Marcelo Castier

Chemical Engineering Program
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Born: November 21, 1957—Rio de Janeiro, Brazil
Nationality: Brazilian

Current position

Adjunct Professor of Chemical Engineering, Texas A&M University at Qatar

Areas of specialization

Thermodynamics • Phase equilibrium • Separation processes • Energy integration • Computer applications in Chemical Engineering

Academic degrees

1981 B.Sc. in Chemical Engineering, "Cum Laude", Federal University of Rio de Janeiro(UFRJ), Rio de Janeiro, Brazil

1985 M.Sc. in Chemical Engineering, Federal University of Rio de Janeiro(UFRJ), Rio de Janeiro, Brazil
Thesis: An Executive Program for Chemical Process Simulation
Supervisor: K. Rajagopal
Comment: the developed program became the seed of PETROX, the in-house process simulator extensively used today by PETROBRAS (the Brazilian oil company) engineers.

1988 Ph.D. in Chemical Engineering, Technical University of Denmark, DTH (now DTU), Lyngby, Denmark
Thesis: Flowsheet Simulation and Chemical and Phase Equilibria
Supervisors: Aage Fredenslund and Peter Rasmussen

Short courses and educational seminars

1986 New Developments in Modeling, Simulation, and Optimization of Chemical Processes,Massachussets Institute of Technology, MIT, USA, July 21-30

1988 Introduction to Industrial Biotechnology, Gesellschaft für Biotechnologische Forschung, GBF, Germany, August-September

1989 First Brazilian School on Computer Algebra, Brazilian Center for Research in Physics, Rio de Janeiro, July 24 – August 4

1992 First School on High Performance Scientific Computing, National Laboratory for Scientific Computing, Rio de Janeiro, Brazil, August 3-7

2012 ABET Program Assessment Basic Workshop, 3-hour workshop, Texas A&M University at Qatar, Doha, Qatar, September 9

2012 Workshop on ABET Self Study Report, presented by Dr. Ed Jones, 3-hour workshop, Texas A&M University at Qatar, Doha, Qatar, May 6

2013 Institute for the Development of Excellence in Assessment Leadership (IDEAL) Accreditation Board for Engineering and Technology (ABET), Tampa, USA, January 7-10

2014 Fundamentals of Safety Management, Texas A&M University at Qatar, Doha, Qatar, September 21

2014 Writing Effective PSAs (Project Safety Analyses), Texas A&M University at Qatar, Doha, Qatar, October 22

2014 Pursuing ABET Accreditation, Engineering Leaders Conference on Engineering Education, Doha, Qatar, November 9

2014 Communicating like an Engineering Leader, Engineering Leaders Conference on Engineering Education, Doha, Qatar, November 9

Online short courses at Texas A&M University at Qatar

2013 Export Controls & Embargo Training - Basic Course

2013, 2016 Financial Conflicts of Interest in Research

2014 Reporting Fraud, Waste and Abuse

2014, 2016 Ethics

2014, 2016 Creating a Discrimination-Free Workplace

2014, 2016 Information Security Awareness

2015, 2016 ACRIC Training - Academic Civil Rights Investigation Committee

2016 TAMUQ Employee Safety Awareness

2016 International Travel Safety: Safe Passage Presentation

Teaching and research experience

Highlights

- Supervisor of 35 M.Sc. dissertations and 8 Ph.D. theses. Currently, supervisor or co-supervisor of 5 M.Sc. students.
- 50+ participations in committees of M.Sc. and D.Sc. theses (In Brazil: Federal University of Rio de Janeiro, Federal University of Bahia, State University of Campinas, State University of Maringá; in Argentina: National Southern University; in Qatar: Texas A&M University at Qatar)
- 7 participations in the search committees for the hiring of faculty members at several Brazilian universities.

Federal University of Rio de Janeiro, Brazil (UFRJ)

1988-2006 *Associate Professor of Chemical Engineering*

Undegraduate courses:

1. Process Engineering
2. Staged Separations
3. Thermodynamics
4. Optimization Applied to Chemical Engineering
5. Numerical Methods Applied to Chemical Engineering
6. Introduction to Chemical Engineering

Graduate courses:

1. Thermodynamics
2. Staged Separations
3. Methods for the Calculation of Thermodynamic Equilibrium
4. Applied Statistical Thermodynamics
5. Chemical Process Design

United Arab Emirates University

2006-2010 *Associate Professor of Chemical Engineering*

Undegraduate courses:

