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Process Simulation of Upgraded Process for Catalytic Synthesis of Methanol

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SPOKE, WP E TASK DI APPARTENENZA

Spoke 8 - Circular economy in agriculture through waste valorisation and recycling

Task 8.2.2 - Thermochemical techniques to produce electricity/heat and advanced fuel from wastes

L'attività di ricerca incrementerà, da TRL-4 a 6, la maturità del processo Biomass to Liquids (bio-metanolo) per applicazioni di taglia < 50 MW LHV. Le principali innovazioni per l'avanzamento di tecnologie BtL, basate su gassificazione di biomassa lignocellulosica, riguardano lo sviluppo di configurazioni ad hoc per i gassificatori, le unità di trattamento del syngas e i reattori di sintesi catalitica dei biofuel; il design e l'integrazione di processo devono essere ottimizzati in funzione delle caratteristiche della biomassa e della taglia limitata dalla filiera di approvvigionamento, al fine di ottenere impianti di ridotta complessità, ma anche efficienti e sostenibili.

ABSTRACT/INTRODUZIONE/BACKGROUND E SCOPO DEL LAVORO

Methanol synthesis is a crucial process in the chemical industry, and its importance is increasing due to its centrality in the ecological transition era. This work focuses on showcasing the upgraded process for methanol synthesis from biogas sources and the development of its digital twin. The process has been upgraded with the design of a dedicated catalyst tailored for small-scale and non-conventional operating conditions. These modifications enabled the refurbishing of unit operations for higher TRL pilot tests. In particular, a field kinetic analysis tool (by HIDEN) and a 3D printer component (by AddCat) have been acquired in a customized nature to be fully integrated with the existing reactors and analytics. The process demonstrates an increase in the methanol yield compared to the pre-existing condition. Furthermore, a new process simulation was developed to study the behavior of the upgraded system under varying operating conditions. This simulation allows for a more detailed exploration of the process performance, facilitating further improvements and scale-up.

MATERIALI/METODI/WORKFLOW CON EVENTUALI GRAFICI/FIGURE/TABELLE/IMMAGINI

The synthesis reactor has been modeled as a multi-tubular heat exchanger with a reactive section inside the tube bundle with a first principle approach. Temperature, pressure and mass fraction profiles are estimated.

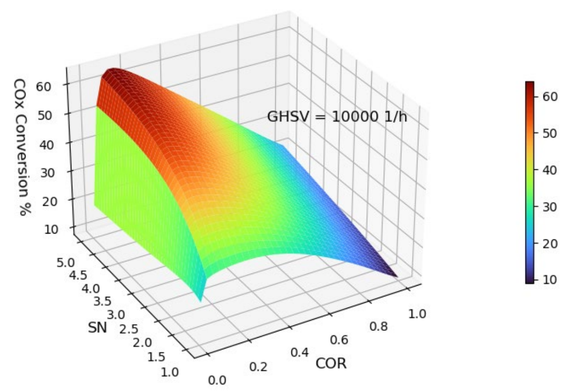
$$\frac{d\omega_i}{dz} = \frac{\varepsilon S_{int}}{m} MW_i \rho_{cat} (1-\varepsilon) \sum_j^{NR} \nu_{i,j}\, r_j$$

$$\frac{dT}{dz} = \pi d_t U (T_s - T) + \frac{\varepsilon S \sum_j^{NR} \Delta H_j^r\, r_j}{m C p_{mix}}$$

$$\frac{dT_s}{dz} = \frac{\pi d_t U}{C p_{oil} m_{oil}} (T - T_s) N_t$$

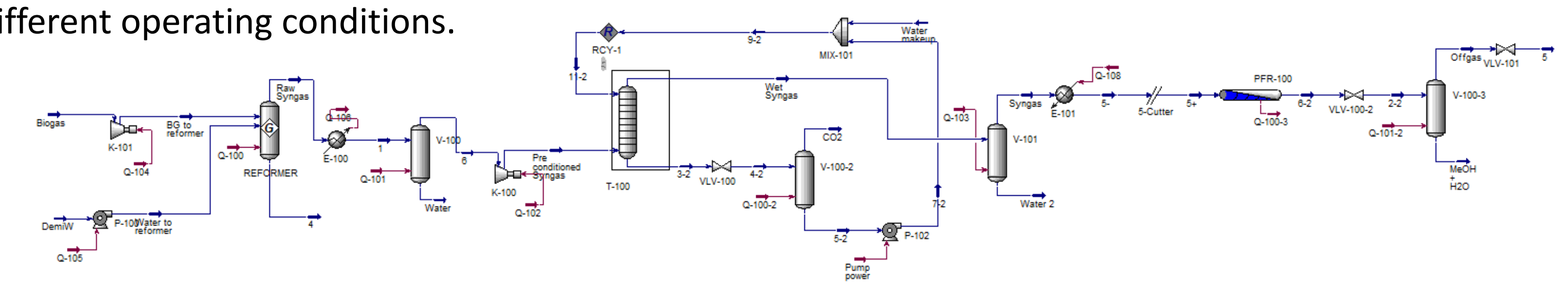
$$\frac{dP}{dz} = -\left(1.75 + 150\left(\frac{(1-\varepsilon)}{Re}\right)\right)\frac{u^2 \rho_g}{d_p}\left(\frac{(1-\varepsilon)}{\varepsilon^3}\right)$$

Definition of optimal operating condition and reactor design based on source quality and quantity.



RISULTATI CON EVENTUALI GRAFICI/FIGURE/TABELLE/IMMAGINI

The site has been refurbished with a kinetic-analysis tool (by HIDEN) and a 3D printer component (by AddCat). A process simulation of the plant has been developed to analyze the performance of the upgraded system under different operating conditions.



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