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CFD coupled mixing cell network modelling of slurry-phase reactor for vacuum residue hydrocracking

Praneet Mishra [a], Tahmeed Aijaz [b], Ashutosh Yadav [a,*]

[a] Department of Chemical Engineering, Indian Institute of Technology, Jammu 181221, J&K, India
[b] Department of Food Technology, IUST Awantipora, Kashmir 192122, J&K, India

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ABSTRACT

The escalating global demand for light-end products, including low-sulfur diesel and gasoline, has prompted refineries to undergo strategic modernization efforts. This involves optimizing processes to efficiently handle heavy crude oil and transform it into high-value, user-friendly products. Slurry-phase hydrocracking is an advancing technology to enhance the production of these essential fuels, aligning with evolving market requirements and environmental regulations. The work encompasses crucial aspects such as potential hydrocracking reactions, lump kinetics, and product yield, all meticulously examined through the modelling and simulation of the Slurry-Phase Reactor (SPR). This study highlights the feasibility of integrating Computational Fluid Dynamics (CFD) simulation with Mixing Cell Network (MCN) modelling of SPR to account back-mixing effects with different lump reaction kinetics. CFD proves its importance for studying SPRs' local hydrodynamics as compared to experimental investigation. Local level hydrodynamics of a lab-scale SPR were investigated and effectively utilized in MCN modelling. It encompasses the validation of product yield distribution derived from the developed MCN and Axial Dispersed Model (ADM) with experimental data and it also includes the comparison of hydrodynamic parameters reported in existing literature. An average absolute error of 3.85 % in the product yield was obtained between experiments and the developed MCN model. The residue conversion of 82.84% was achieved, followed by 29% of asphaltene, to explore insights into physicochemical properties characterized by product distribution. Further, the detailed product distribution and mass yield of each lump kinetic model was reported. Sensitivity analysis was conducted to investigate the impact of dispersion correlation on conversion and the effect of initial bubble size on hydrodynamics and reaction conversion in the SPR.

1. Introduction

The depletion of conventional light crude oil reservoirs and the continuously growing demand for light-end products, such as gasoline, ultra-low sulfur diesel, and kerosene, have attracted increased attention toward developing alternative energy sources [1]. Liquid fuels play a crucial role as an energy medium for petrochemical feedstock and transportation, as evidenced by recent state-of-the-art developments [2]. Technological advancements, such as carbon rejection and hydrogen addition, are employed to enhance the production of liquid fuels. Processes like catalytic cracking, coking, and visbreaking fall under carbon rejection technology, while hydrocracking and hydrotreating are classified under hydrogen addition technology [3]. Hydroprocessing is primarily utilized to convert heavy fractions into light fractions by increasing their hydrogen-to-carbon ratio, thereby enhancing the value of the products through an excess of hydrogen. The Slurry-Phase Reactor (SPR) represents an evolving technology for heavy oil upgradation. Widely employed due to its simple design, minimal pressure drop, ease of maintenance, isothermal operational conditions, operational flexibility, and reduced propensity for coke formation [4]. The SPR demonstrates the ability to treat contaminated feedstock with a low catalyst concentration, achieving high conversion efficiency exceeding 90 % [5]. Within the SPR, the heaviest fraction undergoes thermal cracking, concurrently accompanied by hydrogenation reactions to mitigate coke formation within the reactor. The local

Abbreviations: AR, Aromatics; AS, Asphaltenes; 5-Pham, Five lump kinetic model of Pham et al., (2022) [5]; 5-Sanchez, Five lump kinetic model of Sanchez et al., (2005) [31]; 4-Felix, Four lump kinetic model of Felix et al., (2019) [30]; MD, Middle Distillate; Naph, Naphtha; RE, Resins; SA, Saturates; VGO, Vacuum Gas Oil; VR, Vacuum Residue.

* Corresponding author.
E-mail address: ashutosh.yadav@iitjammu.ac.in (A. Yadav).

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