

# Luís Fernando Mercier Franco

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Born: January 8th, 1988—São Paulo, Brazil  
Nationality: Brazilian

## Professional Experience

2023	<i>Visiting Professor</i> , Reservoir Engineering Research Institute, USA
2022	<i>Associate Professor</i> , University of Campinas, Brazil
2017-2022	<i>Assistant Professor</i> , University of Campinas, Brazil
2016-2017	<i>Postdoctoral Research Associate</i> , Texas A&M University at Qatar, Qatar
2012-2015	<i>Graduate Student</i> , University of São Paulo, Brazil
2013-2014	<i>Research Visitor</i> , University of Notre Dame, USA

## Higher Education

2012-2015	DSC in Chemical Engineering, “Study on the Thermodynamics of Bovine Serum Albumin aqueous solutions: experiments, modeling and molecular simulations”, University of São Paulo, Brazil
2011-2012	MSc in Chemical Engineering, “Study of the solid-liquid equilibrium of systems containing amino acids and proteins”, University of São Paulo, São Paulo ( <i>in Portuguese</i> )
2006-2011	BSc in Chemical Engineering, University of São Paulo, Brazil

## Distinctions and Awards

2023	Fulbright Junior Faculty Member Award
2022	Patron of the Chemical Engineering Class of 2022, University of Campinas
2015	Helmut Knapp Poster Award, European Symposium on Applied Thermodynamics

## Professional Membership

- Elected Director (2023-2025) of the Brazilian Association of Chemical Engineers.

## Journal articles

1. **Franco, LFM**, Pessoa Filho, PA (2011), "On the solubility of proteins as a function of pH: mathematical development and application", *Fluid Phase Equilibr.* 306, 242-250 <https://doi.org/10.1016/j.fluid.2011.04.015>
2. **Franco, LFM**, Pessoa Filho, PA (2013), "On the relationship between the solubility of proteins and the osmotic second virial coefficient", *Braz. J. Chem. Eng.* 30, 95-104 <https://doi.org/10.1590/S0104-66322013000100011>
3. **Franco, LFM**, Mattedi, S, Pessoa Filho, PA (2013), "A new approach for the thermodynamic modeling of the solubility of amino acids and  $\beta$ -lactam compounds as a function of pH", *Fluid Phase Equilibr.* 354, 38-46 <https://doi.org/10.1016/j.fluid.2013.06.009>
4. **Franco, LFM**, Oliveira, CLP, Pessoa Filho, PA (2015), "Thermodynamics of protein aqueous solutions: from the structure factor to the osmotic pressure", *AIChE J.* 61, 2871-2880 <https://doi.org/10.1002/aic.14802>
5. **Franco, LFM**, Castier, M, Economou, IG (2016), "Anisotropic parallel self-diffusion coefficients near the calcite surface: A molecular dynamics study", *J. Chem. Phys.* 145, 084702 <https://doi.org/10.1063/1.4961408>
6. **Franco, LFM**, Castier, M, Economou, IG (2016), "Diffusion in homogeneous and in inhomogeneous media: a new unified approach", *J. Chem. Theory Comput.* 12, 5247-5255 <https://doi.org/10.1021/acs.jctc.6b00653>
7. **Franco, LFM**, Economou, IG, Castier, M (2017), "Statistical mechanical model for adsorption coupled with SAFT-VR Mie equation of state", *Langmuir* 33, 11291-11298 <https://doi.org/10.1021/acs.langmuir.7b02686>
8. **Franco, LFM**, Castier, M, Economou, IG (2017), "Two-body perturbation theory versus first order perturbation theory: A comparison based on the square-well fluid", *J. Chem. Phys.* 147, 214108 <https://doi.org/10.1063/1.4994823>
9. Santos, MS, **Franco, LFM**, Castier, M, Economou, IG (2018), "Molecular dynamics simulation of  $n$ -alkanes and CO<sub>2</sub> confined by calcite nanopores", *Energy & Fuels* 32, 1934-1941 <https://doi.org/10.1021/acs.energyfuels.7b02451>
10. Nikolaidis, IK, **Franco, LFM**, Vechot, LN, Economou, IG (2018), "Modeling of physical properties and vapor-liquid equilibrium of ethylene and ethylene mixtures with equations of state", *Fluid Phase Equilibr.* 470, 149-163 <https://doi.org/10.1016/j.fluid.2018.01.021>
11. Menezes, DES, Ralha, TW, **Franco, LFM**, Pessoa Filho, PA, Robustillo-Fuentes, MD (2018), "Simulation and experimental study of methane-propane hydrate dissociation by high pressure differential scanning calorimetry", *Braz. J. Chem. Eng.* 35, 403-414 <https://doi.org/10.1590/0104-6632.20180352s20160329>

