Corrigendum: Production of Oxymethylene Dimethyl Ethers from Hydrogen and Carbon Dioxide – Part I: Modeling and Analysis for OME_1 & Part II: Modeling and Analysis for $OME_{3\text{-}5}$

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Oxymethylene dimethyl ethers (OME_n) are promising alternatives to fossil fuels as they offer outstanding combustion characteristics and can be produced from H_2 and CO_2 using established process concepts. However, it has remained unknown how efficient a corresponding process is and how the efficiency compares to the production of other synthetic fuels.

In Bongartz et al.[1] and Burre et al.[2], we develop and implement process models for OME_1 and $OME_{3\text{-}5}$ production, respectively. The simulation results are used to calculate the exergy efficiency of both the individual processes and the entire value chains starting from H_2 and CO_2 by considering heat integration based on pinch analysis. For all involved processes, the corresponding model implementations in Aspen Plus have been uploaded to make them accessible for the research community.[3]

The parameters of the kinetic reaction model for the methanol process are taken from Van-Dal and Bouallou[4], who reformulated the original kinetic model of van den Bussche and Froment[5]. In these publications, the kinetic reaction model and corresponding parameters are based on partial pressures. The kinetic model implementation in Bongartz et al.[1] and Burre et al.[2] accidentally used fugacities instead of partial pressures. Due to this discrepancy, the reaction equilibrium is shifted slightly, which has a minor influence on the numerical results (Tab. 1). Additionally, there was a typo

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in the implemented rate constant of one reaction, which, however, did not have a noticeable influence on the results. We replaced the original with the corrected model implementation of the methanol process with the kinetic reaction model based on partial pressures.[3]

Table 1: Results for the reactant, product, and net energy flow rates of the methanol (MeOH) production process per unit mass of methanol produced.

Stream	Mass (kg kg^{-1})	Energy (MJ kg^{-1})
Input		
H_2	**0.196**	
CO_2	**1.428**	
Air	**0.466**	
Electricity		**1.000**
Output		
MeOH	**1**	
Exhaust	**0.593**	
thereof CO_2	**0.051**	
Heat at 234 °C		**1.363**

Additionally, the exergy analysis of the heat-integrated trioxane process in Burre et al.[2] is based on hot and cold composite curves instead of the grand composite curve. Whereas the two representations are equivalent for an energetic analysis (the amount of exchanged energy is the same), heat integration using the grand composite curve results in a lower net exergy demand as the temperature differences between exchanged heat streams are minimized. The original analysis in Burre et al.[2] thus underestimates the exergy efficiency of the heat integrated process.

The exergetically more advantageous heat integration by the grand composite curve has an influence on process efficiencies stated in Burre et al.[2] as follows:

- The overall exergy efficiency of $OME_{3\text{-}5}$ production from H_2 and CO_2 using established process concepts is **55%** (Graphical abstract, Abstract, Section 5.2, Figure 7, and Conclusion).
- If we include H_2 production by alkaline electrolysis, the exergy efficiency of the overall process chain drops to **40%**.
- If we include H_2 production by alkaline electrolysis and CO_2 provision by carbon capture from flue gas, the exergy efficiency of the overall process chain is **37%**.
- The exergy efficiency of the individual trioxane process is **58%** (Section 5.2 and Figure 7).
- If we consider a formaldehyde conversion for the trioxane process of 10% instead of 5%, the

exergy efficiency of the individual trioxane process is **67%** and the exergy efficiency of the overall process chain **58%** (Section 5.2 and Figure 6).

- Considering a pinch-based heat integration throughout the entire process chain (i.e. heat integration not only within the individual processes and subsequent exchange of excess steam between them), the exergy efficiency increases to **57%** (Abstract and Section 5.2).
- If we include H_2 production by alkaline electrolysis and consider heat integration within the entire process chain, the exergy efficiency of the overall process chain is **41%** (Section 5.2).
- If we include H_2 production by alkaline electrolysis, CO_2 provision by carbon capture from flue gas, and consider heat integration within the entire process chain, the exergy efficiency of the overall process chain is **38%** (Section 5.2).

Figure 1 and 2 are the corrected versions of Figure 6 and 7 in the original manuscript.