1. Engineering Materials
2. Engineering Thermodynamics
3. Chemical Engineering Thermodynamics
4. Introduction to Programming
5. Special Topics in Chemical Engineering
6. Graduation Project I and II
7. General Chemistry and Engineering Applications II
8. Process Modeling and Simulation

Graduate courses:

1. Fluid Phase Equilibria
2. Transport Phenomena

Texas A&M University at Qatar

2010-2017 *Professor of Chemical Engineering*

Undegraduate courses:

1. Elementary Chemical Engineering
2. Chemical Engineering Thermodynamics I
3. Chemical Engineering Mass Transfer Operations
4. Chemical Engineering Process Economics, Integration and Simulation

Graduate courses:

1. Applications of Thermodynamics to Chemical Engineering
2. Applied Statistical Mechanics of Fluids
3. Thermodynamics of Oil, Gas, and Water Systems

Texas A&M University at Qatar

2017-2019 *Adjunct Professor of Chemical Engineering*

Short-term assignments

1/1996 – 1/1997 *University of Delaware, USA*, Visiting scholar

3/1996 – 4/1996 *University of Queensland, Australia*, Visiting scholar

8/1999 – 11/1999 *Universidad de Vigo, Spain*, Visiting professor

4/2006 – 6/2006 *University of Delaware, USA*, Fulbright senior visiting scholar

Languages

Mother tongue: Portuguese

Excellent knowledge of: English and Spanish (Diploma of Spanish as a Foreign Language, Superior Level, University of Salamanca)

Fair knowledge of: French (CEFFAR Diploma) and Danish

Administrative/scientific activities

At the Federal University of Rio de Janeiro, Brazil (UFRJ)

7/1992–12/1993 Associate Director for Graduate Studies, Research and Development, Escola de Química (School of Chemistry)

12/1999–12/2001 Elected representative of Associate Professors at the Center of Technology (equivalent to the Deanship of Engineering)

12/1998–11/2000 Head of the Graduate Course (M.Sc. and D.Sc. programs) on Technology of Chemical and Biochemical Processes, Escola de Química (School of Chemistry)

2003–2006 Elected member of the University-level Council for Research and Graduate Studies

For Brazilian agencies

1993 Member of the Pilot Commission for the evaluation of Chemistry and Chemical Engineering courses in Brazil, Ministry of Education, Brasília, Brazil, 1993.

1998 Member of the evaluation team of Chemical Engineering courses in Brazil, Ministry of Education, May 1998.

2003

Member of the ad-hoc Committee for evaluation of Chemical Engineering research proposals, Brazilian National Research Council (CNPq), Brasília, Brazil, July, 2003.

At the United Arab Emirates University

2006–2009 Head of the Research Committee, Department of Chemical and Petroleum Engineering

2006–2009 Member of the Research Committee, College of Engineering

2009–2010 Course Coordinator of Engineering Thermodynamics

At Texas A&M University at Qatar

8/2010–2015 Chair of the Continuous Assessment and Improvement Committee, Chemical Engineering Program

8/2010–2015 Member of the Texas A&M University at Qatar ABET Committee

1/2011–8/2017 Chair of the Undergraduate Curriculum Changes Committee, Chemical Engineering Program

9/2010–8/2017 Liaison between the Undergraduate Curriculum Changes Committee in Qatar and the Undergraduate Committee at the Artie McFerrin Department of Chemical Engineering in College Station, TX

2/2013–4/2013 Research Standards Officer at the Qatar campus, Ex Officio Chair

2/2013–4/2013 Chair of Inquiry Committee to Assess Allegations of Scientific Misconduct

2010–2013 Member of the Strategic Committee, Chemical Engineering Program

2011–8/2017 Member of the Graduate Studies Committee of the Chemical Engineering Program

4/2011–8/2017 Member of the Distinguished Lecture Series Committee

2011–2017 Member of Honor Code Panels (on several occasions)

2012–2015 Member of the Awards Committee, Chemical Engineering Program

2012 Member of Honor Code Appeal Panel, February 7

2012 Member of Research Award Committee

2012 Member of the Selection Committee for the Association of Former Students - College Level Distinguished Achievement Teaching Award

2012–2016 Member of the Faculty Grievance Review Committee – elected by Chemical Engineering faculty members in January 2012, reelected in May 2014

2013–2015 Member of the Field Appropriate Subcommittee (FA-SC) of the Chemical Engineering Program (the FA-SC screens requests for promotion)

2013–current Faculty fellow of the Mary Kay O'Connor Process Safety Center – Qatar