12. Tsimpanogiannis, IN, Moulτος, OA, **Franco, LFM**, Spera, MBM, Erdos, M, Economou, IG (2019), "Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies", *Mol. Sim.* 45, 425-453 <https://doi.org/10.1080/08927022.2018.1511903>
13. **Franco, LFM** (2019), "On the structure of a confined ideal gas: A statistical mechanical description with an external field", *Fluid Phase Equilibr.* 489, 99-103 <https://doi.org/10.1016/j.fluid.2019.02.014>
14. Lopes, JT, **Franco, LFM** (2019), "New Thermodynamic Approach for Nonspherical Molecules Based on a Perturbation Theory for Ellipsoids", *Ind. Eng. Chem. Res.* 58, 6850-6859 <https://doi.org/10.1021/acs.iecr.9b00766>
15. Araújo, IS, **Franco, LFM** (2019), "A model to predict adsorption of mixtures coupled with SAFT-VR Mie Equation of state", *Fluid Phase Equilibr.* 496, 61-68 <https://doi.org/10.1016/j.fluid.2019.05.021>
16. da Costa, BLV, Raghavendran, V, **Franco, LFM**, Chaves Filho, AB, Yoshinaga, MY, Miyamoto, S, Basso, TO, Gombert, AK (2019), "Forever panting and forever growing: physiology of *Saccharomyces cerevisiae* at extremely low oxygen availability in the absence of ergosterol and unsaturated fatty acids", *FEMS Yeast Res.* 19, foz054 <https://doi.org/10.1093/femsyr/foz054>
17. Lopes, JT, **Franco, LFM** (2020), "Prediction of isochoric heat capacity: Discrete versus continuous potentials", *Fluid Phase Equilibr.* 520, 112380 <https://doi.org/10.1016/j.fluid.2019.112380>
18. Bartolomeu, RAC, **Franco, LFM** (2020), "Thermophysical properties of supercritical H<sub>2</sub> from Molecular Dynamics simulations", *Int. J. Hydrog. Energy* 45, 16372-16380 <https://doi.org/10.1016/j.ijhydene.2020.04.164>
19. Fiates, J, Zhang, Y, **Franco, LFM**, Maginn, EJ, Doubek, G (2020), "Impact of anion shape on Li<sup>+</sup> solvation and on transport properties for lithium-air batteries: a molecular dynamics study", *Phys. Chem. Chem. Phys.* 22, 15842-15852 <https://doi.org/10.1039/D0CP00853B>
20. Spera, MBM, **Franco, LFM** (2020), "Surface and confinement effects on the self-diffusion coefficients for methane-ethane mixtures within calcite nanopores", *Fluid Phase Equilibr.* 522, 112740 <https://doi.org/10.1016/j.fluid.2020.112740>
21. Bartolomeu, RAC, Lopes, JT, Spera, MBM, **Franco, LFM** (2020), "Derivative properties data for hydrogen-ethylene supercritical mixtures using a SAFT EoS and a SAFT force field", *J. Chem. Eng. Data* 65, 5735-5742 <https://doi.org/10.1021/acs.jced.0c00699>
22. Paixão, VP, **Franco, LFM**, Dangelo, JVH (2020), "Simulation and Design of a Water-Gas Shift Catalytic Multitubular Reactor with Integrated Heat Exchange", *Ind. Eng. Chem. Res.* 59, 21429-21438 <https://doi.org/10.1021/acs.iecr.0c03262>

