

# Lucas Francisco dos Santos

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## PERSONAL STATEMENT

Lucas is a lifelong learner passionate about problem-solving using model-based and data-driven approaches. He has worked with optimization, machine learning, modeling, and simulation in python, Julia, Matlab, GAMS, Pyomo, and JuMP since 2018. He has specialized in using machine learning and optimization to solve challenging decision-making tasks with chemical process simulators.

## EXPERIENCE

### Researcher @ State University of Maringa - Ago. 2018 – Jun. 2023 (4 yrs. 10 mos.)

*Onsite - Brazil*

- Global optimization of chemical process simulator assisted by machine learning models that replace simulations reducing computation time by more than 10,000 times;
- Derivative-free optimization of black-box simulations encompassing genetic algorithms, particle swarm, Nelder-Mead, and Bayesian optimization.
- Results showed consistent economic, energy, and environmental gains in chemical processes that were published in 5 papers in high-impact scientific journals.

### Researcher @ University of Alicante - Jan. 2022 – Jan. 2023 (1 yr.)

*Onsite - Spain*

- Development of nonlinear optimization models with black-box chemical process simulations embedded in JuMP (Julia) using state-of-the-art gradient-based solvers;
- Elaboration of automatic differentiable thermodynamic models in Julia aimed at optimizing chemical processes;
- Application to the optimal design of natural gas liquefaction processes enhanced energy efficiency.

### Researcher @ ETH Zürich - Ago – Nov. 2022 (4 mos.)

*Onsite - Switzerland*

- Development of mixed-integer linear optimization models of the European natural gas supply chain considering disruptive scenarios due to geopolitical reasons and based on its trade, price, and demand data and projections.
- Application of machine learning models to determine environmental impacts of the resulting natural gas supply chains with MSE in the order of  $10^{-8}$  and computation time from  $\approx 1$  min to  $10 \mu s$  compared to rigorous simulation.
- A web application was delivered for simulating and visualizing the supply chain and environmental impact results.

## EDUCATION

### Ph.D. in Chemical Engineering

Aug. 2019 – Jun. 2023

*State University of Maringa*

Supervisors: Professor Mauro Antônio da Silva Sá Ravagnani, PhD  
Professor Caliane Bastos Borba Costa, PhD

*University of Alicante (double degree)*

Supervisors: Professor José Antonio Caballero Suárez, PhD

Thesis: Optimization of chemical process simulation: application to optimal rigorous design of natural gas liquefaction processes.

### Master's degree in Chemical Engineering

Aug. 2018 – Aug. 2019

*State University of Maringa (UEM)*

GPA: 10/10

Supervisors: Professor Mauro Antônio da Silva Sá Ravagnani, PhD  
Professor Caliane Bastos Borba Costa, PhD

Dissertation: Optimal synthesis of work and heat exchange networks

### Bachelor in Chemical Engineering

Graduated in Jul. 2018

*State University of Maringa (UEM)*

GPA: 8.8/10

*University of California, Santa Barbara (UCSB)*

Set. 2015 – Jul. 2016

Fulbright undergraduate exchange student – fully funded scholarship.

GPA: 3.76/4.00

## PROFESSIONAL SKILLS

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- **Programming:** Python, Julia, MATLAB, git, HTML, CSS.
- **Software:** Aspen HYSYS, GAMS, DWSIM, Pyomo, Brightway2, JuMP, TensorFlow, Scikit-Learn, pandas, numpy.
- **Technical:** Optimization; Mathematical modeling; Surrogate modeling; Chemical process simulation, design, and synthesis; Machine learning; Software engineering, Life cycle assessment.
- **Personal strengths:** Strong work ethic; Problem solver; Project-oriented; Approachable; Critical thinking; Team player.
- **Languages:** Portuguese (native); English (fluent); Spanish (advanced).

## RESEARCH PROJECTS

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2023 – Ongoing (ETH Zürich):

Environmental impact assessment of the EU's plans to restructure the natural gas supply and demand

2022 – Ongoing (University of Alicante and State University of Maringa):

Optimization of implicit thermodynamic models with automatic differentiation in Julia

2022 – Ongoing (University of Alicante and State University of Maringa):

Subgradient for primal-dual interior point optimization of nondifferentiable black-box models

2021 – Ongoing (State University of Maringa):

Development of a free tool for optimization of chemical processes using DWSIM and Python

2019 – Ongoing (State University of Maringa and University of Alicante):

Surrogate-based optimization of chemical process simulation

## MAIN PUBLICATIONS

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Multi-objective simulation–optimization via kriging surrogate models applied to natural gas liquefaction process design

LF Santos, CBB Costa, JA Caballero, MASS Ravagnani  
Energy, 262, 125271, 2023

Framework for embedding black-box simulation into mathematical programming via kriging surrogate model applied to natural gas liquefaction process optimization.

LF Santos, CBB Costa, JA Caballero, MASS Ravagnani  
Applied Energy, 310, 118537, 2022

Framework for Embedding Process Simulator in GAMS via Kriging Surrogate Model Applied to C3MR Natural Gas Liquefaction Optimization

LF Santos, CBB Costa, JA Caballero, MASS Ravagnani  
Chemical Engineering Transactions, 88, 475-480, 2021

Kriging-assisted constrained optimization of single-mixed refrigerant natural gas liquefaction process

LF Santos, CBB Costa, JA Caballero, MASS Ravagnani  
Chemical Engineering Science, 241, 116699, 2021

Design and optimization of energy-efficient single mixed refrigerant LNG liquefaction process

LF Santos, CBB Costa, JA Caballero, MASS Ravagnani  
Brazilian Journal of Chemical Engineering, 1-14, 2021

Synthesis and optimization of work and heat exchange networks using an MINLP model with a reduced number of decision variables

LF Santos, CBB Costa, JA Caballero, MASS Ravagnani  
Applied Energy, 262, 114441, 2020

Mass-transfer driven spinodal decomposition in a ternary polymer solution

DR Tree, LF Dos Santos, CB Wilson, TR Scott, JU Garcia, GH Fredrickson  
Soft Matter, 15 (23), 4614-4628, 2019

## CONGRESS PRESENTATIONS

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- ESCAPE-32: 32<sup>nd</sup> European Symposium on Computer Aided Process Engineering – INP Toulouse, June 2022.
- II Brazilian Congress on Process Systems Engineering – Universidade Federal do Paraná, May 2022
- PRES'21: 24<sup>th</sup> Conference on Process Integration for Energy Saving and Pollution Reduction – Brno University of Technology, November 2021.
- I Brazilian Congress on Process Systems Engineering – Universidade Federal do Rio de Janeiro, May 2019
- IV Symposium of Paraná for process modeling, simulation, and control – Universidade Federal do Paraná, March 2019