2013–current Member of the Gas and Fuel Research Center

2014–2016 Member of the Advanced Scientific Computing Group

2016–current Member of the Advanced Scientific Computing Center

2014–2016 Member of the Institutional Excellence Working Group

2014–2017 Member of the Academic Civil Rights Investigation Committee (ACRIC)

2015–2016 Member of the Task Force to Better Bridge Science and Engineering Courses

2015–2016 Chair of the Search Committee for the Hiring of Chemical Engineering Faculty

2015–2016 Member of following Award Committees: Richard Ewing Award for Excellence in Student Research, Faculty Excellence Award, Faculty Research Excellence Award, Research Excellence Award for Early Career Faculty, Research Fellow Excellence Award, Research Team Excellence Award

2015-2016 Chair of the 2016-2020 Strategic Plan Focused Leadership KPI (Key Performance Indicators) Committee

2016 Member of the 2016-2021 Strategic Plan Committee

2016 Member of the Faculty Performance Improvement Plan Oversight Committee

2016 Member of the Aggie Life 102 Committee

2016 Peer-elected faculty senator (effective from September 2016) of Texas A&M University

2016-2017 Faculty Senate Caucus leader of Texas A&M University at Qatar

Scientific events

2002 Co-president of the VI Iberoamerican Conference on Phase Equilibria and Fluid Properties for Chemical Process Design, EQUIFASE 2002, October 12-16, Foz do Iguaçu, Brazil.

2011 Member of the Scientific Committee of the VI Brazilian Congress of Applied Thermodynamics – CBTERMO 2011, November 22-25, Salvador, Brazil.

2011 Chair of the roundtable on solar energy, National Academy of Engineering Grand Challenges Forum: Global Perspective and Local Outlook, Qatar University, Administration Building, Conference Hall, Monday, May 9, 2011.

2011 President of the Scientific Committee of the I Brazilian Congress on Rheology, May 10-11, Rio de Janeiro, Brazil.

2012 Member of the International Scientific Committee of the IX Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – EQUIFASE 2012, October 8-12, Puerto Varas,

Chile.

2013 Member of the Local (Brazil/Argentina) Organizing Committee of the 2013 PPEPPD Conference – the 13^{th} International Conference on Properties and Phase Equilibria for Chemical Process Design, which is the leading world conference in this field, Puerto Iguazu, Argentina.

2013 Chair of session at 2013 PPEPPD Conference – the 13^{th} International Conference on Properties and Phase Equilibria for Chemical Process Design, Puerto Iguazu, Argentina.

2013 Member of the Scientific Committee of the VII Brazilian Congress of Applied Thermodynamics – CBTERMO 2013, November 3-6, Uberlândia, Brazil.

2014 Chair of session, Workshop on Natural Gas Monetization, March 27-8, Montgomery, TX, USA.

2014 Chair of the Selection Committee for the Best Paper Award at the Workshop on Natural Gas Monetization, March 27-28, Montgomery, TX, USA.

2014 Chair of session 1B, Engineering Education II, at the 2014 Engineering Leaders Conference on Engineering Education, November 9, Doha, Qatar.

2014 Member of the Selection Committee for the Best Paper Award at the 2014 Engineering Leaders Conference on Engineering Education, November 9, Doha, Qatar.

2015 Chair of session, Qatar Process Safety Symposium, March 30-31, Doha, Qatar.

2015 Chair of session, European Symposium on Applied Thermodynamics, June 11-14, Athens, Greece.

2015 Member of the International Scientific Committee of the X Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – EQUIFASE 2015, June 28 to July 1, Alicante, Spain.

2015 Chair of the Selection Committee for the Esteban A. Brignole Award, awarded during the X Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – EQUIFASE 2015, June 28 to July 1, Alicante, Spain.

2015 Chair of session and presenter of the Esteban A. Brignole Award ceremony, X Iberoamerican Conference on Phase Equilibria and Fluid Properties for Chemical Process Design - EQUIFASE 2015, June 28-July 1, Alicante, Spain.

2015 Member of the Scientific Committee of the VIII Brazilian Congress of Applied Thermodynamics – CBTERMO 2015, November 17-20, Aracaju, Brazil.

2015 Co-organizer (with Ioannis Economou and Mert Atilhan) of the Conference in Recognition of the Career Achievements of Professor Kenneth R. Hall, December 3, Doha, Qatar.

2016 Chair of session at the Qatar Fertiliser Company – Texas A&M University at Qatar Conference 2016, January 14, Doha, Qatar.

