Short-cut statistical models for estimating the consumption of energy utilities in chemical batch plants

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The minimization of energy consumption in the chemical industry is one of the key principles of green chemistry. This has led to the development of evaluation tools, which include energy use as a metric, not only in academia but also in the industry. The use of these evaluation tools requires process specific data of energy consumption, which is usually scarce particularly in multiproduct and multipurpose batch plants.

In this study we focus on shortcut models for estimating the consumption of energy utilities (steam, cooling water, brine, etc.) in chemical batch plants. For this purpose, we developed statistical models, namely probability density functions (PDF) and classification trees on the basis of real production data. These models take the form of generic intervals defined as interquartile ranges derived from the PDF parameters, and as classes derived from the classification trees. The use of the models is possible at different levels of process design, the minimal required information being the reaction type. The PDF models were assessed with diverse metrics for the goodness-of-fit and the classification trees by means of cross-validation. Additionally, the transparency of the classification trees facilitated the analysis of the effect of the predictor variables (i.e., reaction type and operational parameters) upon the consumption of the energy utilities, resulting in a set of dominating, descriptive classification rules.

The prediction performance of both types of models was further evaluated in case studies. The validation results show that the statistical models proposed in this work provide satisfactory interval estimations for energy consumption, for instance similar to the expected accuracy of cost estimations in early process design phases (i.e., 30-40% modeling estimation error). Moreover, we have applied the PDF models to a case study for the production of the intermediate substance 4-(2-methoxyethyl)-phenol, which can be produced from seven different synthesis routes. In a previous work, a decision-making framework, which considers environmental and economic proxy indicators for screening of chemical batch process alternatives during early phases of process design (Albrecht et al., 2010), was applied to the same case study. Both methodologies allow a ranking of the different synthesis routes. It is demonstrated that the results depicted in this case study show the

applicability of the PDF models – considering median values or intervals – for a fast ranking of process alternatives with respect to energy consumption, when only the reaction synthesis routes are known at early stages of process design. The PDF models provided a similar ranking compared to more complex indicators (i.e., mass loss index, energy loss index, productivity loss index) which require more detailed chemical and process information.

These new shortcut models developed in this work, especially the classification trees, represent a potentially useful tool for estimating energy utility consumption of production processes, when limited process information is available or when overwhelming processes have to be screened in short time (e.g., early design phase screening of process alternatives, life cycle assessment studies, etc.). Even though the PDF models also allow reasonable predictions of energy utility consumption, their most interesting potential applications will be for providing a benchmark framework for labelling chemical reaction types and rigorous uncertainty analysis.

Finally, the short-cut models are put into perspective with respect to a set of previously developed methodologies for estimation of energy consumption developed in the Safety and Environmental Technology Group of ETH (Szijjarto et al., 2008, Wernet et al., 2009, Rerat et al., 2012, Pereira et al., 2013) based on standard process documentation, rules of thumb, expert knowledge, and thermodynamic principles. Depending on the application target, the proper use of these models is summarized, mentioning the modeling challenges for further research.

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