Vinicius Viena Santana

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EDUCATION

2021 – On going **PhD in Chemical and Biological Engineering**, University of Porto and MIT Portugal, Portugal

2019 – 2019 **Integrated Master in Chemical Engineering**, University of Porto, Portugal - Diploma Recognition

2013 – 2019 **Bachelor in Chemical Engineering**, Federal University of Bahia, Bahia, Brazil

LANGUAGES

Portuguese Mother tongue **English** Advanced (C1 - IELTs overall score 7.0)

German Basic

RESEARCH INTEREST

- Processing Modelling, Simulation and Optimization
- Artificial Intelligence Applied to Process Systems Engineering
- Natural Gas Reforming Process and Technologies
- Blue Hydrogen Economy

RESEARCH PROJECTS

2023 – On going — Intelligent control system for BCS operation in the field and under maximum flow condition, Petrobras, Brazil
Ph.D. Student Fellow

2021 – On going — Scientific Machine Learning and Hybrid Modeling Applied to Industrial Engineering - Towards Feasible Industrial AI.
Ph.D. Candidate at MIT Portugal Program - Data Science for Digital Transformation in Manufacturing

2021 – 2021 — Design of Hybrid - Pressure swing adsorption/Simulated moving bed process for olefin separation, Korean Research Institute of Chemical Technology, South Korea.
Master Student Fellow

2019 – 2021 — Artificial Intelligent oriented Cyclic Adsorption Separation and Reaction Processes Optimization and Control(AICySPrOC), UPorto, Portugal.
Master Student Fellow

2017 – 2019 — Transient analysis of true/simulated moving bed reactors: A case study on the synthesis of n-Propyl propionate, UPorto, Portugal.
Scientific Initiation Fellow

2015 – 2017 — Evaluation of the effects of gas mixtures, numerical methods and equations of state for the characterization of centrifugal compressors with uncertainties.
Scientific Initiation Fellow

2014 – 2015 — Evaluation of MgO/Fe3O4 e Al-SBA 15 catalysts for the production of biofuel from palm oil using membrane reactor.
Scientific Initiation Fellow

TRANSFER OF TECHNOLOGY

2022 – present — *AIKognitos* - A startup to promote the digital and smart transformation of the chemical industry.
Startup proposal in top 3 in the AINanoTEC Entrepreneurial Program.
Co-Creator

PUBLICATIONS

I contributed to the publication of 16 manuscripts, having an h-index of 5. Among these publications, I am a corresponding author in 3 and first author in 6.

PEER-REVIEWED PAPERS

2023 — 1. **Vinicius V. Santana**; Costa, Erbet A.; Rebello, Carine M.; Ribeiro, Ana Mafalda; Rackauckas, Chris; B. R. Nogueira, Idelfonso. "Efficient hybrid modeling and sorption model discovery for non-linear advection-diffusion-sorption systems: A systematic scientific machine learning approach". ArXiV (2023): doi:https://arxiv. org/abs/2303.13555. Pre-print and Submitted to Chemical Engineering Science.

2. Queiroz, Luana P.; Rebello, Carine M.; Costa, Erbet A.; **Vinicius V. Santana**;Rodrigues, Bruno C. L.; Rodrigues, Alírio E.; Ribeiro, Ana M.; Nogueira, Idelfonso B. R.. "Generating Flavor Molecules Using Scientific Machine Learning". ACSOmega 8 12 (2023): 10875-10887. doi:http://dx.doi.org/10.1021/acsomega.2c07176.

3. Queiroz, Luana P.; Rebello, Carine M.; Costa, Erbet A.; **Vinicius V. Santana**;Rodrigues, Bruno C. L.; Rodrigues, Alírio E.; Ribeiro, Ana M.; Nogueira, Idelfonso B. R.. "A Reinforcement Learning Framework to Discover Natural Flavor Molecules". Foods 12 6 (2023): 1147. doi:http://dx.doi.org/10.3390/foods12061147.

4. **Vinicius V. Santana**; Martins, Márcio A. F.; Loureiro, José M.; Ribeiro, Ana M.;Queiroz, Luana P.; Rebello, Carine M.; Rodrigues, Alírio E.; Nogueira, Idelfonso B.R.. "Novel Framework for Simulated Moving Bed Reactor Optimization Based on Deep Neural Network Models and Meta-heuristic Optimizers: An Approach with Optimality Guarantee". ACS Omega 8 7 (2023): 6463-6475. doi:http://dx.doi.org/10.1021/acsomega.2c06737.