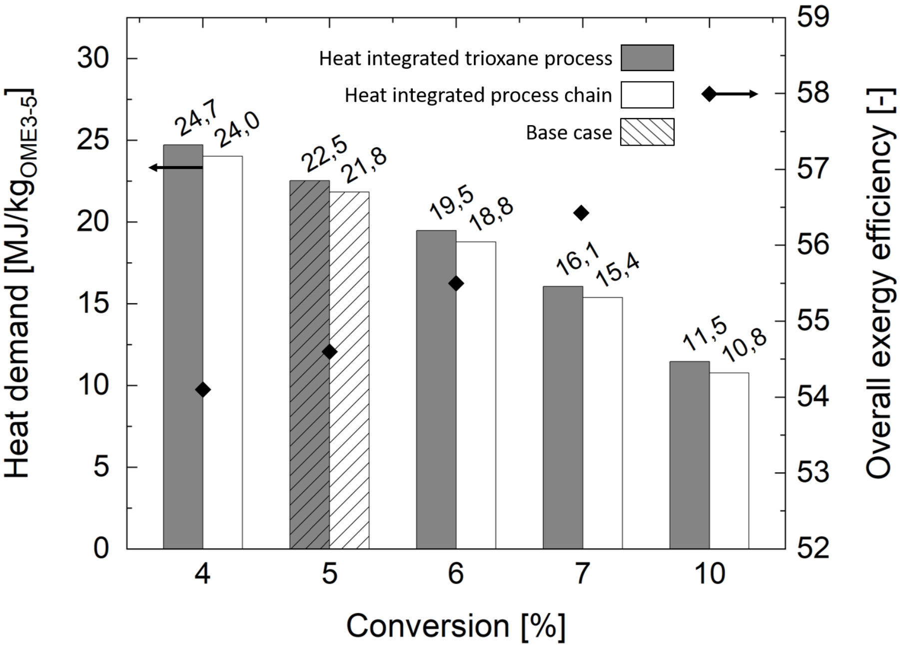

Figure 1: The influence of the conversion of FA to trioxane on the energy demand of the separately heat integrated trioxane production process, as well as on the overall energy demand of the entire process chain. Additionally, the exergy efficiency of the overall process chain starting from H_2 and CO_2 is shown.

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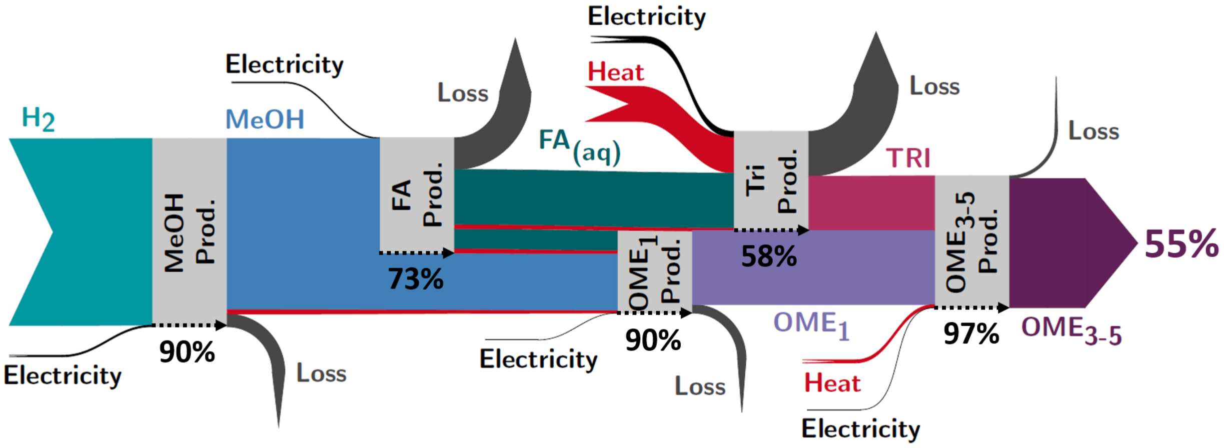

Figure 2: Sankey diagram of exergy flows within the reference process chain for the production of 1 kg $OME_{3\text{-}5}$. The gray boxes denote the different process steps and the percentages are the exergy efficiencies of these separate steps. The overall exergy efficiency from H_2 to $OME_{3\text{-}5}$ is **55%**.

References

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