2016 Chair of session *Energy 1*, at the Texas A&M University at Qatar Annual Research Showcase 2016, April 12, Doha, Qatar.

2016 Chair of session, Qatar Process Safety Symposium, April 18-19, Doha, Qatar.

2016 Co-organizer of the event: Thermodynamics in the Chemical Product and Process Design: News Challenges, New Methods - Celebrating the the 60^{th} Anniversary of Prof. Frederico Wanderley Tavares (Termodinâmica no Projeto de Processos e Produtos Químicos: Novos Desafios, Novos Métodos - Celebrando o 60º Aniversário do Prof. Frederico Wanderley Tavares), July 8, Rio de Janeiro, Brazil.

2017 Member of the Scientific Committee of EQUIPETRO 2017 (1^{st} Meeting on Phase Equilibrium in Petroleum; I Encontro sobre Equilíbrio de Fases em Petróleo), March 22-24, Salvador, Brazil.

2017 Member of the Scientific Committee of the IX Argentinian Congress of Chemical Engineering, 6-9 August, Bahia Blanca, Argentina.

2017 Member of the Organizing Committee of the IX Brazilian Congress of Applied Thermodynamics – CBTERMO 2017, October 23-26, Porto Alegre, Brazil.

2018 Member of the International Scientific Committee of the XI Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – EQUIFASE 2018, October 22-25, Córdoba, Argentina.

2018 Chair of the round table: Teaching Thermodynamics for Chemical Engineering in the XXI Century, XI Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – EQUIFASE 2018, October 22-25, Córdoba, Argentina.

Editorial duties

2001–2005 Associate Editor of the Brazilian Journal of Chemical Engineering

2006–2007 Associate Editor of the Emirates Journal for Engineering Research

2009–2011 Member of the Editorial Board: Recent Patents on Chemical Engineering (published by Bentham Science Publishers)

2014– Associate editor of the Brazilian Journal of Chemical Engineering

2000– Referee for the following technical journals: AIChE Journal, Asia Pacific Journal of Chemical Engineering, Biomass & Bioenergy, Brazilian Journal of Chemical Engineering, Canadian Journal of Chemical Engineering, Catalysis Today, Chemical Engineering Communications, Chemical Engineering Education, Chemical Engineering Science, Computer Applications in Engineering Education, Computers and Chemical Engineering, Fluid Phase Equilibria, Fuel, Industrial & Engineering Chemistry Research, International Journal of Greenhouse Gas Control, Journal of Chemical and Engineering Data, Journal of Chemical Thermodynamics, Journal of Molecular Liquids, Journal of Solution Chemistry, Journal of Supercritical Fluids, Journal of Thermodynamics, Korean Journal of Chemical Engineering, Oil and Gas Science and Technology, Latin American Applied Research, Polymer Engineering and Science, Separation Science and Technology, Thermochimica Acta.

Referee for several conferences and for funding agencies from Brazil and other Latin American countries.

Distinctions and achievements

1975 *Member of the Honor Group of the Santo Antonio Maria Zaccaria High School* (dedicated to students with outstanding academic performance at the institution), Rio de Janeiro, Brazil, granted in 1975.

1976 *Ranked first in the entrance exams to the School of Chemistry*, Federal University of Rio de Janeiro, Brazil (out of approximately 1000 candidates).

1981 *"Cum Laude" Undergraduate Diploma* in Chemical Engineering.

11/1991 *First place in the public selection* for Assistant Professor in Chemical Process Design, School of Chemistry, Federal University of Rio de Janeiro, Brazil.

Supervisor (or co-supervisor) of distinguished research done by undergraduate students, at five occasions, in different technical meetings.

2000–2006 Fellow of the "Scientists of Our State" program, in three consecutive two-year periods. Granted by the State of Rio de Janeiro Science Foundation (FAPERJ) to few distinguished researchers working in the State.

2006 *Fulbright Senior Visiting Scholar* at the University of Delaware. Granted by the Fulbright Commission, Department of State, USA, 2006 (only person in all fields of Engineering to be granted a Fulbright scholarship in Brazil, in 2005).

2012 Granted a *"rolling appointment"* by Texas A&M University at Qatar (There is no tenure at TAMUQ: a "rolling appointment", which is an appointment with automatic renewal, contingent on performance, is the closest equivalent).

