Uncertainty and sensitivity analysis of model outputs in process industries: A critical review and perspectives in the era of digitalization and artificial intelligence

Gürkan Sin

Department of Chemical and Biochemical Engineering, Process and Systems Engineering Centre (PROSYS), Technical University of Denmark, Copenhagen, Denmark; gsi@kt.dtu.dk).

Abstract

In today's chemical industries commercial software tools employing state-of-the-art models and advanced optimization and control algorithms are used at different stages of the project life cycle, from early stages performing scale-up and conceptual process design, front-end engineering design to retrofitting and optimization studies at the plant commissioning/operation stage. The impact of advanced process modeling and simulation, optimization and control is profound and has become mainstream in the chemical industries due to the significant economic benefits achieved. These are amongst crown achievements of the process systems engineering community in Chemical Engineering discipline through research in mathematical programming, modeling, process synthesis and design and process control that has been performed in the past decades. Today there are new driving forces affecting the bottom line of chemical industries but also universities alike namely digitalization, machine learning/Artificial Intelligence (AI), climate change, decarbonization, sector coupling through renewable energy, etc. These technologies open up new horizons for industry to become more efficient, to decrease CO_2 footprint and to develop innovative products and services. As model-based engineering becomes more established as enabling technology to address these challenges, in this talk we review the critical role of uncertainty and sensitivity analysis methods starting from the fundamental theory of Monte Carlo integration to sensitivity analysis using variance decomposition methods. Here an important distinction between when a study is about uncertainty and when it is about sensitivity analysis will be discussed. A number of applications of uncertainty and sensitivity analysis from process systems engineering which employs largely first principles/mechanistic models are presented: These examples include a range of engineering problems related to model identification/parameter estimation (in process/property modeling) to process synthesis and design and optimization. From these experiences, a critical analysis of the theory and pitfalls encountered in the application of uncertainty & sensitivity analysis in wider process systems engineering is presented. In the second part of the talk, a critical attention is given to the need to provide model prediction error (uncertainty quantification) of machine learning as well as deep learning/graph neural network models that are becoming popular in this emerging AI paradigm. While a wide range of methods for uncertainty assessment for such deep learning models are proposed from the larger deep learning community (from ensemble modeling to last layer dropout, etc), these methods are mostly pragmatic and heuristics in nature. Therefore the importance of benchmarking and critically assessing the quality of uncertainty quantification methods should remain an important point of attention. This aspect will be discussed on a study that deals property prediction of chemical compounds using graph neural networks.
Stepping back from these particular examples, and looking ahead at the big picture, we see that many engineering decisions relies on computational analysis/calculations that employs a range of models some increasingly sophisticated (be it mechanistic, machine learning/deep learning or a hybrid combination). In this regard, proper identification and systematic study of potential sources

of uncertainty and assessment of their consequences to such decisions will remain relevant and important problem. This field is truly fascinating with many scientific and engineering challenges to address.