23. AlYazidi, A, **Franco, LFM**, Economou, IG, Castier, M (2021), “Modeling confined fluids with the multicomponent potential theory of adsorption and the SAFT-VR Mie equation of state”, *Fluid Phase Equilibr.* 534, 112941 <https://doi.org/10.1016/j.fluid.2021.112941>
24. Gonçalves, AF, **Franco, LFM** (2021), “On the conversion of the confined ideal gas distribution between the canonical and the grand canonical ensembles”, *Fluid Phase Equilibr.* 533, 112962 <https://doi.org/10.1016/j.fluid.2021.112962>
25. Vicentini, R, da Silva, LM, Franco, DV, Nunes, W, Fiates, J, Doubek, G, **Franco, LFM**, Freitas, RG, Fantini, C, Zanin, H (2021), “Raman probing carbon & aqueous electrolytes interfaces and molecular dynamics simulations towards understanding electrochemical properties under polarization conditions in supercapacitors”, *J. Energy Chem.* 60, 279-292 <https://doi.org/10.1016/j.jechem.2021.01.003>
26. Lopes, JT, **Franco, LFM** (2021), “A possible way to explicitly account for different molecular geometries with an equation of state”, *J. Mol. Liq.* 330, 115676 <https://doi.org/10.1016/j.molliq.2021.115676>
27. Lopes, JT, Romano, F, Grelet, E, **Franco, LFM**, Giacometti, A (2021), “Phase behavior of hard cylinders”, *J. Chem. Phys.* 154, 104902 <https://doi.org/10.1063/5.0040942>
28. Spera, MBM, **Franco, LFM** (2021), “The effect of thermal gradients on adsorption”, *Fuel* 295, 120553 <https://doi.org/10.1016/j.fuel.2021.120553>
29. Nobre, NEL, **Franco, LFM** (2021), “Isochoric heat capacity of confined fluids: the effect of pore width”, *Fluid Phase Equilibr.* 549, 113202 <https://doi.org/10.1016/j.fluid.2021.113202>
30. de Souza, NB, Lopes, JT, **Franco, LFM** (2021), “Thermodynamic perturbation theory coefficients for ellipsoidal molecules”, *Fluid Phase Equilibr.* 549, 113209 <https://doi.org/10.1016/j.fluid.2021.113209>
31. **Franco, LFM**, Pessôa Filho, PA (2022), “Mathematical Description of the Enzymatic Activity of Proteins with Ionizable Groups Exhibiting Deviations from the Henderson-Hasselbalch Equation”, *Appl. Biochem. Biotechnol.* 194, 1221-1234 <https://doi.org/10.1007/s12010-021-03700-y>
32. Gonçalves, AF, Castier, M, **Franco, LFM** (2022), “The role of cross-association between carbon dioxide and hydrogen sulfide using the SAFT-VR Mie equation of state”, *Fluid Phase Equilibr.* 559, 113493 <https://doi.org/10.1016/j.fluid.2022.113493>
33. Paixão, VP, **Franco, LFM**, Dangelo, JVH (2022), “Thermoeconomic analysis of conventional and recuperative ORC for heat recovery of exothermic reactions”, *Therm. Sci. Eng. Prog.* 33, 101347 <https://doi.org/10.1016/j.tsep.2022.101347>