4/2014 Co-supervisor (with Dr. Nimir Elbashir) of the M.Sc. thesis "Multiphase Equilibrium of Fluids Confined in Fischer-Tropsch Catalytic Systems" for which Samah Warrag received Texas A&M University at Qatar's *Richard E. Ewing Award for Excellence in Student Research.*

3/2015 Co-supervisor (with Dr. Luc Véchot) of Rym Kanes, the first student recognized with the *Qatar Process Safety Symposium's Process Safety Excellence Student Award.*

2015– *Outstanding reviewer (achieved: March 2015), International Journal of Greenhouse Gas Control*, for being within the top 10th percentile of reviewers for the Journal, in terms of the number of manuscript reviews completed in the previous two years.

4/2016 Co-supervisor (with Prof. Ioannis Economou) of Noura A. A. Dawash, recognized with the *TAMUQ Chemical Engineering Program Graduate Student Award.*

4/2016 Co-supervisor (with Prof. Ioannis Economou) of the M.Sc. thesis "Thermodynamic Modeling of Fluids Confined in Porous Media" for which Noura A.A. Dawass received Texas A&M University at Qatar's *Richard E. Ewing Award for Excellence in Student Research.*

4/2016 Five-year service award, Texas A&M University at Qatar.

4/2017 Co-supervisor (with Prof. Ioannis Economou) of Muaz Selam, recognized with the *TAMUQ Chemical Engineering Program Graduate Student Award.*

4/2017 Co-supervisor (with Dr. Luc Véchot) of Abdulla Al-Mohannadi and Rashid Al-Muhannadi, students recognized with the *Qatar Process Safety Symposium's Process Safety Excellence Student Award.*

Consulting

1994–1995 Consulting work for PETROBRAS (the Brazilian Oil Company) on the Characterization of Oil Fractions and Simulation of Hydrotreating Processes (in joint work with Profs. E.M. Queiroz, J.L. Medeiros and O.Q. Araújo).

2006 Consulting work for PETROBRAS on DME (dimethyl ether) production.

2006 Consulting work for PETROBRAS on the thermodynamic modeling of systems with amines and glycols.

2006 Consulting work for PETROBRAS on the dynamic simulation of flash drums.

Recent research funding

2011–2012 Thermodynamic Properties of Polar Compounds and Mixtures Using the Mattedi-Tavares-Castier Equation of State, *Qatar National Research Fund - Undergraduate Research Experience Program* (QNRF-UREP), PI: Marcelo Castier, January, 2011-January 2012, approximately US$ 20000.00.

2011–2012 Vapor-Liquid Equilibrium of Aqueous Electrolyte Solutions Using the Electrolattice Equation of State, QNRF-UREP, PI: Marcelo Castier, July, 2011-July 2012, approx. US$ 10000.00.

2012–2013 Thermodynamic Speed of Sound from Equations of State, QNRF-UREP, PI: Marcelo Castier, February, 2012–January 2013, approx. US$ 20000.00.

2012–2016 Utilization of MRI and NMR in the Visualization of Fischer-Tropsch Synthesis Reaction Behaviors, *Qatar National Research Fund - National Priorities Research Program* (QNRF-NPRP), PI: Nimir Elbashir, co-PI: Marcelo Castier, co-PI: Prof. Lynn Gladden, approximately US$ 1050000.00, of which about US$ 80000.00 under my responsibility.

2013–2016 Fluid Separations by Adsorption in Porous Solids, QNRF-NPRP, PI: Marcelo Castier, co-PI: Frederico Wanderley Tavares, co-PI: Stanley I. Sandler, approximately US$ 900000.00, of which about US$ 600000.00 under my responsibility.

2013–2014 Thermodynamic properties of aqueous electrolyte solutions using the Q-electrolattice equation of state, QNRF-UREP, PI: Marcelo Castier, March, 2013 – February 2014, approximately US$ 20000.00.

2014 Modeling CO_2 Storage in Aquifers and Deep Oceans with the Q-electrolattice Equation of State, *Qatar National Research Fund - Post-Doctoral Research Associate Program* (QNRF-PDRA), granted to Dr. André Zuber under my supervision in 2014, US$ 295558.20 – unused because Dr. Zuber joined the Technical Federal University of Paraná, in Brazil.

2015–2018 Design and Optimization of Highly Productive Zeolitic Imidazolate Framework, ZIF-8, Membranes for Industrial Propylene/Propane Separations, QNRF – NPRP – 7, Lead PI: Hae-Kwon Jeong, co-PIs: Ioannis Economou and Marcelo Castier, approximately US$ 900000.00, of which about US$

300000.00 under my responsibility.

