System analysis, modelling, and sustainability assessment – multicriteria optimization of electrochemical processes

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Ten Fraunhofer Institutes led by the Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT have joined forces to work on the Fraunhofer lighthouse project ”Electricity as a Resource”. Their aim is to develop and optimize processes that enable low-carbon power to be used to synthesize important base chemicals. In this lecture results from the system analysis, modelling and the sustainable assessment are presented.

Process design is a multicriteria task, where a good balance between conflicting objective functions must be found by choosing a suitable set of design variables. Model-based simulation and optimization have become important tools which help the process engineer in identifying promising alternatives. In this contribution, a prototypical integrated simulation platform is presented which consists of a thermodynamic simulation of a commercial flowsheet simulator on the one hand and of a life cycle assessment module on the other hand. Based on this integrated simulation, numerically efficient sensitivity studies and multicriteria optimization studies are carried out, where adaptive strategies are pursued such that only a minimal number of simulation runs are needed in order to achieve a maximal gain in information about the process.

This framework is applied to an electrochemical process, consisting in the electro synthesis of H_2O_2. Therefore, a user-defined module was implemented into the commercial flowsheet simulator, and combined with additional standard unit-operations for downstream separation. Due to the integration of the flowsheet simulator and the sustainability assessment module, both process-relevant and environmentally relevant KPIs[1] can be quantified and optimized. The results clearly

[1] KPI: key performance indicators

show the tradeoffs between the objectives and allow to make the planning horizon transparent.

Especially**,** LCA[2] results were compared to corresponding conventional chemical production and recommendations were deduced. Concerning the LCA, additional CO_2 conversion pathways in order to produce different chemicals were investigated.

Since energy demand is a crucial factor for the costs and sustainability of the production process, energy scenarios for the years 2020, 2030, 2040 and 2050 were defined. The scenarios were used to calculate the environmental impacts of electricity provision. Recommendations for the coupling of chemical production with the energy market were drawn.

Main CO_2 sources in Germany were investigated and visualized in maps to identify potential production sites. The maps show the CO_2 amounts of different sources and differentiate between the quality of the available CO_2 supply (e.g. low and high CO_2-concentrations).

Apart from the environmental assessment an integrative sustainability concept was applied to identify additional crucial sustainability aspects like the development of investments, human capacities and know how.

Two stakeholder dialogues were realized with stakeholders from the chemical industry and the energy sector. The first dialogue focused on the coupling of a fluctuating energy offer and the chemical industry and research demands for electrochemical processes. The second dialogue focused on the energy markets and on molecules produced by electrochemistry with high added value.

[2] LCA: life cycle assessment