

Simultaneous Multiobjective Chemical Model Fitting of Online Measurements: Calorimetry, Spectroscopy and Gas Uptake

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With modern online instrumentation it is now possible to follow the course of a chemical reaction using a variety of techniques simultaneously (e.g. calorimetry, spectroscopy and gas consumption/production).

In this work a multi-objective genetic algorithm has been developed for the optimization of a chemical model simultaneously against multiple measurements from any variety of instrumentation. Current techniques for the fitting of chemical models to measured kinetic data struggle when faced with data from different types of instrumentation. The data from different instrumentation have different error structures, different information content and often observe different physical phenomenon. Combining the data into a single objective function for optimization is difficult with no good general techniques available. Furthermore, combining the data into a single objective function leaves the user with little insight into whether the same chemical model or model parameters are really suitable for each type of measurement. Rather than combining the data into a single objective function, the ranking of solutions within the genetic algorithm is done using the multi-objective Pareto optimal set. The final output of the algorithm is an optimized Pareto optimal set showing the trade off between the different objective functions for a range of parameter values. The final Pareto optimal is then further refined using multi-objective local optimization.

The approach has been demonstrated using simultaneously measured calorimetric and mid-IR spectroscopic data of the two-step epoxidation of 2,5-di-tert-butyl-1,4-benzoquinone. Preliminary results of the application to data of the hydrogenation of aromatic nitro compounds will be introduced. For this case the additional online hydrogen uptake measurement is considered. The results show that the multi-objective genetic algorithm is a powerful method for the evaluation of a chemical model against data from different sources and for the determination of the appropriateness of a chemical model.