2016–2019 Development of a State-of-the-Art Thermodynamic Model for Mixtures Containing Water, Carbon Dioxide, Salts and Hydrocarbons in Bulk and in Confinement, QNRF – NPRP – 8, Lead PI: Ioannis Economou, approximately US$ 900000.00, of which about US$ 300000.00 under my responsibility.

2016–2017 Simulation of Emergency Relief from Vessels with Runaway Reactions, QNRF-UREP, PI: Marcelo Castier, approximately US$ 20000.00.

2016–2017 Redefine the Education Experience via Augmented Reality Tools, TAMUQ, Lead PI: Konstantinos Kakosimos, PIs: Ghada Salama and Marcelo Castier, US$ 12000.00.

Invited presentations

All titles in English for convenience: some of the presentations were in Portuguese or Spanish.

1988 Thermodynamic Analysis of an Alcohol Distillery, Gesellschaft für Biotechnologische Forschung (GBF) - Braunschweig – Germany, August, 1988.

1989 Calculation of Chemical and Phase Equilibria in Non-ideal Systems, Federal University of Uberlândia, Brazil, May, 1989.

1991 Automatic Implementation of Thermodynamic Models by Means of Computer Algebra, First Meeting "Il Mondo Nuovo", Department of Theoretical Physics, Catholic University of Petropolis, Brazil, October, 1991.

1991 Automatic Drawing of Phase Diagrams for Polymer Systems, Federal University of Uberlândia, Brazil, December, 1991.

1994 An Introduction to Mathematica, Department of Chemical Engineering, University of Delaware, USA, February, 1994.

1994 Energy Integration of Chemical Processes: Heat Exchanger Network Synthesis, Rural Federal University of Rio de Janeiro, April, 1994.

1995 Calculation of Critical Points with Free Energy-Based Mixing Rules Using the Method of Homotopic Continuation, Department of Chemical Engineering, University of Delaware, January, 1995.

1997 Recent Advances in Thermodynamics Applied to Chemical Engineering Problems, Federal University of Minas Gerais, Brazil, November, 1997.

1998 Separations, Thermodynamics and Interfacial Phenomena: Comments of the Brazilian Group, Pan-American Workshop to Promote Collaboration in Chemical Engineering, Rio de Janeiro. August, 1998.

1999 Thermodynamic Equilibrium Calculations in Systems Subject to the Effect of External Fields, Fifth Iberoamerican Conference on Phase Equilibria for Chemical Process Design (EQUIFASE'99), Vigo, Spain, June, 1999.

1999 Use of Global Optimization Techniques for Fitting Vapor-Liquid Equilibrium Data, University of Vigo, Vigo, Spain, November, 1999.

2002 Methods of Thermodynamics in the Analysis of Particulate Systems, XXX Brazilian Conference on Particulate Systems (ENEMP), São Carlos, SP, Brazil, October, 2002.

2003 The New Challenges of Thermodynamics Applied to Chemical Engineering, Fluminense Federal University, Niterói, RJ, Brazil, December, 2003.

2005 Computer Modeling of the Physical Properties of Pure Substances and Mixtures, VIII Meeting on Computational Modeling, Nova Friburgo, Brazil, November, 2005.

2006 Thermodynamic Properties and Phase Equilibria for Chemical Process Design: an Overview of Research in Rio de Janeiro, Universities of Notre Dame and of Delaware, USA, June, 2006.

2006 Thermodynamic Properties of Petroleum Fluids by Molecular Simulation and Equations of State, United Arab Emirates University, Al Ain, UAE, October, 2006.

2011 Phase Equilibrium Problems Inspired by Accidental Fluid Leaks, invited speaker of the VI Brazilian Congress of Applied Thermodynamics, Salvador, State of Bahia, Brazil, November, 2011 (also presented at the Petroleum Institute, Abu Dhabi, United Arab Emirates, January 11, 2012)

2012 Um Modelo Internacional de Formação em Engenharia? (An International Model for Engineering Education?), Brazilian Meeting on Chemical Engineering Education (ENBEQ), Búzios, Brazil, September 12, 2012.

2012 Applying Thermodynamics to Process Safety, Adsorption, and Electrolyte Solutions – with an Eye on Education, Qatar University, Doha, Qatar, November 21, 2012.

2013 From Test Tubes to Fracking: Mathematical Modeling in Chemical Engineering (Do Frasco ao "Fracking": Modelagem Matemática na Engenharia Química), Universidade Regional do Noroeste do Estado do Rio Grande do Sul, Ijuí, October 16, 2013.

