Saman Naseri Boroujeni

MARIE SKŁODOWSKA-CURIE POSTDOCTORAL FELLOW

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Education

2020-2024 **PhD in Chemical Engineering**

Technical University of Denmark (DTU), Kgs. Lyngby, Denmark

Thesis: *Ion-ion association in electrolyte solutions: a theoretical investigation* Supervisors: Prof. Georgios M. Kontogeorgis, Assoc. Prof. Xiaodong Liang, and Dr. Bjørn Maribo-Mogensen

- Collaborated with a global team of thermodynamics specialists on an ERC Advanced Grant project ("New Paradigm in Electrolyte Thermodynamics"), developing a novel equation of state for electrolyte solutions.
- Pioneered the study, benchmarking, and development of models for electrical conductivity of electrolyte solutions, culminating in two original predictive models.
- Engineered a new open-source Julia software package for predicting thermodynamic properties, pending release alongside associated publications.

2016-2019 **MSc in Petroleum Engineering**

Sharif University of Technology (SUT), Tehran, Iran

GPA: 17.66 / 20 — Top of class

Thesis: *Development of a new simulation tool to study asphaltene precipitation and deposition in oil well columns* Supervisors: Prof. Vahid Taghikhani and Prof. Saeid Jamshidi

- Investigated asphaltene precipitation challenges in petroleum wellbores, developing innovative predictive solutions for the oil and gas industry.
- Developed an asphaltene precipitation module within the PVT Pro software in collaboration with MAPSA Co., significantly extending the software's capabilities.
- Created **MAD-ADEPT**, a commercialised software package for modelling asphaltene deposition on wellbore surfaces.

2012-2016 **BSc in Petroleum Engineering**

Petroleum University of Technology (PUT), Ahwaz, Iran

GPA: 18.56 / 20 — Top of class

- Graduated as top student in the class, demonstrating exceptional academic performance across all core petroleum engineering disciplines.

Professional Experiences

Nov 2025 - Present **Marie Skłodowska-Curie Postdoctoral Fellow**

Imperial College London, London, UK

- Developed ML-based models for prediction of physicochemical properties of ionic liquids, enabling faster and more reliable candidate screening.
- Developing COSMO-SAC and SAFT-γ Mie equation of state for accurate thermodynamic property prediction of ionic liquids.
- Designed a reinforcement learning framework for goal-directed discovery of API ionic liquids, combining GNN property oracles with multi-objective molecular generation.
- Developed and released openAPIILDesign, an open-source Python package for end-to-end API ionic liquid design integrating predictive and generative models.

Feb 2024 - Nov 2025 **Postdoctoral Research Associate**

Imperial College London, London, UK

- Optimised parameter estimation for equations of state using quantum chemistry data, significantly improving thermodynamic property prediction accuracy.
- Benchmarked the SAFT-γ Mie equation of state on pharmaceutical systems, improving reliability and efficiency in API property prediction.
- Developed COSMO-NET, a machine learning model for predicting molecular descriptors from quantum chemistry calculations.
- Built predictive models for thermodynamic properties of active pharmaceutical ingredients and contributed to molecular and process design for API manufacturing.

Nov 2021- Apr 2022 **Guest PhD Researcher**

Hafnium Labs Aps., Copenhagen, Denmark

- Contributed to the development and implementation of thermodynamic models for electrolyte solutions within the Q-props™ commercial software in Julia.
- Performed rigorous benchmarking of associative primitive models for electrostatic interactions, refining model accuracy in electrolyte systems.

Jun 2020 - Oct 2020 **Back End Scientific Developer**

ESTD (RETINA Suite), Tehran, Iran

- Developed deep learning surrogate models that enhanced hydrocarbon reservoir simulation efficiency, significantly reducing computational time in the RETINA Suite.
- Implemented advanced ML techniques to build predictive models, improving the accuracy of complex reservoir simulations.

Mar 2017 - May 2020 **Technical Software Developer**

Abdal Industrial Projects Management Co. (MAPSA), Tehran, Iran

- Developed and implemented multiphase flow models in the Flow Pro software using C++ and Qt, enhancing simulation capability for complex fluid dynamics.
- Advanced the PVT Pro software by building robust multiphase phase equilibrium calculations, delivering more accurate predictions of phase behaviour.

