Highly integrated process equipment from Additive Manufacturing: Digital Process Engineering tool chain for more efficient P2X high pressure reactions

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Highlights

- Metal 3D printing (PBF-LB/M) of high-pressure equipment for methanol synthesis
- Fully digital workflow in the design and manufacturing process with cross-linked simulations
- Design automation for mass customized process equipment
- First prototypes

1. Introduction

Equipment for process and reaction technology can benefit from advantages of Additive Manufacturing (AM) technologies which are accessible through a fully digital chain of digital process engineering, digital 3D equipment design, application-specific geometry optimization and digital manufacturing [1]. Digital workflows enable an automated optimization and design of devices for efficient mass customization [2]. AM-made tailor-made porous metal structures [3] enable high process intensification.

This paper presents an approach for designing such equipment using a digital twin approach.

2. Methods

To design and manufacture process equipment by Metal Laser Beam Powder Bed Fusion (PBF-LB/M) 3D printing technology, we followed two approaches for a digital workflow. For the modelling, the P2X high pressure (> 50 bar) reaction for methanol synthesis was chosen:

$$3\ H_2\ (g) + CO_2\ (g) \rightarrow H_3COH\ (g) + H_2O\ (g)$$

In the joint research project 3D-PROCESS, research partners evaluated different digital toolchains to generate a manufacturable 3D model for the case of

1. Reactor system: thermodynamic modelling including catalytic kinetics given into a pre-defined 3D structure generation from software Rhinoceros/Grasshopper and structural refinement with optimizer software (ambiguous research approach)
2. Separation technology: thermodynamic heat transfer modelling including phase change / condensation, leading to a generic design realized as a fully parameterized model in 3D design software NX CAD (more state-of-the-art industrialized approach)

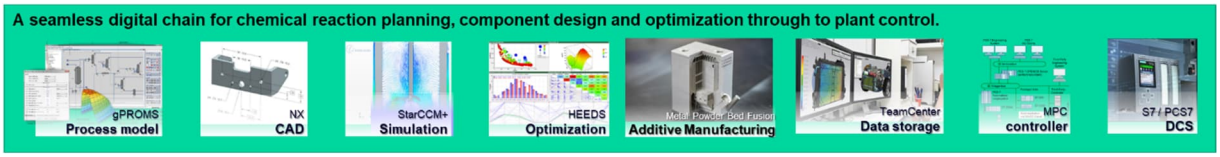

Figure 1. Digital software toolchain for the design, manufacturing, and operation of customized AM parts.

For the digital software tool chain, an analysis of several aspects using different digital twin approaches is required:

- A parameterized digital 3D **CAD model** was created, which serves as basis for different simulation analyses (as described in the next steps) and is input for the AM printing process.
- Finite Element Method (**FEM**) for calculation of structural stress for the reactor and for mechanical stabilization of the separation system was applied.
- **CFD simulation** calculates the fluid flow and thermal behavior of educts and products in the reactor structure, as well as thermomechanical behavior of the metal equipment.
- Effective nonlinear **optimization** was used to optimize the structure.
- **Process simulation** is used to simulate the kinetic behavior within the reactor and integration into the complete process plant.

Calculations are done to solid metal and, as replacement material, also to porous metal sections.

3. Results and discussion

Different equipment is generated for CO_2-based P2X methanol synthesis. To speed up the reactor development workflow, a novel reactor design automation toolbox has been developed as described by Kaya and Klahn [2]. In this toolbox, the user provides input parameters such as inlet flow rate, temperature, pressure, syngas concentration, catalyst diameter, density, porosity and kinetic equations of the reaction. The channel lengths are adapted to the required residence time. The reaction and cooling behavior are optimized using 3D CFD simulation and the structure mechanical behavior using FEA simulation, leading to automatically generated shapes in approx. 50 minutes.

The separator contains the classical equipment like a heat exchanger, reaction chamber as well as separation including sensors positions, but densely packed and integrated into one single piece of metal. The prototype has been validated by physical tests using pressure test beds in the laboratory.

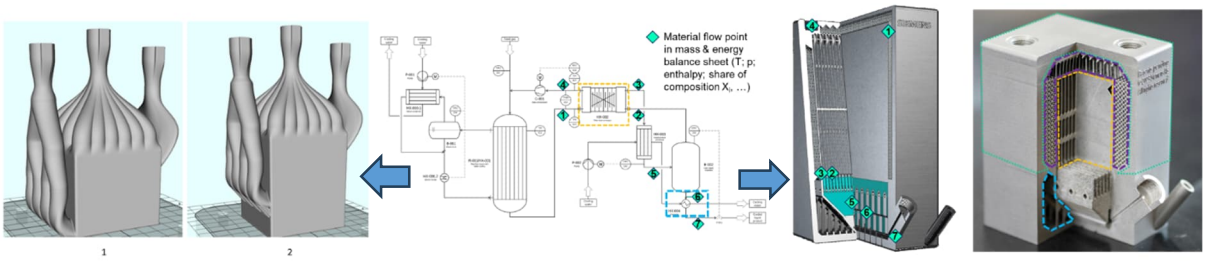

Figure 2. Reactor and feed-effluent heat exchanger/cooler/condenser units in process diagram (middle) leading to a generative reactor design (left), and highly integrated separator, 3D CAD models (middle), prototype (right)

4. Conclusions

A proof of concept has been successfully conducted to design and manufacture customized chemical equipment with Additive Manufacturing.

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Keywords
Circularity; Additive Manufacturing; Simulation; Methanol Synthesis