

## WP4 TASK 4.1

# Dynamic modelling of synthesis processes

## ABSTRACT

The objective of WP 4.1 was to develop dynamic process models in Aspen Dynamics to effectively handle variations in electrolytic hydrogen input in green methanol and catalytic methanation processes. Based on prior modeling experience the modeling was divided into two parts, a crude methanol production (a mixture of methanol and water from methanol synthesis) and methanol purification. By this way, only the crude methanol process needs to be dynamically modeled. The results show that the minimum load of the model is around 20%, with maximum allowable ramping rates of 3.25%/minute for ramp-down and 2.10%/minute for ramp-up between full and minimum load. With the constructed control structure, the model demonstrates that the process can effectively handle continuous variations of electrolytic H<sub>2</sub> input.

## MOTIVATION

Renewable power is intermittent and therefore integration of synthesis processes with power and hydrogen production is not straightforward. Traditional synthesis processes are designed to operate at steady state with almost constant feed rate of raw materials. Variation of feed rate might be a cause problem in process operation. To facilitate process operation in variable conditions, processes need to be designed and operated to handle fast process variations. The motivation for this work was to develop a process model for methanol production which can operate at variable feed conditions. A new design for process syntheses and control structures needs to be invented and implemented.

## RESULTS

A dynamic Aspen plus simulation model was developed for the process including the necessary control structures to facilitate methanol production with intermittent renewable power generation. The flowsheet of the process is given in Figure 1. With the constructed control structure, the model demonstrates that the process can effectively handle continuous

variations of electrolytic H<sub>2</sub> input. The dynamic model was used to test different scenarios of power variation.

It was found that for dynamic operation it is best to divide the process into two parts: 1) Production of crude methanol (mixture of methanol and water), and 2) continuous separation of methanol from water. Only the crude methanol production part needs to be modelled dynamically.

The results show (see Figure 2 for details) that the minimum load of the model is around 20%, with maximum allowable ramping rates of 3.25%/minute for ramp-down and 2.10%/minute for ramp-up between full and minimum load. The main reason for the minimum load point is the operational lower limit of the compressors.