2022

1. B. R. Nogueira, Idelfonso; **Vinicius V. Santana**; Ribeiro, Ana M.; Rodrigues, Alírio E.. "Using scientific machine learning to develop universal differential equation for multicomponent adsorption separation systems". The Canadian Journal of Chemical Engineering 100 9 (2022): 2279-2290. doi:http://dx.doi.org/10.1002/cjce.

2. B. R. Nogueira, Idelfonso ; Dias, Rafael O.M.; Rebello, Carine M.; Costa, Erbet A.; **Vinicius V. Santana**; Rodrigues, Alírio E.; Ferreira, Alexandre; Ribeiro, Ana M.. "A novel nested loop optimization problem based on deep neural networks and feasible operation regions definition for simultaneous material screening andprocess optimization". Chemical Engineering Research and Design 180 (2022):243-253. doi:http://dx.doi.org/10.1016/j.cherd.2022.02.013.

3. **Vinicius V. Santana**; Gama, Marlon S.; Loureiro, Jose M.; Rodrigues, Alírio E.; Ribeiro, Ana M.; Tavares, Frederico W.; Barreto, Amaro G.; Nogueira, Idelfonso B.R.. "A First Approach towards Adsorption-Oriented Physics-Informed Neural Networks: Monoclonal Antibody Adsorption Performance on an Ion-Exchange Column as a Case Study". ChemEngineering 6 2 (2022): 21. doi:http://dx.doi.org/10.3390/chemengineering6020021.

4. Costa, Erbet A.; Rebello, Carine M.; **Vinicius V. Santana**; Rodrigues, Alírio E.; Ribeiro, Ana M.; Schnitman, Leizer; Nogueira, Idelfonso B. R.. "Mapping Uncertainties of Soft-Sensors Based on Deep Feed forward Neural Networks through a Novel Monte Carlo Uncertainties Training Process". Processes 10 2 (2022): 409. doi:http://dx.doi.org/10.3390/pr10020409.

5. Rebello, Carine M.; Marrocos, Paulo H.; Costa, Erbet A.; **Vinicius V. Santana**; Rodrigues, Alírio E.; Ribeiro, Ana M.; Nogueira, Idelfonso B. R.. "Machine Learning-Based Dynamic Modeling for Process Engineering Applications: A Guideline for Simulation and Prediction from Perceptron to Deep Learning".Processes 10 2 (2022): 250. doi:http://dx.doi.org/10.3390/pr10020250.

2021

1. Regufe, Maria João; **Vinicius V. Santana**; Ferreira, Alexandre F. P.; Ribeiro, Ana M.; Loureiro, José M.; Nogueira, Idelfonso B. R.. "A Hybrid Modeling Framework for Membrane Separation Processes: Application to Lithium-Ion Recovery from Batteries". Processes 9 11(2021): 1939. doi:http://dx.doi.org/10.3390/pr9111939.

2. Regufe, Maria João; **Vinicius V. Santana**; Márcio André Fernandes Martins; Alexandre F.P Ferreira; José Miguel Loureiro; Alírio Egidio Rodrigues; Ana Mafalda Almeida Peixoto Ribeiro; Idelfonso Bessa dos Reis Nogueira. "Adsorption material composition and process optimization, a systematic approach based on Deep Learning". IFAC-PapersOnLine (2021).

3. **Vinicius V. Santana**; Martins, Márcio A.F.; Loureiro, José M.; Ribeiro, Ana M.; Rodrigues, Alírio E.; Nogueira, Idelfonso B.R.. "Optimal fragrances formulation using a deep learning neural network architecture: A novel systematic approach". Computers & Chemical Engineering 150 (2021): 107344. doi:http://dx.doi.org/10.1016/j.compchemeng.2021.107344.

4. **Vinicius V. Santana**; Martins, Márcio A. F.; Rodrigues, Alírio E.; Loureiro, José M.; Ribeiro, Ana M.; Nogueira, Idelfonso B. R.. "Abnormal Operation Tracking through Big-Data-Based Gram–Schmidt Orthogonalization: Production of n-Propyl Propionate in a Simulated Moving-Bed Reactor: A Case Study".Industrial & Engineering Chemistry Research (2021): doi:http://dx.doi.org/10.1021/acs.iecr.1c00214.

