user story

Applying *kinetics* to Simulate Fischer Tropsch

Hydrocarbon fuels from CO/H_2

SUMMARY

- Detailed microkinetics model (with novel features including surface coverage profiles) coupled with advanced parameter estimation techniques used to study FT synthesis on $Co/\gamma-Al_2O_3$.
- Great agreement with experimental data

The Fischer–Tropsch (FT) synthesis is a key process in the gas to liquids technology that enables synthetic fuels and lubricants production. This is of increasing importance given the scarcity and cost of conventional petroleum-derived hydrocarbons. Due to the large number of reacting species, readsorption and conversion of primary products, difficulties in measuring surface intermediates, and coverage-dependent reaction rates, detailed mechanistic modelling of the FT synthesis is highly complex.

THE CHALLENGE

To devise a chemical characterisation of the FT synthesis with semi-automated estimations for the large number of free parameters (i.e. pre-exponential factors and activation energies) that are required in order to correctly predict the overall behaviour of the system.

SOLUTION

A detailed microkinetic description of the FT reactions on a $Co/\gamma-Al_2O_3$ catalyst over the full range of syngas has been developed and coupled with a two-stage parameter estimation method based on a quasi-random global search followed by a local optimisation technique.

RESULT

Figures 1 (C1 compounds) and 2 (Olefins) show a good agreement between the model and the experimental data. Figure 3 (Below) presents a unique feature of this model, the fractional surface coverage profiles. These are key parameters for a correct modelling of the FT synthesis.

Figure 1

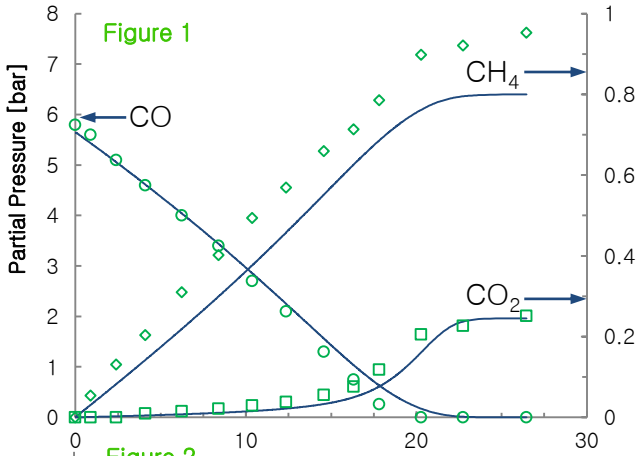


Figure 2

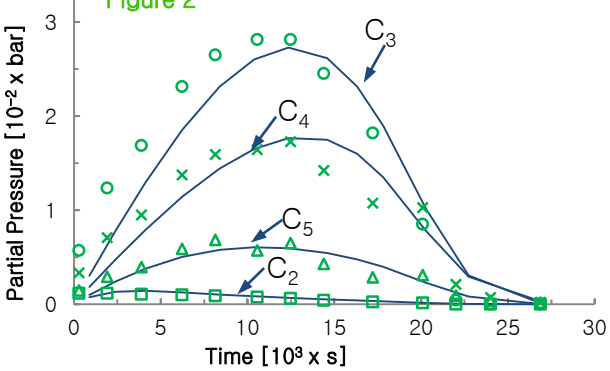
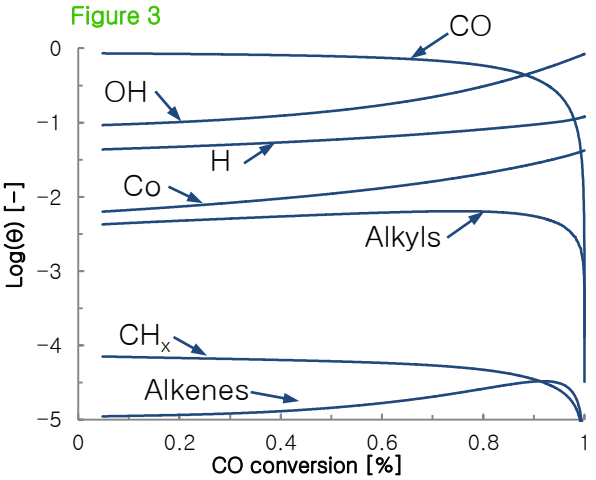


Figure 3



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