Grants Awarded

2025	**€ 276,187**	MSCA Postdoctoral Fellowship — Marie Skłodowska-Curie Actions, Horizon Europe, European Union (Grant No. 101201955).
2023	**€ 1,000** (7,500 DKK)	Otto Mønsted Foundation travel grant — AIChE Annual Meeting, Orlando, USA.
2022	**€ 1,000** (7,500 DKK)	Otto Mønsted Foundation travel grant — Thermodynamics Conference, Bath, UK.

Awards & Honors

- Best poster award winner, CERE/KT Consortium Meeting, Helsingør, 2023.
- Best MSc thesis selected by Iranian Association of Chemical Engineers, 2020.

Teaching & Supervision

Supervision & Leadership

- Co-supervisor of master's and PhD students in Chemical Engineering — Imperial College London, UK.
- Workshop leader, CEDAR CDT training programme — Imperial College London, UK.
- Workshop leader, CMAC Open Days 2025 — CMAC, UK.

Postgraduate & Master's

- TA, Advanced Process Optimisation — Imperial College London.
- TA, Advanced Course on Thermodynamic Models (PhD summer school) — DTU, Denmark.
- TA, Chemical Engineering Model Analysis — DTU, Denmark.

Undergraduateπ

- TA, Physical Chemistry — Imperial College London.
- TA, Thermodynamics II — Sharif University of Technology.
- TA, Chemistry I — Petroleum University of Technology.
- TA, Organic Chemistry — Petroleum University of Technology.

Skills

Programming Language: Python, C++, Julia.

AI/DL: Scikit-learn, Numpy, Matpilotlib, PyTorch, PyTorch Geometric, Pandas, SciPy.

Engineering Tools: RDKit, Gaussian, gPROMS, ChemProp, DeepChem.

Soft Skills: Problem Solving, Algorithmic Thinking, Learning Agility, Teamwork

Publications List

2026

1. **Naseri Boroujeni, S.**, Bernet T., Paliwal S., Standish R., Wehbe M., Jackson G., and Galindo A., and Adjiman C. S. 2026. Predictive Modelling of Thermophysical Properties of Active Pharmaceutical Ingredients: A Systematic Evaluation of SAFT-γ Mie and COSMO-SAC (in preparation).
2. Paliwal S., Bernet T., **Naseri Boroujeni, S.**, Zhan Z., Haslam A. J., Adjiman C. S., Jackson G., and Galindo A. 2026. Solubility prediction of paracetamol and salicylic acid: the role of intramolecular hydrogen bonds (in preparation).
3. **Naseri Boroujeni, S.**, Galindo A., Jackson G. and Adjiman C. S., 2026. COSMO-NET: Fast and Accurate Machine Learning Surrogates for COSMO-based Molecular Descriptors. Molecular Systems Design & Engineering (in peer-review).

2024

4. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2024. Response to “Comment on ‘Binding Debye–Hückel theory for associative electrolyte solutions’” [J. Chem. Phys. 159, 154503 (2023)]. The Journal of Chemical Physics, 161 (15), p.057103.
5. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2024. Theoretical and Practical Investigation of Ion-ion Association in Electrolyte Solutions. The Journal of Chemical Physics, 160 (15), p.154509.
6. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2024. Novel Model for Predicting the Electrical Conductivity of Multisalt Electrolyte Solutions. The Journal of Physical Chemistry B, 128 (2), pp.536-550.

2023

7. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2023. New Electrical Conductivity Model for Electrolyte Solutions Based on the Debye-Hückel-Onsager Theory. The Journal of Physical Chemistry B, 127(46), pp.9954-9975.
8. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2023. Binding Debye–Hückel Theory for Associative Electrolyte Solutions. The Journal of Chemical Physics, 159 (15), p.154503.
9. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2023. Mean Ionic Activity Coefficient of Associative Electrolyte Solutions: A Comparison Study. Journal of Molecular Liquids, 386, p.122509.
10. **Naseri Boroujeni, S.**, Maribo-Mogensen, B., Liang, X. and Kontogeorgis, G.M., 2023. On The Estimation of Equivalent Conductivity of Electrolyte Solutions: The Effect of Relative Static Permittivity and Viscosity. Fluid Phase Equilibria, 567, p. 113698.

2022

11. **Naseri Boroujeni, S.**, Liang, X., Maribo-Mogensen, B. and Kontogeorgis, G.M., 2022. Comparison of Models for The Prediction of The Electrical Conductivity of Electrolyte Solutions. Industrial & Engineering Chemistry Research, 61(8), pp.3168-3185.