34. Spera, MBM, Braga, FN, Bartolomeu, RAC, Economou, IG, **Franco, LFM** (2022), “Diffusion of fluids confined in carbonate minerals: A molecular dynamics simulation study for carbon dioxide and methane–ethane mixture within calcite”, *Fuel* 325, 124800 <https://doi.org/10.1016/j.fuel.2022.124800>
35. de Souza, NB, Lopes, JT, **Franco, LFM** (2022), “Thermodynamic perturbation theory coefficients for hard spherocylinders and cylinders”, *Fluid Phase Equilibr.* 561, 113543 <https://doi.org/10.1016/j.fluid.2022.113543>
36. Lyra, EP, **Franco, LFM** (2022), “Deriving force fields with a multiscale approach: from ab initio calculations to molecular-based equations of state”, *J. Chem. Phys.* 157, 114107 <https://doi.org/10.1063/5.0109350>
37. Germiniani, LGL, Beppu, MM, **Franco, LFM** (2022), “Densities of the Standard Amino Acids in Aqueous Solutions via Molecular Dynamics Simulations”, *J. Chem. Eng. Data* 67, 797-808 <https://doi.org/10.1021/acs.jced.1c00645>
38. Santos, MS, Hamza, M, **Franco, LFM**, Castier, M, Economou, IG (2022), “Molecular Understanding of Enhanced Hydrocarbon Recovery Processes: Role of Local Self-Diffusion Coefficients of Complex Mixtures”, *Energy Fuels* 36, 8301-8310 <https://doi.org/10.1021/acs.energyfuels.2c01031>
39. Gonçalves, AF, Castier, M, **Franco, LFM** (2023), “Capillary condensation: Limitations of the multicomponent potential theory of adsorption (MPTA)”, *Fluid Phase Equilibr.* 569, 113759 <https://doi.org/10.1016/j.fluid.2023.113759>
40. Coelho, FM, **Franco, LFM**, Firoozabadi, A (2023), “Thermodiffusion of CO<sub>2</sub> in Water by Nonequilibrium Molecular Dynamics Simulations”, *J. Phys. Chem. B* 127, 2749-2760 <https://doi.org/10.1021/acs.jpccb.2c08260>
41. **Franco, LFM et al.** (2023), “A competency-based chemical engineering curriculum at the University of Campinas in Brazil”, *Educ. Chem. Eng.* 44, 21-34 <https://doi.org/10.1021/acs.jpccb.2c08260>
42. Gonçalves, AF, **Franco, LFM**, Castier, M (2023), “Adsorption in a centrifugal field: a thermodynamic analysis”, *Fluid Phase Equilibr.* 572, 113820 <https://doi.org/10.1016/j.fluid.2023.113820>
43. **Franco, LFM**, Firoozabadi, A (2023), “Computation of Shear Viscosity by a Consistent Method in Equilibrium Molecular Dynamics Simulations: Applications to 1-Decene Oligomers”, *J. Phys. Chem. B*, 127, 10043-10051 <https://doi.org/10.1016/j.fluid.2023.113820>
44. Coelho, FM, **Franco, LFM**, Firoozabadi (2023), “Effect of Salinity on CO<sub>2</sub> Thermodiffusion in Aqueous Mixtures by Molecular Dynamics Simulations”, *ACS Sustain. Chem. Eng.*, 11, 17086-17097, <https://doi.org/10.1021/acssuschemeng.3c05269>

