Application of Optimal Experimental Design to Thermodynamic Property Measurements

Ophelia Frotscher [S]
Applied Thermodynamics, Chemnitz University of Technology, Chemnitz, SN, Germany

Roland Herzog
Numerical Mathematics, Chemnitz University of Technology, Chemnitz, SN, Germany

Markus Richter [C]
Applied Thermodynamics, Chemnitz University of Technology, Chemnitz, SN, Germany
m.richter@mb.tu-chemnitz.de

Thermodynamic properties of energy carriers and ecofriendly refrigerants are of large interest in the context of the energy transition. In process design and simulation, such properties are calculated with equations of state (EOS), which are typically based on experimental data. Here, fast and reliable thermodynamic property measurements are extremely desirable. In case the form of the EOS is known, optimal experimental design (OED) can be used to calculate (T, p) state points at which thermodynamic properties are supposed to be measured as the basis for the fitting process. This reduces the required experimental time and effort and also improves the EOS towards a more reliable parameter fit. The mathematical methods of OED have been known for several decades. In the field of thermodynamic property research, however, the potential seems widely unused. Reasons could be (1) the time-consuming implementation of the mathematical algorithms, (2) the necessary sequential design within the measurement process and (3) a lack of knowledge about the form of the EOS, which will be fitted to the measured data. In this work, OED will be introduced in conjunction with (p, v, T) data for liquid substances and applied to linear and non-linear models. We demonstrate the potential of OED by combining experiment and EOS development. The approaches for linear and non-linear models are explained. It will be shown how OED can be used to compare different forms of EOS since the selection of the model's form is often not possible before the first experiments are conducted. Furthermore, the implementation of different objective criteria in the context of EOS development will be discussed. With the goal to achieve more efficient and less time-consuming measurement programs as well as an accelerated way of modeling thermodynamic properties, the current limitations are discussed, and possible solutions are presented.