

Performances of a non-conventional methanol reactor

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Methanol, a liquid-phase fuel, is increasingly recognized as a valuable energy carrier due to its high energy density, compatibility with the existing transport and storage infrastructure, and it is a valuable raw material in the chemical industry. In 2020, the global methanol production was approximately 110 million metric tons: around 80% of the total was used in the chemical industry while, the remaining 20% was utilized as a fuel source [1]. Projections indicate a significant expansion in the worldwide methanol demand, potentially reaching 500 million metric tons by 2050, driven by both energy applications and chemical manufacturing [1]. The core of methanol synthesis is the reactor: several configurations have been described in the literature and are commercially available, with defined advantages and disadvantages [2].

In this work, a non-conventional reactor configuration of shell-and-tube type, with catalyst on the tube-side and coolant on the shell-side, and with the shell-side split into two zones (double-zone methanol reactor - DZMR) is proposed to evaluate its performances in methanol synthesis. Two fractions of coolant are fed into both shell-side zones, which are hydraulically connected via a peripheral annular duct that surrounds the tube bundle and that is defined by the shell wall. Specifically, this annular duct is present only in the second shell-side zone. The second fraction of coolant is hence introduced into this peripheral duct so that this secondary coolant stream flows only through the second shell-side zone. Overall, the proposed configuration allows for having globally non-isothermal conditions on the coolant-side to better exploit thermodynamic and kinetic benefits.

The DZMR is modelled in Aspen Plus while syngas is used as the feed and diathermic oil (Therminol 66) is used as the coolant. The catalyst ($\text{Cu/ZnO/Al}_2\text{O}_3$) is loaded into tubes where the syngas is flowing. Different operating schemes are investigated and compared in terms of methanol productivity, yield, conversion and coolant consumption.

Results show that when the first shell-side zone works in non-isothermal conditions and the second shell-side zone works in isothermal conditions, methanol production (328 tonMeOH/year), yield and conversion (41%) are the highest, and the required coolant flowrate is the smallest (6223 kg/h). The obtained performances are better compared to an existing shell-and-tube reactor cooled by boiling water and in once-through configuration.

Keywords: *methanol synthesis, double-zone methanol reactor, modelling, simulation*

References [1] E. Anetjarvi, E. Vakkilainen, K. Melin, *Energy* (2023) 127202; [2] Manenti, F., Bozzano, G., *Progress in Energy and Combustion Science*, (2016) 56, 71-105