Dynamic modeling of small-scale methanation reactor

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Chemical energy storage via power-to-methane technology has become one of the most promising options to store redundant renewable energy on a large scale, due to the existing infrastructure of methane storage (the natural gas grid). The power-to-methane technology is expected to be coupled directly with renewable electricity sources without an electrical battery as a buffer. In such a case, dynamic response of a power-to-methane system, particularly the isothermal methanation reactor, is critical to ensure safe and efficient operation. Thus, in this study, the dynamic modeling and response of small-scale methanation reactors are investigated, based on experimental data obtained from the facilities available in the EnergyPolis building.

The key tasks involved include:

1. 2D or 3D dynamic modeling of the existing methanation reactors with Aspen Custom Modeler with the dimension data provided for each reactor. Collect the differential equations involved and formulate soundly in Aspen Custom Modeler.
2. Steady-state parameter estimation with available experimental data to obtain the unknown parameters relevant for heat and mass transfer as well as reaction kinetics. If dynamic experimental data is available, dynamic parameter estimation can be performed to get more reasonable estimation of these parameters.
3. Based on the developed models, investigate the influence of inlet velocity, inlet temperature, operating pressure, feed composition, cooling facility on the reactor performance, e.g., carbon conversion rate and catalyst de-activation.
4. Investigate the difference of dynamic response between the methanation of carbon dioxide and synthesis gas.

Skill requirement:

- Familiar with modeling of chemical processes and Aspen Plus, best with Aspen Custom Modeler
- Familiar with programming language and logics, best with C and C++
- Familiar with the concepts of power-to-methane and solid-oxide electrolysis