji, Ming Zhao, Geoff Wang

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1 Computational fluid dynamic simulation of a sorption-

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4 Guozhao Ji^a, Ming Zhao^{a,*} and Geoff Wang^b

⁵ ^a School of Environment, Tsinghua University, Beijing 100084, China

⁶ ^b School of Chemical Engineering, the University of Queensland, Brisbane, Qld 4072,

7 Australia

8 * Corresponding Author. Tel: +86 10 62784701. Email: ming.zhao@tsinghua.edu.cn

9 Abstract

To understand the reaction process of methane steam reforming in a sorption 10 enhanced membrane reactor (SEMR), a computational fluid dynamic (CFD) model 11 was developed to simulate the methane (CH₄) steam reforming in a palladium-based 12 membrane reactor using a Ni-based catalyst and Na₂ZrO₃ CO₂ sorbent. The CFD 13 14 model gained the insight of details in the reactor which could not be obtained by experiment. With the detailed information, this model detected the difference of 15 reaction kinetics and fluid dynamic conditions in a SEMR and a traditional membrane 16 reactor (MR). The comparison suggests that sorption-enhanced membrane reactor not 17 only decreases CO₂ fraction, but also improves hydrogen (H₂) production by 18 increasing reaction rates, CH₄ conversion and H₂ yield. The poisoning effect of carbon 19 monoxide (CO) on the palladium membrane can also be minimized by reduced CO 20

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