2013 Thermodynamic Sound Speed: Algorithm and Applications (Velocidade termodinâmica do som: algoritmo e aplicações), School of Chemistry, Federal University of Rio de Janeiro, October 23, 2013.

2013 Engenharia Química: Desafios para os Próximos 50 anos (Chemical Engineering: Challenges for the Next 50 Years), XIII Annual Colloquium on Chemical Engineering (special event celebrating 50 years of graduate studies in Chemical Engineering in Brazil), Chemical Engineering Program, COPPE, Federal University of Rio de Janeiro, October 25, 2013.

2013 Thermodynamics Applied to Process Safety, Adsorption, and Electrolyte Solutions – with an Eye on Chemical Engineering Education (Termodinâmica Aplicada à Segurança de Processos, Adsorção e Soluções Eletrolíticas - com um Olho na Formação de Engenheiros Químicos), Federal University of Paraná, Brazil, December 12, 2013 (updated version of the seminar presented in 2012 at Qatar University).

2014 Using Computer Algebra to Speed up Code Development: A Chemical Engineer's Perspective, Texas A&M at Qatar Advanced Scientific Computing Workshop, May 11, 2014.

2014 Modeling and Applications of the Thermodynamic Properties of Pure Substances and Mixtures, Texas A&M at Qatar Advanced Scientific Computing Group's Workshop on Collaboration Opportunities in Computational Science and Engineering 2014, June 8, 2014.

2014 Texas A&M University at Qatar Graduate Studies; University of São Paulo; State University of Campinas; Federal University of Santa Catarina; State University of Maringá; Federal University of Rio de Janeiro; Federal Fluminense University; State University of Rio de Janeiro; Federal University of Paraná; August 18-28, 2014.

2014, 2015 Applying Thermodynamics to Flow Processes and Confined Fluids – with an Eye on Education, University of São Paulo, August 18, 2014; Federal University of Santa Catarina, August 20, 2014; Federal University of Bahia, February 26, 2015.

2015 Simulation of Leaks and Venting Operations with Rigorous Evaluations of the Thermodynamic Properties, School of Chemistry, Federal University of Rio de Janeiro, May 21, 2015.

2015 Thermodynamic Modeling of the Properties of Confined Fluids: Advances and Challenges (Modelado Termodinámico De Propiedades De Fluidos Confinados: Avances y Desafíos), Plenary lecture at the VIII Argentinian Congress of Chemical Engineering, August 2-5, Buenos Aires, Argentina.

2015 Undergraduate and Graduate Studies in Chemical Engineering at Texas A&M University: Opportunities in Texas and Qatar (Graduação e Pós-Graduação em Engenharia Química na Texas A&M University: Oportunidades no Texas e Qatar), Federal Technological University of Paraná, August 10, Francisco Beltrão, Brazil.

2015 The Importance of Thermodynamic Properties on Equipment and Process Design (A Importância de Propriedades Termodinâmicas no Projeto de Equipamentos e Processos), invited seminar at the I Chemical Engineering Academic Week, Federal Technological University of Paraná, November 13, Francisco Beltrão, Brazil.

2015 Thermodynamic Models for Fluids Confined in Porous Media (Modelos termodinâmicos para fluidos confinados em meios porosos), invited opening lecture of the VIII Brazilian Congress of Applied Thermodynamics – CBTERMO 2015, November 17-20, Aracaju, Brazil.

2015 Volume-based flash calculations: applications to process safety and confined fluids, invited seminar at the Université de Pau et des Pays de l'Adour, November 26, Pau, France.

2015 Fluid Properties in Porous Media via Molecular Dynamics and Multipotential Theory of Adsorption, presentation at the Conference in Recognition of the Career Achievements of Professor Kenneth R. Hall, Texas A&M University at Qatar, December 3, Doha, Qatar.

2016 Thermodynamic Modeling of Fluids Confined in Porous Media: an Overview of Selected Approaches, invited lecture at the 2016 PPEPPD Conference – the 14^{th} International Conference on Properties and Phase Equilibria for Chemical Process Design, which is the leading world conference in this field, May 23, Granja (Porto), Portugal.

2016 The Professional Trajectory of Prof. Frederico Wanderley Tavares (A Trajetória Profissional do Prof. Frederico Wanderley Tavares), co-presenter: Prof. Krishnaswamy Rajagopal, Federal University of Rio de Janeiro, July 8, Rio de Janeiro, Brazil.