2020

1. **Vinicius V. Santana**; Martins, Márcio A.F.; Rodrigues, Alírio E.; Loureiro, José M.;Ribeiro, Ana M.; Nogueira, Idelfonso B.R.. "Transient Analysis of True/SimulatedMoving Bed Reactors: A Case Study on the Synthesis of n-Propyl Propionate".Computers & Chemical Engineering (2020): 106820. doi:http://dx.doi.org/10.1016/j.compchemeng.2020.106820.

2. Nogueira, Idelfonso B.R.; **Vinicius V. Santana**; Rodrigues, Alírio E.; Loureiro, José M.; Ribeiro, Ana M.. "Dynamics of a True Moving Bed Reactor: Synthesis of n-Propyl Propionate and an alternative optimization method". Chemical Engineeringand Processing - Process Intensification 148 (2020): 107821. doi:http://dx.doi.org/10.1016/j.cep.2020.107821.

3. Nogueira, Idelfonso B.R.; Martins, Márcio A.F.; Requião, Reiner; Oliveira, Amanda R.; **Vinicius V. Santana**; Koivisto, Hannu; Rodrigues, Alírio E.; Loureiro, José M.; Ribeiro, Ana M.. "Optimization of a True Moving Bed unit and determination of its feasible operating region using a novel Sliding Particle Swarm Optimization". Computers & Industrial Engineering 135 (2019): 368-381. doi:http://dx.doi.org/10.1016/j.cie.2019.06.020.

CONFERENCE PAPER

2019

Vinicius Viena Santana; Márcio A.F. Martins; Ana Mafalda Ribeiro; José M. Loureiro; **Vinicius V. Santana**. Dynamic response to process disturbances – An analysis of TMBR model in transient regime. *I Brazilian Congress on Process Systems Engineering.*

CONFERENCE POSTER

2022

Vinicius V. Santana; Ana Mafalda Ribeiro; Nogueira, Idelfonso B.R.. Advancing Scientific Machine Learning in Physical Sciences: Applications in Process SystemsEngineering. *MIT Portugal Annual Conference.*

DISTINCTIONS AND AWARDS

- Award-Winning poster in Data Science at the 2022 MIT Portugal Annual Conference. `https://mitportugal.mit.edu/poster-gallery`

THESIS/DISSERTATION

2019 Dynamics of Simulated Moving Bed Reactors: Synthesis of n-Propyl Propionate and Transient Analysis *Bachelor, Federal University of Bahia & Master, University of Porto, Faculty of Engineering.*

PROGRAMMING SKILLS

- **Python**: 4 years programming in Python for machine learning (ML) and PSE - personal projects in https://github.com/viniviena/Projects
- **Julia Language**: 2 years programming in Julia for ML and PSE - published paper with Julia Lab's co-PI Chris Rackauckas in scientific machine learning https://github.com/viniviena/ude_chromatography)

TEACHING

2016 – 2017 Chemistry
Volunteer High-School Teacher - Teached chemistry for socially vulnerable students preparing for high-school national exam.
Federal University of Bahia, Brazil

STUDENT SUPERVISION

MASTER'S

2022 – present Luana Queiroz
Supervisor
Bridging Fundamental and Process Scales by Scientific Machine Learning
Master in Chemical Engineering, University of Porto, Portugal.

UNDERGRADUATE

2021 – present Eduarda Augusto
Supervisor
A data scraping tool for digital documents applied to collect information on perfume descriptors
Chemical Engineering, University of Porto, Portugal.

2020 – present Bruno Rodrigues
Supervisor
A web scraping tool to collect information about perfume evaluation by customers.
Chemical Engineering, University of Porto, Portugal.

REVIEWER

- Canadian Journal of Chemical Engineering, Wiley

NON-ACADEMIC PROFESSIONAL EXPERIENCES

Feb 2019 – Feb 2020 Braskem, S/A. Industrial Innovation Intern. Collaborated with Engineers and Data scientists to create predictive models for PVC quality control and improvement.Perfoermed mass and energy balance of 100kT/year capacity PVC plant for CO2 and energy benchmark. Identified and mitigated brittle fracture risk for designed natural gas facility rigorous simulations.

May 2021 – Aug 2021 SENAI CIMATEC, Brazil. Artificial Intelligence Consultant - High-Performance Computing Center. Collaboration with Engineers, Computer Scientists and Meterologists to build machine learning models from massive data (1 TB to 10 TB) aiming at short- and medium-term wind and solar energy forecasting using Python libraries (pandas, tensorflow, numpy, Dask) and git for version control.