45. de Souza, NF, Picard, C, **Franco, LFM**, Coasne, B (2024), “Thermal Conductivity of a Fluid-Filled Nanoporous Material: Underlying Molecular Mechanisms and the Rattle Effect”, *J. Phys. Chem. B*, 128, 2516-2527, <https://doi.org/10.1021/acs.jpcb.3c07088>
46. Polat, HM, Coelho, FM, Vlugt, TJH, **Franco, LFM**, Tsimpanogiannis, IN, Moulton, OA (2024), “Diffusivity of CO<sub>2</sub> in H<sub>2</sub>O: A Review of Experimental Studies and Molecular Simulations in the Bulk and in Confinement”, *J. Chem. Eng. Data*, 69, 3296-3329, <https://doi.org/10.1021/acs.jced.3c00778>
47. Gonçalves, AF, Amancio, RJ, Castier, M, **Franco, LFM** (2024), “Classical Density Functional Theory Consistent with the SAFT-VR Mie Equation of State: Development of Functionals and Application to Confined Fluids”, *J. Chem. Eng. Data*, 69, 3645-3659, <https://doi.org/10.1021/acs.jced.4c00020>
48. Costa, LF, Germiniani, LG, **Franco, LFM** (2024), “An analysis of the dipalmitoylphosphatidylcholine bilayer gel phases predicted with molecular dynamics simulations using force fields from the GROMOS family”, *Fluid Phase Equilib.*, 583, 114115, <https://doi.org/10.1016/j.fluid.2024.114115>
49. Sermoud, VM, Gonçalves, AF, Barreto Jr, AG, **Franco, LFM**, Tavares, FW, **Castier, M** (2024), “Classical density functional theory of confined fluids: From getting started to modern applications”, *Fluid Phase Equilib.*, 586, 114177, <https://doi.org/10.1016/j.fluid.2024.114177>
50. Coelho, FM, Vinogradov, J, Derksen, JJ, **Franco, LFM** (2024), “Electrokinetic properties of NaCl solution via molecular dynamics simulations with scaled-charge electrolytes”, *J. Chem. Phys.*, 161, 044508, <https://doi.org/10.1063/5.0219098>
51. Canzian, EP, Cruz, AA, Mazza, R, **Franco, LFM** (2024), “Phase equilibrium calculations with specified vapor fraction”, *Fluid Phase Equilib.*, 589, 114274, <https://doi.org/10.1016/j.fluid.2024.114274>
52. Weidmann, AB, **Franco, LFM**, Sum, AK, Pessôa Filho, P de A (2024), “Dissociation temperature of gas hydrates through isenthalpic-isobaric molecular dynamics simulations”, *J. Chem. Phys.*, 161, 174505, <https://doi.org/10.1063/5.0234866>
53. Coelho, FM, **Franco, LFM** (2024), “The Interplay between Dynamics and Structure on the Dielectric Tensor of Nanoconfined Water: Surface Charge and Salinity Effect”, *J. Phys. Chem. B* (accepted)

Invited Lectures and Presentations on international meetings

- de Souza, NF, Benelli, FE, Quinzio, MJ, Rodrigues-Reartes, SB, Franco, LFM, Cismondi-Duarte, M, “Enthalpy and Entropy of Mixing of Hydrocarbon Mixtures: Insights from Molecular Simulations”, *In: 12<sup>th</sup> Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design - Equifase*, Évora, Portugal (oral)
- 2023 de Souza, NF, Picard, C, Franco, LFM, Coasne, B, “Heat transfer mechanisms in confined fluids: a molecular dynamics study”, *In: 16<sup>th</sup> International Conference on Properties and Phase Equilibria for Product and Process Design - PPEPPD*, Tarragona, Spain (oral)
- 2022 Franco, LFM, “Confinement effects: what we can learn from molecular simulations”, *In: 14<sup>th</sup> Brazilian Meeting on Adsorption - EBA*, Brasília, Brazil (Invited Lecture)
- 2018 Franco, LFM, “Thermodynamics of confined fluids”, *In: 11<sup>th</sup> Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design - Equifase*, Córdoba, Argentina (Invited Lecture)
- 2017 Franco, LFM, Economou, IG, Castier, M, “An extension of SAFT-VR Mie to predict confined fluid properties: application to adsorption isotherms”, *In: 29<sup>th</sup> European Symposium on Applied Thermodynamics - ESAT*, Bucharest, Romania (oral)
- 2017 Franco, LFM, Castier, M, Economou, IG, “A theoretical expression for the residual Helmholtz free energy due to confinement effect: application to adsorption isotherms using SAFT-VR Mie”, *In: SAFT conference*, Heidelberg, Germany (oral)
- 2016 Franco, LFM, Castier, M, Economou, IG, “Molecular Simulation of Confined Fluids: Pure components and mixtures”, *In: 14<sup>th</sup> International Conference on Properties and Phase Equilibria for Product and Process Design - PPEPPD*, Porto, Portugal (poster)
- 2015 Franco, LFM, Oliveira, CLP, Pessôa Filho, PA, “On the structure factor of proteins in aqueous solutions”, *In: 28<sup>th</sup> European Symposium on Applied Thermodynamics - ESAT*, Athens, Greece (poster)
- 2015 Franco, LFM, Zhang, Y, Pessôa Filho, PA, Maginn, EJ, “On the universal reference for Walden plot”, *In: 28<sup>th</sup> European Symposium on Applied Thermodynamics - ESAT*, Athens, Greece (oral)
- 2014 Franco, LFM, Oliveira, CLP, Pessôa Filho, PA, “On the behaviour of the attractive potential of globular proteins: analytical expression and experimental determination of the structure factor”, *In: 23<sup>rd</sup> International Conference on Chemical Thermodynamics - ICCT*, Durban, South Africa (oral)
- 2013 Franco, LFM, Pessôa Filho, PA, “Insights on solid-liquid equilibrium operations in the downstream processing of proteins”, *In: 13<sup>th</sup> International Conference on Properties and Phase Equilibria for Product and Process Design - PPEPPD*, Puerto Iguazu, Argentina (oral)
- 2012 Franco, LFM, Mattedi, S, Pessôa Filho, PA, “Solid-liquid equilibrium of amino acids and  $\beta$ -lactam compounds as a function of pH”, *In: 22<sup>nd</sup> International Conference on Chemical Thermodynamics - ICCT*, Búzios, Brazil (poster)
- 2012 Franco, LFM, Pessôa Filho, PA, “A theoretical study on the relationship between protein solubility and the osmotic second virial coefficient”, *In: 22<sup>nd</sup> International Conference on Chemical Thermodynamics - ICCT*, Búzios, Brazil (poster)