2020

12. **Naseri, S.**, Jamshidi, S. and Taghikhani, V., 2020. A New Multiphase and Dynamic Asphaltene Deposition Tool (MAD-ADEPT) to Predict the Deposition of Asphaltene Particles on Tubing Wall. Journal of Petroleum Science and Engineering, 195, p.107553.

Conference Presentations

2025

1. PPEPPD, Bad Gögging, Germany, 2025. Poster: Estimating Parameters of SAFT-γ Mie Equation of State Using COSMO-SAC Generated Pseudo Data. **S. Naseri Boroujeni**, George Jackson, Amparo Galindo, Claire Adjiman.
2. Molecular Systems Engineering Seminar, London, UK, 2025. Invited Talk: Benchmarking the Predictive Capabilities of the SAFT-γ Mie Eos for Properties of Interest in Pharmaceutical Systems. **S. Naseri Boroujeni**.

2024

3. The Sargent Centre for Process Systems Engineering Industrial Consortium Meeting, London, UK, 2024. Poster: Estimating Parameters of SAFT-γ Mie Equation of State Using COSMO-SAC Generated Pseudo Data. **S. Naseri Boroujeni**, George Jackson, Amparo Galindo, Claire Adjiman.
4. 28th Thermodynamics Conference, Delft, The Netherlands, 2024. Oral: Benchmarking the Predictive Capabilities of the SAFT-γ Mie Eos for Properties of Interest in Pharmaceutical Systems. **S. Naseri Boroujeni**, Thomas Bernet, Benjamin Tan, Ahmed Alyazidi, Shubhani Paliwal, George Jackson, Amparo Galindo, Claire Adjiman.
5. Molecular Systems Engineering Seminar, London, UK. Invited Talk: Ion-ion Association in Electrolyte Solutions: A Theoretical Investigation. **S. Naseri Boroujeni**.

2023

6. AIChE Annual Meeting, Orlando, USA, 2023. Oral: A Unified Model for the Thermodynamic, Transport, and Physical Properties of Associative Electrolyte Solutions. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
7. AIChE Annual Meeting, Orlando, USA, 2023. Oral: Binding Debye-Hückel Equation of State for Charged Hard Sphere Fluids. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
8. CERE and KT Consortium Annual Discussion Meeting, Helsingør, Denmark, 2023. Oral: Ion-ion Association in Electrolyte Solutions; A Theoretical Study of Mean Ionic Activity Coefficient, Electrical Conductivity, and Relative Static Permittivity. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
9. CERE and KT Consortium Annual Discussion Meeting, Helsingør, Denmark, 2023. Poster: Debye-Hückel Based Theories for Thermodynamic and Transport Properties of Charged Hard Sphere Fluids. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
10. PPEPPD, Tarragona, Spain, 2023. Poster: A New Model for the Electrical Conductivity of Electrolyte Solutions from the Debye-Hückel-Onsager Theory. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.

2022

11. 32nd ESAT, Graz, Austria, 2022. Oral: Electrical Conductivity of Associative Electrolyte Solutions. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
12. 32nd ESAT, Graz, Austria, 2022. Poster: A Predictive Analysis of Electrical Conductivity Models for Electrolyte Solutions. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
13. 27th Thermodynamics Conference, Bath, UK, 2022. Poster: A Predictive Analysis of Implicit Solvent Models for Associative Electrolyte Solutions. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
14. 27th Thermodynamics Conference, Bath, UK, 2022. Poster: Thermodynamic Properties of Associative Electrolyte Solutions; An Implicit Solvent Model. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
15. CERE and KT Consortium Annual Discussion Meeting, Snekkersten, Denmark, 2022. Oral: Ion-ion Association Insight from Electrical Conductivity and Mean Ionic Activity Coefficient. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.
16. CERE and KT Consortium Annual Discussion Meeting, Snekkersten, Denmark, 2022. Poster: Thermodynamic Properties of Associative Electrolyte Solutions; A Chemical Approach. **S. Naseri Boroujeni**, B. Maribo-Mogensen, X. Liang, and G. M. Kontogeorgis.

2021

17. CERE and KT Consortium Annual Discussion Meeting, online, 2021. Oral: An Evaluation Study of the Reliability and Applicability of Current Electric Conductance Models in Electrolyte Solutions. **S. Naseri Boroujeni**, X. Liang, B. Maribo-Mogensen, and G. M. Kontogeorgis.