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Coach	**Supervisor(s)**	**Funding**
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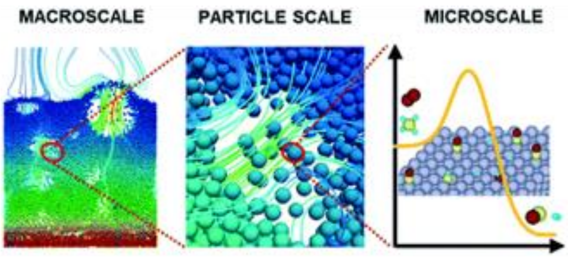
Study on Methane pyrolysis using Computational fluid dynamics coupled with the Discrete Element Method

Aim

This thesis aims to provide more insight into the thermocatalytic decomposition of methane known as methane pyrolysis using solid catalyst particles in a gas-solid fluidized bed reactor. The study of the process using Computational Fluid Dynamics coupled with the Discrete Element Method (CFD-DEM) employing an Eulerian-Lagrangian approach, coupled with microkinetic reaction mechanisms, will shed light on the process and possible approaches for process intensification.

Justification



Different scales of the thermocatalytic decomposition of methane with solid catalyst

Hydrogen production, particularly through methane pyrolysis, is a key energy source for achieving zero emissions in Europe by 2050 under the Paris Agreement[1]. This process, which converts methane into hydrogen and solid carbon, offers lower costs by leveraging the carbon market, compared to other methods like steam methane reforming and water splitting that are costly and environmentally challenging. However, methane pyrolysis, while promising, has its own limitations in productivity, process uncertainties, and operational challenges due to carbon formation [2].

To overcome these challenges and enhance the production rate and efficiency, there is a need for optimization and further studies for the development of this process. The proposed master thesis seeks to address critical challenges in the methane pyrolysis for carbon nanomaterials and hydrogen production through CFD studies. The thesis will aim to bridge this gap by employing CFD simulation as a powerful tool to present a comprehensive study of the pyrolysis reactor and help with development of new design and technologies for this process. The proposed method combines Computational Fluid Dynamics (CFD) to study fluid behaviour with Discrete Element Method (DEM) for modeling particle movement and interactions in simulations. It also accounts for inter-phase interactions by linking momentum, heat, and mass transfer between phases in the simulation, providing a detailed and dynamic portrayal of the system. By using simulation studies, the research will provide essential insights and data for optimizing process conditions, particularly for maximizing the production as a CFD guided design.

Program

1. Literature review on the simulation approaches to methane pyrolysis.
2. Study of the fluidized bed reactors
   - Get acquainted with open-source software OpenFOAM and our in-house solvers catchyFOAM [3] and catchy-CFDEM [4]
   - Performing non-reactive and reactive CFD simulation of the process.
3. Validating the simulation results, post-processing of the results and investigating the effects of various parameters.

References

[1] European Climate Foundation, https://europeanclimate.org/net-zero-2050/.
[2] J. Raza, A. et al., Renewable and Sustainable Energy Reviews. 2022, 168.
[3] L. A. Vandewalle, et al., Energy & Fuels. 2021, 35.
[4] F. Wéry, et al., Chemical Engineering Journal. 2023, 455.

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