Edgar Ivan **Sanchez Medina**

Doctoral researcher at MPI-Magdeburg | M.Sc. Chemical Engineering from Imperial College London

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I am passionate about using and developing Machine Learning methods for science applications, specifically, in chemical engineering systems from the molecular scale up to the plant scale. My main expertise revolves around **Graph Neural Networks** for molecular and mixture property prediction. I am also interested in **data-driven optimization**. I enjoy gaming, reading and walking around the city or in nature.

Formation

(expected) 2024 **PhD in Process Systems Engineering**, Max Planck Institute for Dynamics of Complex Technical Systems and Otto von Guericke University.

2019 **M.Sc. in Advanced Chemical Engineering with Process Systems Engineering**, Imperial College London. (Graduated with Distinction)

2018 **B.Eng. Chemical Engineering**, National Autonomous University of Mexico (UNAM). (Honorable mention)

Experience

Nov. 2019 – present | **Doctoral researcher, MPI-Magdeburg and Otto von Guericke University, Germany**
- GNNs for molecular and mixture property prediction.
- ML for process optimization.

Python · PyTorch · RDKit · Github · Aspen Plus · Aspen HYSYS · CasADI

May 2018 – Jul. 2018 | **Research intern, The University of Manchester, UK**
- Coded stochastic optimization algorithms for bioprocess systems applications.

Python

May 2018 – Jul. 2018 | **Electricity market analyst, Bravos Energía, Mexico**
- Developed an electricity tariffs model for forecasting until 2032 in the Wholesale Mexican electricity market.

VBA · Microsoft Excel

Jun. 2017 – Sep. 2017 | **Research assistant, McMaster University, Canada**
- Studied the dynamic behavior of semi-continuous distillation systems

Aspen Plus · Aspen Dynamics

Feb. 2017 – Jun. 2017 | **Research assistant, University of California-Riverside, USA**
- Turbidity experiments for the analysis of antiscalants used in Reverse Osmosis desalination plants.

Jun. 2016 – Aug. 2016 | **Research intern, University of Maryland, USA**
- Molecular dynamics of water-oil-alcohol systems.

NAMD · VMD

Teaching and Mentoring

2022 | **Lecturer, Otto von Guericke University, Germany**
- Machine Learning in Chemical Engineering - 4 CP (Summer semester)

2019 - 2022 | **Teaching assistant, Otto von Guericke University, Germany**
- Machine Learning in Chemical Engineering - 4 CP (Summer semester)
- Process Systems Engineering - 5 CP (Winter semester)

2021 - 2022 | **M.Sc. Theses supervised, Otto von Guericke University and TU-Chemnitz, Germany**
- Viswa Sunkavalli, *Graph Neural Networks for the prediction of environmental indicators of molecules*.
- Manoj Mangipudi, *Gaussian processes for the prediction of molecular EHS properties*.
- Anahita Iravanizad, *Enriching Graph Neural Network Input via Random Walks on Graphs*.
- Rahul Bankala, *Multi-objective optimization of an organic Rankine cycle system using Gaussian processes*.

Projects

Graph Neural Networks for the prediction of infinite dilution activity coefficients 2021 - 2022

Code Paper AIChE Annual Meeting 2022

GNN and hybrid GNN-mechanistic models for predicting activity coefficients at infinite dilution of binary mixtures.

PyTorch Geometric | RDKit | Pandas

Aspen Plus and Aspen HYSYS - Python connection 2021

Aspen Plus connection Aspen HYSYS connection

Connection between the process simulators Aspen Plus and Aspen HYSYS with Python.

Python

Pedagogical implementation of optimization methods used in ML 2020

Code

Jupyter Notebook with pedagogical implementations of common optimization algorithms used in ML (e.g., Gradient Descent, RMSProp, Adam, Constraint Newton's method and Interior Point method).

Numpy | Matplotlib | SciPy

Stochastic optimization algorithms 2018

Website

Implementation of Particle Swarm Optimization, Simulated Annealing, Tabu Search and Genetic Algorithm.

Numpy | Matplotlib

Publications

2022 Medina, E.I.S., Linke, S., Stoll, M. and Sundmacher, K., 2022. **Graph neural networks for the prediction of infinite dilution activity coefficients**. Digital Discovery, 1(3), pp.216-225.

2021 Iravanizad, A., Medina, E.I.S. and Stoll, M., 2021. **RaWaNet : Enriching Graph Neural Network Input via Random Walks on Graphs**. arXiv preprint arXiv:2109.07555.

2021 Medina, E.S., Linke, S. and Sundmacher, K., 2021. **Prediction of bioconcentration factors (BCF) using graph neural networks**. In Computer Aided Chemical Engineering (Vol. 50, pp. 991-997). Elsevier.

2021 Medina, E.S., Vallejo, D.R., Chachuat, B., Sundmacher, K., Petsagkourakis, P. and del Rio-Chanona, E.A., 2021. **Acyclic modular flowsheet optimization using multiple trust regions and Gaussian process regression**. In Computer Aided Chemical Engineering (Vol. 50, pp. 1117-1123). Elsevier.

2020 McBride, K., Sanchez Medina, E.I. and Sundmacher, K., 2020. **Hybrid semi-parametric modeling in separation processes : a review**. Chemie Ingenieur Technik, 92(7), pp.842-855.

2019 Jain, T., Sanchez, E., Owens-Bennett, E., Trussell, R., Walker, S. and Liu, H., 2019. **Impacts of antiscalants on the formation of calcium solids : Implication on scaling potential of desalination concentrate**. Environmental Science : Water Research & Technology, 5(7), pp.1285-1294.

2018 Madabhushi, P.B., Medina, E.I.S. and Adams II, T.A., 2018. **Understanding the dynamic behaviour of semi-continuous distillation**. In Computer Aided Chemical Engineering (Vol. 43, pp. 845-850). Elsevier.

Outreach and Volunteering

2019-2022 Part of the executive board and organizing team of the International Meeting of Artificial Intelligence and its Applications (**RIIAA**) in LATAM. Summer schools and conference (virtual and on-site) organization.

Languages

English ●●●●●
Spanish ●●●●●
German ●○○○○

Soft-skills training

- Visual storytelling
- Scientific Writing
- Communication