Technische Universität Braunschweig

Wissenschaftliche*r Mitarbeiter*in (m/w/d) im SPP 2403 Carnot-Batterien

Prediction and surrogate modelling of thermodynamics properties of mixtures with application to the inverse design under uncertainty

Befristet (3 Jahre), TV-L E13, 100%

Hintergrund zum SPP (aus Pressemitteilung):

The energy supply is intended to be primarily secured in the future using sustainable but fluctuating energy sources such as wind and solar power. In order to achieve this, a large quantity of energy storage is required to provide energy when, for example, the sun is not shining. One possibility for this is the storage of electrical energy in the form of heat, which can later be converted back. This involves the coupling of high-temperature heat pumps with storage systems, as well as heat engines for the subsequent provision of electrical energy. Such systems are referred to as Carnot batteries and offer the potential for cost-effective energy storage. However, due to the multitude of design parameters, there is not yet a systematic methodology for their design and evaluation within a future energy system.

To address this issue, in 2022 the German Research Foundation (Deutsche Forschungsgemeinschaft) decided to establish the Priority Program 2403 "Carnot Batteries: Inverse Design from Market to Molecule," within which 17 individual projects have now been approved for the first funding period of three years. Researchers from all over Germany will work on developing fundamental design concepts and methods that, starting from market criteria, comprehensively analyze overall systems. They will also develop design methodologies, utilizing expertise on the required machinery, storage systems, and working fluids (molecules), which are also represented in the priority program.

The project

The selection of a suitable working fluid poses a significant challenge in the design of a thermodynamic process. As various requirements must be met by a working fluid, mixtures are increasingly gaining importance to achieve the desired combination of properties. Highly accurate multiparameter Helmholtz Equation of State (HEOS) models represent the state of the art for describing fluid data, but their evaluation is computationally intensive, making them unsuitable for optimization applications. Additionally, they do not allow for the consideration of mixtures for which no mixing models or parameters are available.

The aim of this project is to overcome these two limitations in the application of HEOS in the working fluid selection process. One objective is the development of Gaussian Process (GP) surrogate models for the efficient description of substance properties in optimization. New potential mixtures should be considered by adjusting their mixture parameters to results from molecular simulations. To account for deviations between the HEOS models and molecular simulation results, a stochastic HEOS modeling approach is pursued, for which stochastic GP surrogate models are also generated. These stochastic GP surrogates are then used for calculating substance properties in an optimization process to identify suitable mixtures for a specific application. Thus, the modeling approach pursued in this proposal enables robust optimization by considering the uncertainties of the underlying models.

Description of the Position

The position is split 50% between the Institute of Thermodynamics (Research Group of Prof. G. Raabe) and 50% at the Institute for Acoustics and Dynamics (Research Group of Prof. U. Römer) and is initially limited to an expected duration of 3 years. Its purpose is to contribute to the qualification of young scientists and provides the opportunity for pursuing a doctoral degree or further academic qualification. Compensation is in accordance with the collective agreement, ranging up to salary level 13 TV-L, depending on responsibilities and fulfillment of personal requirements; full-time employment (100% position).

Tasks:

- Development of GP surrogate modeling for highly accurate multiparameter HEOS using a selected model system (water-ethanol or water-ammonia), comparison in terms of accuracy and efficiency with other modeling approaches.
- Development of stochastic HEOS models and their surrogates.
- Development of optimization algorithms for the inverse design of thermodynamic processes, considering uncertainties.

Your profile:

- Above-average completion of a master's degree in mechanical engineering or related fields.
- Good fundamental knowledge in thermodynamics.
- Basic understanding of surrogate modeling or quantification of uncertainties.
- Programming skills
- Team and communication skills, flexibility, motivation, and the ability to work independently.

What we offer:

- Research on a socially relevant and scientifically challenging topic.
- Engaged and interdisciplinary supervision.
- A pleasant office atmosphere – but home office is possible.
- Participation in the education program of the Graduate Academy Grad$^{TUBS.}$

Application:

Please submit your written application, including the usual comprehensive documents and your desired start date, preferably by email and preferably in PDF format, by 15th September 2023 to: G.Raabe@tu-braunschweig.de or U.Roemer@tu-braunschweig.de