## Grants

Since 2017, more than USD 3,250,000 from agencies and companies have been granted to fund research.

1. “Development of a in-line emulsion characterization system based on ultrasound”, (co-PI with AMF Fileti), Petrobras, USD 220,000, (12/18-01/24)
2. “Junior Professor Grant”, (PI), University of Campinas, USD 3,000, (02/18-02/19)
3. “Production and process technologies for oil refining”, (co-PI with MC Costa), ANP, USD 740,000, (01/19-present)
4. “Molecular Dynamics of Confined Fluids: equilibrium and transport properties”, (PI), FAPESP, USD 64,000, (02/19-present)
5. “Remodeling of the Laboratory of Complex Systems Engineering - LESC”, (PI), University of Campinas, USD 5,000, (03/20-03/21)
6. “Chemical modifications on the PPE’s surfaces with antiviral agents for controlling Covid-19”, (co-PI with MM Beppu), CAPES, USD 435,000, (07/20-present)
7. “Molecular simulation of confined fluids for industrial applications”, (PI), FAPESP, USD 7,000, (05/22-04/24)
8. “Dense gas flow through Gas Lift Valves”, (co-PI with RA Mazza), Petrobras, USD 800,000, (01/23-present)
9. “Engineering and screening new solid sorbents for CO<sub>2</sub> capture using a multiscale computational approach”, (PI), TotalEnergies, USD 1,000,000, (12/23-present)

## Consultancy Services

1. (2023) Beiersdorf, Consultancy services to develop a process simulator to compute the internal pressure in vessels;
2. (2023) Inpasa, Consultancy services to compute CO<sub>2</sub> emissions.

## Doctoral Dissertations Directed

1. Juliane Fiates (joint with Gustavo Doubek), “Understanding the role of electrolytes and electrodes on Li-air batteries through molecular dynamics simulation”, 2020, (Currently Postdoctoral Research Associate, @Newcastle University, UK)
2. Joyce Tavares Lopes, “Monte Carlo simulations and Equations of State based on perturbation theory”, 2020, (Currently Senior C++ Developer @ToffeeX, UK)



