Adem R.N. Aouichaoui

ML and Molecular Researcher

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I am a motivated and ambitious academic specializing in machine learning and molecular science, with extensive experience in mathematical modelling, computer-aided molecular design, and advanced machine learning techniques. Throughout my PhD and postdoctoral research, I have focused on various facets of molecular property modelling, including quantitative structure property relations (QSPRs) using descriptors and machine learning as well as graph neural networks (GNNs). Through publications and presentation, I have communicated my findings on an international level. I am eager to leverage this opportunity to advance my academic career by extending the field of applicability of QSPRs, and molecular screening , further honing my skills and contributing to this exciting field.

Skills

- Thermodynamic Modelling
- Coding: Python, MATLAB, GAMS
- Mathematical Modelling
- Optimization
- Machine Learning
- Solution-oriented
- Creativity
- Positive Attitude
- Clear Communication
- Collaboration

Experience

Postdoctoral Researcher, Technical University of Denmark (DTU) *2023 - present*

- Accelerated Innovation in Manufacturing Biologics (AIM-BIO) project: development of digital models for ion exchange chromatography to build a digital plant as part of the ongoing digitalisation effort at DTU and NC State
- Machine-learning for energy and process optimisation (MLEEP): scoping and identification of energy and process optimisation potentials, feasibility studies, mechanistic modelling

Research Assistant, Technical University of Denmark (DTU) *2021 - 2021*

- Quantification of Nitrous Oxide emissions from wastewater treatment plants using deep neural networks
- Performing sensitivity analysis of model inputs to gain process insights

Doctor of Philosophy (PhD), Technical University of Denmark (DTU) *2019 - 2023*

- Topic: Machine learning for new and improved molecular property models
- Main contributions:
  - Developed a novel hierarchal graph neural network model (GNN) that integrates three different views of the molecule to predict 30 different thermophysical properties of interest to the process systems engineering field. The model provides state-of-the-art performance for many properties and a new take on interpretability by highlighting groups rather than atoms
  - Improved the performance of group additivity models (group-contribution models) for a wide range of properties through a systematic approach for outlier detection
  - Performed uncertainty to evaluate the reliability of the model prediction
- Teaching activities: separation processes, safety and risk assessment, uncertainty and sensitivity analysis (PhD level), process design
- Project supervision: 6 M.Sc. thesis and 2 B.Eng projects
- External research stay at Hamburg University of Technology (TUHH): integrating OpenCOSMO-RS in computer-aided molecular design

Dissemination

Peer-reviewed Journal Article

- **Aouichaoui, A. R.**, Fan, F., Abildskov, J., & Sin, G. (2023). Application of Interpretable Group-embedded Graph Neural Networks for Pure Compound Properties. Computers & Chemical Engineering, 176, 108291
- **Aouichaoui, A. R.**, Fan, F., Mansouri, S. S., Abildskov, J., & Sin, G. (2023). Combining Group-Contribution Concept and Graph Neural Networks Toward Interpretable Molecular Property Models. Journal of Chemical Information and Modeling, 63(3), 725-744
- **Aouichaoui, A. R.**, Mansouri, S. S., Abildskov, J., & Sin, G. (2022). Uncertainty Estimation in Deep Learning-based Property Models: Graph Neural Networks Applied to The Critical Properties. AIChE Journal, 68(6), e17696

Selected Peer-reviewed Conference Proceedings

- **Aouichaoui, A. R.**, Mansouri, S. S., Abildskov, J., & Sin, G. (2022). Application of Outlier Treatment Towards Improved Property Prediction Models. In Computer Aided Chemical Engineering (Vol. 51, pp. 1357-1362). Elsevier
- **Aouichaoui, A. R.**, Cogliati, A., Abildskov, J., & Sin, G. (2023). S-GNN: State-Dependent Graph Neural Networks for Functional Molecular Properties. In Computer Aided Chemical Engineering (Vol. 52, pp. 575-581). Elsevier
- **For more papers, visit google scholar: https://tinyurl.com/5dwrm2fc**

Selected Conference Presentations

- **Aouichaoui, A. R.**, Mansouri, S. S., Abildskov, J., Sin, G. (2021). Benchmarking Uncertainty Quantification Methods for Property Prediction Models: Application to Group-Contribution Models, **Keynote lecture** at the 13th European Congress of Chemical Engineering (ECCE), Berlin, Germany, (Online), September 2021
- **Aouichaoui, A. R.**, Fan, F., Mansouri, S. S., Abildskov, J., & Sin, G. (2021). Combining Functional Groups and Graph Neural Networks Towards Interpretable Molecular Property Models, Oral presentation at the 2022 American Institute of Chemical Engineers (AIChE) annual meeting, Phoenix, AZ, USA, November 2022
- **Aouichaoui, A. R.**, Fan, F., & Sin, G. (2022). An Interpretable Graph Neural Network-based Property Prediction, Oral presentation at the 32nd European Symposium of Computer Aided Process Engineering (ESCAPE-32), Toulouse, France, June 2022
- Summary: American Institute of Chemical Engineers (AIChE x 3), European Symposium of Computer Aided Process Engineering (ESCAPE x 4), European symposium of applied thermodynamic (ESAT x 1), European Congress for Chemical Engineers (ECCE x 2)

Awards

- Recipient of the Otto Mønsted travel grant (3 times of total of 1,000 USD each)
- Recipient of a 1,000 USD grant from *teknisk kemi fund*
- Best poster presentation at two industry-academia meetings:
  - The process systems engineering center (PROSYS) Annual Research Day 2022
  - The KT-Consortium Annual Meeting 2023
- Best poster at the annual research day of the Chem. Eng. department

Education

M.Sc. Chemical Engineering (Hons), Technical University of Denmark (DTU) *2017-2019*

- Thesis: Computer-aided molecular design for solvent selection in extractive distillation (A+)
- Focus: process & thermodynamic modelling and mathematical optimization
- External stay: Monash University, Melbourne, Australia
- GPA 3.7-3.9

B.Eng. Chemical & Bio-Engineering, Technical University of Denmark (DTU) *2017-2019*

- Thesis: P-V-T modelling using the BWR equation of state for energy recovery applications
- GPA 3.7