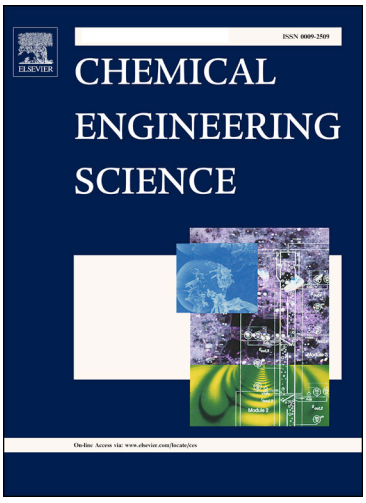

Molecular dynamics simulation of methane hydrate formation on metal surface with oil

Mucong Zi, Daoyi Chen, Guozhong Wu

PII: S0009-2509(18)30448-2
DOI: https://doi.org/10.1016/j.ces.2018.06.070
Reference: CES 14344

To appear in: *Chemical Engineering Science*

Received Date: 9 January 2018
Revised Date: 13 June 2018
Accepted Date: 25 June 2018

Please cite this article as: M. Zi, D. Chen, G. Wu, Molecular dynamics simulation of methane hydrate formation on metal surface with oil, *Chemical Engineering Science* (2018), doi: https://doi.org/10.1016/j.ces.2018.06.070

Molecular dynamics simulation of methane hydrate formation on metal surface with oil

Mucong Zi [†,‡], Daoyi Chen[†,‡], Guozhong Wu[*,†,‡]

[†] Division of Ocean Science and Technology, Graduate School at Shenzhen, Tsinghua University, Shenzhen 518055, China

[‡] School of Environment, Tsinghua University, Beijing 100084, China

* Corresponding Author

E-mail: w.guozhong@sz.tsinghua.edu.cn

Tel: +86-0755-26030544

ABSTRACT

Microsecond molecular dynamics simulations were performed to investigate the methane hydrate formation on smooth and rough metal surface covered with water, light oil, and heavy oil with asphaltenes, respectively. The growth and crystallization of methane hydrates were characterized by the four-body order parameter and the face-saturated incomplete cage analysis. Results highlighted the priority for hydrate growth inside the groove of rough metal surface, from which the hydrate grew upwards to the outside of the groove and then to the water-gas interface. It clearly