3. Marcelle Bruna de Mendonça Spera, “On the diffusion of confined hydrocarbon mixtures via Molecular Dynamics simulation”, 2021, (Currently Postdoctoral Research Associate, @University of Stuttgart, Germany)
4. Luiz Guilherme Lomônaco Germiniani (joint with Marisa M. Beppu), “Computational modeling of molecular interactions of amino acids and peptides”, 2021, (Currently Postdoctoral Research Associate, @University of Campinas, Brazil)
5. Vitor Pirovani Paixão (joint with José Vicente H. Dangelo), “Shift reactor design with integrated heat exchange and waste heat usage”, 2022, (Currently Process Engineer @Petrobras, Brazil)
6. Emerson Parazzi Lyra, “Propriedades de copolímeros em bloco anfífilos em solução” (*in Portuguese*), 2023, (Currently Postdoctoral Research Associate, @University of Campinas, Brazil)
7. André de Freitas Gonçalves (joint with Marcelo Castier), “Estudo de equilíbrio de fases em sistemas confinados” (*in Portuguese*), 2024, (Currently Postdoctoral Research Associate, @University of Campinas, Brazil)

## Doctoral Dissertations under Direction

1. Rodrigo Amaral Coutinho Bartolomeu, “Modelagem e inversão matemática da atenuação acústica para determinação da distribuição do tamanho de gotas em emulsões” (*in Portuguese*), 2019-present
2. Arthur Benigno Weidmann (joint with Pedro de A. Pessoa Filho), “Simulação de Dinâmica Molecular de hidratos de gás” (*in Portuguese*), 2020-present
3. Larissa Fernandes Costa, “Dinâmica Molecular da interação de compostos desinfetantes com o envoltório do SARS-CoV-2” (*in Portuguese*), 2020-present
4. Nikolas Ferreira de Souza, “Estudo das metodologias de cálculo de propriedades de transporte em meios confinados por dinâmica molecular” (*in Portuguese*), 2020-present
5. Felipe Mourão Coelho, “Simulações de dinâmica molecular para estudo de propriedades de equilíbrio de misturas de fluidos confinados” (*in Portuguese*), 2021-present
6. Nathan Barros de Souza, “New equation of state for mixtures of nonspherical molecules based on statistical mechanics”, 2022-present
7. Estefânia Pintor Canzian, “Termodinâmica de Não-Equilíbrio aplicada a reservatórios de óleo & gás” (*in Portuguese*), 2022-present
8. Gilberto Ribeiro Pinto Júnior, “Aplicação de simulações Rede Boltzmann para compreensão de difusão em mesoescala em meios porosos” (*in Portuguese*), 2024-present

9. Gabriel Pereira da Silva, “Propriedades de transporte de mecânicas de materiais adsorptivos para captura de CO<sub>2</sub> via dinâmica molecular” (*in Portuguese*), 2024-present
10. Ana Paula de Barros Barreto Mazó, “Determinação de isotermas de adsorção de CO<sub>2</sub> em diferentes materiais adsorptivos por GCMC” (*in Portuguese*), 2024-present

## Master Dissertations Directed

1. Isa Silveira de Araújo, “Modeling of mixture adsorption: an extension of SAFT-VR Mie Equation of State”, 2019, (Currently PhD candidate, @University of Texas, USA)
2. Rodrigo Amaral Coutinho Bartolomeu, “Estudo de nanovazamento de hidrogênio confinado por simulações de dinâmica molecular” (*in Portuguese*), 2019, (Currently PhD candidate, @University of Campinas, Brazil)
3. Lucas Giuliano Murgida de Moraes, “Flow in porous media and adsorption of binary fluids via Lattice Boltzmann Method”, 2020, (Currently PhD candidate, @University of Campinas, Brazil)
4. Natália Esperança Lisboa, “Calor específico a volume constante de fluidos confinados: efeito do tamanho de poro” (*in Portuguese*), 2021
5. Flávia Nogueira Braga, “Study of diffusion aspects in confined media subject to external electric potential for application in catalysis via Molecular Dynamics simulations”, 2022, (Currently PhD candidate, @University of Aveiro, Portugal)
6. Nathan Barros de Souza, “Teoria de perturbação termodinâmica para corpos convexos rígidos ” (*in Portuguese*), 2022, (Currently PhD candidate, @University of Campinas, Brazil)
7. Rodolfo José Amâncio, “Simulação molecular de alcanos lineares sob confinamento: avaliação de propriedades de conformação e termos de perturbação termodinâmica usando teorias BH e WCA” (*in Portuguese*), 2024, (Currently Data Scientist @Albert Einstein, Brazil)
8. Bruno Salomão Leão (joint with Bradley Olsen from MIT and Marisa M. Beppu from Unicamp), “Development of a canonicalization algorithm for BigSMILES and a syntax for representing coarse-grained polymers”, 2024, (Currently Consultant @Visagio, Brazil)