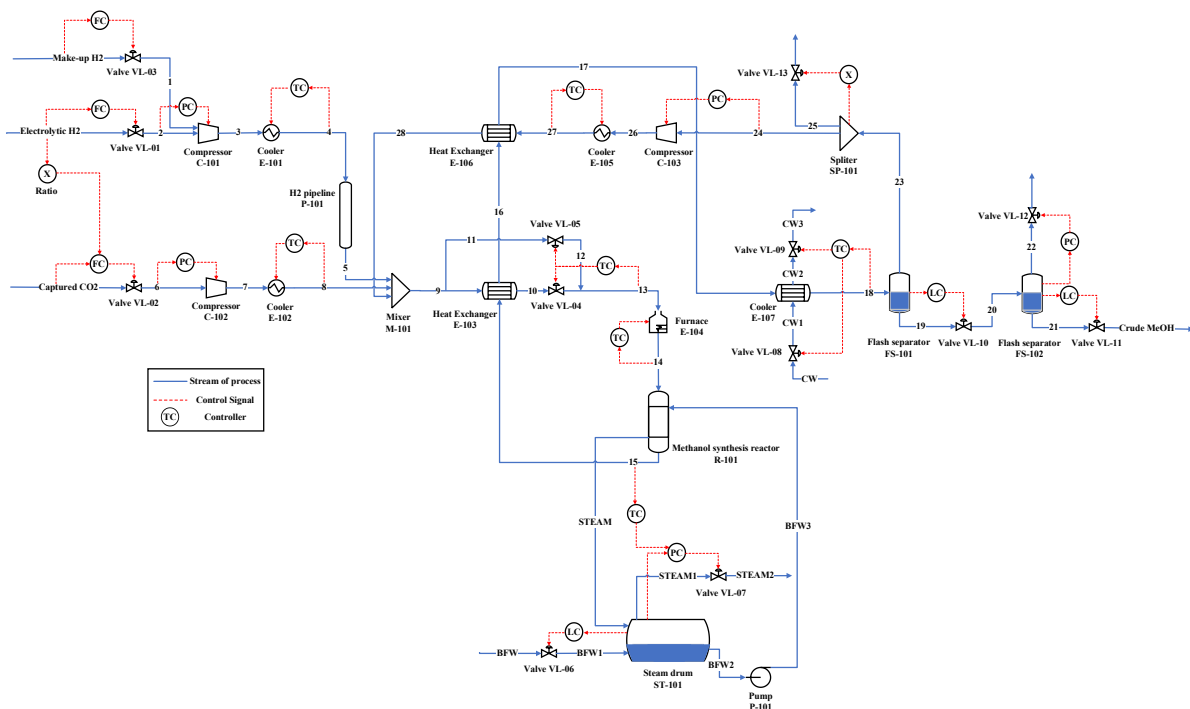
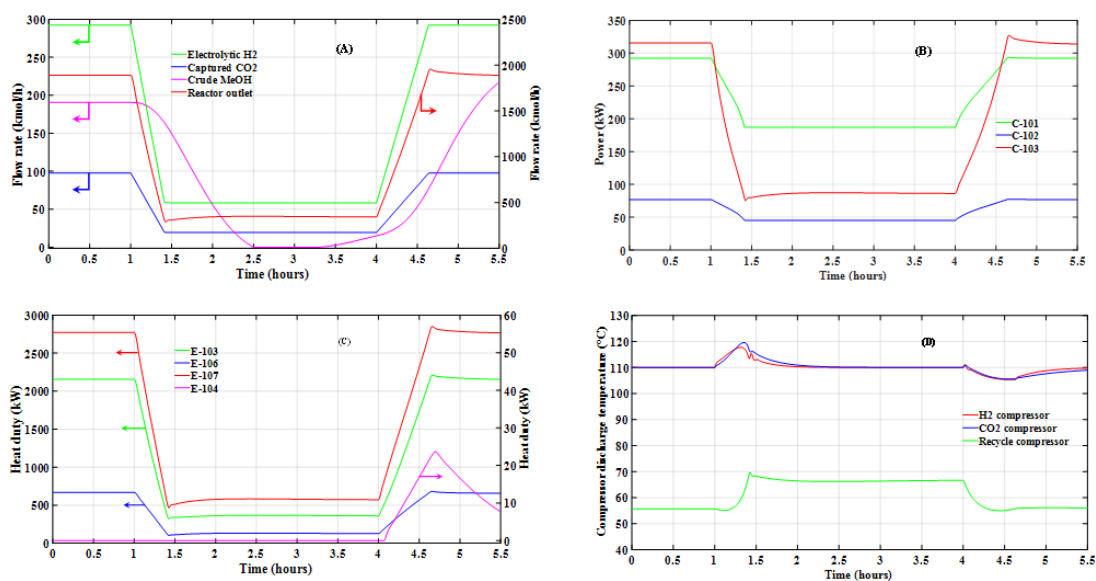


Figure 1. Flowsheet and plantwide control structure for crude methanol synthesis.



**Figure 2. Simulation results showing a) the variation of the feed streams and reaction products, b) power of the compressors, c) heat duties of heat exchangers, d) compressor discharge temperatures.**

### APPLICATIONS/IMPACT

The results of the project allow a better design of synthesis plants that can be operated under variable feed rate. The results also show what the operational limits of the processes are and how the limits can be extended to efficiently utilize variable power in a flexible way. The results also give ideas about the still existing process bottlenecks, for example the operational limits of compressors, and how these limitations could be potentially improved. Furthermore, the results can be used to evaluate the possible need and size of intermediate hydrogen storages to minimize the overall production and storage costs.

### MAIN CONTACT

Arto Laari, LUT School of Engineering Science, arto.laari@lut.fi

### AUTHORS

Hung Nguyen, Arto Laari