Development of a New Library in OpenFOAM for Simulations of Reacting Flows with Surface Reactions

Danh Nam Nguyen[1], Jae Hun Lee[1], Hae Won Seo[2], Hyung Jun Ahn[2], Chun Sang Yoo[1*]

[1]Department of Mechanical Engineering, UNIST

Unist-Gil, Ulsan, 44919, Republic of Korea

[2]Hydrogen and Low Carbon Energy R&D Lab, POSCO Holdings

Cheongam-ro, Pohang, 37673, Republic of Korea

Abstract

Recently, hydrogen (H_2) production has gained significant attention since H_2 has emerged as an effective and clean alternative to fossil fuels, especially in the power generation sector, to meet carbon neutrality by 2050. While many experimental studies on the H_2 production from catalytic ammonia (NH_3) decomposition have been conducted, the numerical investigation on this field is limited due to lacking sufficient computational fluid dynamics (CFD) package for public use to handle surface reactions occurring in catalytic processes. In that context, we developed a new surface chemistry library in OpenFOAM (OF) platform, a free and robust open-source CFD package, to provide a sufficient CFD tool for researchers working on this field and combustion community since there is no such library officially available in OF. The developed library can handle several types of typical surface reaction rate models consisting of the basic Arrheninus form, sticking coefficient, and surface coverage dependence models. It was validated against experimental data and previous studies by performing two dimensional (2-D) simulations of fixed packed-bed catalytic reactors. The results showed a good agreement between predicted and benchmark data, implying that our implementation is proper, and our developed library can be used for simulations of catalytic processes with the utilizations of detailed micro chemical kinetic models.

*Correspondence to: csyoo@unist.ac.kr