## Master Dissertations under Direction

1. Luiz Felipe Joana Ribeiro, “Cálculo da produção de entropia local em escoamentos turbulentos” (*in Portuguese*), 2022-present
2. Thiago Ferrazin Fernandes, “Cálculos ab initio para predição das interações cruzadas de misturas de CO<sub>2</sub> em materiais adsorventes” (*in Portuguese*), 2024-present

## Postdoctoral Researchers under Direction

1. Dr. André de Freitas Gonçalves, 2024-present
2. Dr. Emerson Parazzi Lyra, 2024-present
3. Dr. Luiz Guilherme Lomônaco Germiniani, 2021-present

## Postdoctoral Researchers Directed

1. Dr. Arley Alles Cruz, 2022-2024 (Currently Postdoctoral Research Associate, UNIT, Brazil)
2. Dr. Daniela da Silva Damaceno, 2020-2021, (Currently Research Scientist, SINTEF Energe Research, Norway)
3. Dr. Lilian Caroline Kramer Biasi, 2020-2021, (Currently Postdoctoral Research Associate, University of São Paulo, Brazil)

## Services Activities at Unicamp

- Head of Teaching of the School of Chemical Engineering (2023-present);
- Vice Head of Teaching of the School of Chemical Engineering (2021-2023);
- Representative of the Technological Area at the Consulting Board of the Cátedra Sérgio Vieira de Mello (2021-present);
- Representative of the Associate Professors at the University Board (2022-present);
- Representative of the Assistant Professors at the University Board (2019-2022);

## Graduate courses taught at Unicamp

- IQ401 - Thermodynamics
- IQ475 - Topics on Chemical Systems
- IQ620 - Thermodynamics II
- IQ707 - Molecular simulation for the calculation of petroleum-based fluid properties

## Undergraduate courses taught at Unicamp

- EQ045 - Topics on Chemical Processes I
- EQ048 - Topics on Computational Tools for Chemical Engineering
- EQ101 - Introduction to Processes and Chemical Industry
- EQ201 - Mass and Energy Balances
- EQ210 - Modeling in Engineering 1 (*new curriculum*)
- EQ211 - Macroscopic Balances (*new curriculum*)
- EQ213 - Kinetic and Thermodynamic Models (*new curriculum*)
- EQ220 - Numerical Methods (*new curriculum*)
- EQ240 - Engineering and Society 1 (*new curriculum*)
- EQ415 - Thermodynamics I
- EQ481 - Introduction to Chemical Engineering
- EQ541 - Transport Phenomena I
- EQ601 - Chemical Engineering Laboratory I
- EQ801 - Chemical Engineering Laboratory III
- EQ922 - Chemical Process Design

## Agency Review Activities

- ACS PRF
- CNPq
- FAPESP
- FAEPEX
- SDummont - LNCC

## Journal Review Activities

- ACS Applied Materials & Interfaces
- Adsorption
- Applied Energy
- Brazilian Journal of Chemical Engineering
- Canadian Journal of Chemical Engineering

- Computers and Mathematics with Applications
- Computational Materials Science
- Energy & Fuels
- European Physical Journal Plus
- Fuel
- Fluid Phase Equilibria
- Industrial & Engineering Chemistry Research
- Journal of Chemical & Engineering Data
- Journal of Chemical Thermodynamics
- Journal of Physical Chemistry
- Journal of Molecular Liquids
- Journal of Molecular Modeling
- Journal of Natural Gas Science and Engineering
- Journal of Supercritical Fluids
- Langmuir
- Microelectronics Reliability
- Molecular Physics
- Physical Chemistry Chemical Physics