## Production of the future

## Abstract englisch

Project Title	Short title: MultiEfficiency
	Full title: Efficient feedstock use for multi-component systems in the chemical industry
Synopsis	Process optimization in the chemical industry is very complex, particularly when it comes to alternating feedstocks and process parameters. Hitherto, mathematically based models are state of the art for process optimization. A limitation of these models is the fact that any changes are included too late/sluggishly in the process. Therefore, the optimization potential of chemical processes isn't fully exploited yet. As an alternative, thermodynamic models could be used instead of mathematical approaches. Based on thermodynamic models, dynamic real-time optimizations could be implemented. For this purpose, a real-time registration and use of the plant parameters should be carried out. Therefore, focus of the project is the development of such a real-time system for the chemical industry, enabling predestination and simultaneous optimization of control parameters for production.
Summary / Abstract	<b>Initial situation:</b> The chemical industry comprises considerably complex processes, due to the great variety of variables and degrees of freedom (e.g., pressure, temperature, composition, mass flow etc.). For this reason, process optimization is a very complex task, particularly when it comes to alternating feedstocks and process parameters. Currently, mostly <b>mathematical</b> optimization models are used. Although such models are capable of accounting for variation of parameters and dynamics, extrapolation of such models beyond their validity ranges runs the risk of violating physical or thermodynamic constraints. This may result in suboptimal results and/or considerable uncertainties when operating modes approach their limiting conditions. In that case, mathematical optimization models find their limits. To overcome such limitations, the use of rigorous <b>thermodynamic</b> approaches instead of mathematical models could be considered. However, optimization based on thermodynamic models is not yet state of the art in chemical industry. A prerequisite for such an approach is the use of real-time data from the chemical plant as an input for the dynamic optimizer based on thermodynamics. The combination of rigorous thermodynamics and dynamic optimization at present would be unprecedented and has a great potential for various kinds of production plants in the chemical industry, particularly when it comes to alternating feedstocks and process parameters. Hence, dynamic optimization based on thermodynamics provides the basis of this project, aiming at a considerable increase of efficiency for chemical plants. As an example, 1% increase of the efficiency of a chemical plant corresponds to an annual cost reduction of apprx. EUR 19m.

	<b>Problem definition:</b> A new approach for real-time process optimization is required, which is particularly reliable when operating modes approach their limiting conditions. This requires implementation of real-time data from the plant, aiming at a prompt determination of parameters for optimal plant operation. Such an optimization is not possible using mathematical models because thousands of parameters would have to be computed in real-time, and results are prone to considerable uncertainties due to error propagation, especially in limiting conditions of operation. Hence, the new approach will be based on rigorous thermodnamic models.
	<b>Aims:</b> (1) Development of an approach for prediction and optimization of control parameters for a chemical plant, based on an existing plant. (2) Development of a system by which essential input parameters, like boiling curves, density and composition of a multicomponent system, can be determined in real-time. (3) Development of a application-oriented output for plant operators which displays the recommended operating parameters, enabling the operators to adjust actual plant parameters according to the recommended values. (4) The software application to be developed should be easily implementable into the existing production control system of every industrial plant.
	<b>The methodology (excl. project management):</b> Comprises the following working packages: AP2 – investigation & analysis of the technical solution approaches; AP3 – development of a static and dynamic real-time simulation model for characterization of a multicomponent system and for estimation of recommended operating parameters; AP4 – simulation and validation (i.e., comparison with data from an existing plant) based on the example of a benzene production plant; AP5 – development of a strategy for the implementation of the new approach in the control system of a chemical plant; AP6 – final evaluation and recommendations for further steps to be taken;
	<b>Targeted results:</b> (1) The prototype of a new approach for real-time optimization of chemical plants based on rigorous thermodynamics. (2) A rigorous thermodynamic model (static as well as dynamic) and results when applied to an existing plant. (3) The sensitization of the plant staff (operators gets used to considering recommendations from the optimizer) (4) Availability of verified simulation results based on the example of an existing benzene production plant (5) standardization of the prototype system in view of scalability and portability.
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