2016 Addressing Local Problems to Solve Global Problems (Abordando Problemas Locais para Solucionar Problemas Globais), Inaugural class (online from Doha, Qatar) of the Graduate Program on Chemical and Biochemical Technology, Federal University of Rio de Janeiro, September 26, Rio de Janeiro, Brazil.

2016 Ethical Concerns in Globalization of Western Engineering Education, presentation during the panel *Reassessing Western Engineering Education in a Globalized World*, International Ethics Summit - Morality in the Global Era: Theory, Policy, and Praxis, December 4–6, Doha, Qatar.

2017 Thermath-XSEOS-YouThermo: from an Alphabet Soup to an Educational Project, Panel on the *Teaching Thermodynamics* Workshop, European Symposium of Applied Thermodynamics, May 18–21, Bucharest, Romania.

2017 Short course (in Portuguese): XSEOS – a Friendly Computational Environment to Learn Thermodynamics (XSEOS – um Ambiente Computacional Amigável para Aprender Termodinâmica), Universidade Federal Tecnológica do Paraná, Campus Francisco Beltrão, 9 and 10 October 2017.

2017 Short course (in Portuguese): XSEOS – a Friendly Computational Environment to Learn and Teach Thermodynamics (XSEOS – um Ambiente Computacional Amigável para Ensinar e Aprender Termodinâmica), V Brazilian School of Thermodynamics, 23 October 2017.

2017 An External View on Quality (in Portuguese), 50^{th} Anniversary of the Graduate Program on Chemical and Biochemical Process Engineering, School of Chemistry, Federal University of Rio de Janeiro, 15 December 2017.

2018 Short course (in Spanish): XSEOS – a Friendly Computational Environment to Learn and Teach Thermodynamics (XSEOS – un Ambiente Computacional Amigable para Enseñar e Aprender Termodinámica), Universidad Nacional de Córdoba, Argentina, 1-2 March 2018.

2018 Applications of thermodynamics to process safety and to supersonic fluid separators, XI Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – EQUIFASE 2018, October 22-25, Córdoba, Argentina. (to occur)

2018 Merging Tradition and Avant-Garde in the Study of Confined Fluids (in Portuguese), XVIII Annual Colloquium of Chemical Engineering Program, COPPE, Federal University of Rio de Janeiro, 7 November 2018, Rio de Janeiro, Brazil. (to occur)

Publications in scientific journals

References

[1] G. D. Barbosa, M. L. D'Lima, S. M. H. Daghash, M. Castier, F. W. Tavares, and L. Travalloni. Cubic equations of state extended to confined fluids: new mixing rules and extension to spherical pores. *Chemical Engineering Science*, 184:52–61, 2018.

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Freely available software

XSEOS

XSEOS is an Excel add-in to calculate physical properties using excess Gibbs free energy models and equations of state, primarily aimed at undergraduate education but also useful for graduate education and research. The current version has more than 42000 lines of Visual Basic code to compute several thermodynamic properties with many of the models most commonly used for chemical process design.

URL: http://people.qatar.tamu.edu/marcelo.castier/index.htm

THERMATH

THERMATH is written in the Mathematica programming language. Thermath takes advantage of Mathematica's ability to perform analytical differentiation and integration. Given the expression of an excess Gibbs energy model or of an equation of state, Thermath obtains the expressions of several thermodynamic expressions (e.g., activity or fugacity coefficients, excess or residual properties, etc.) and their derivatives, analyzes them searching for common terms, and automatically

generates efficient codes to implement them as Fortran, Visual Basic, or Matlab procedures. The current version of Thermath has about 7000 lines of code for the required symbolic manipulations.

Audiovisual productions

2016 **YouThermo** Channel on Youtube, co-founder, with Dr. André Zuber from the Technical Federal University of Paraná (Brazil). The channel produces educational videos about Chemical Engineering Thermodynamics and related topics. Channel created on 9 November 2016 and launched publicly on 4 January 2017.

For the YouThermo Channel

2016 **Making sense of pressure-enthalpy diagrams** (URL: Electronic link)

2016 **Isentropic compression** (URL: Electronic link)

2016 **Isentropic compression with the Soave-Redlich-Kwong equation of state** (URL: Electronic link)

2016 **Visualization of liquid-liquid separation** (URL: Electronic link)

2016 **Visualization of solid-liquid separation** (URL: Electronic link)

2016 **Visualization of bubble point** (URL: Electronic link)

2016 **Visualization of dew point** (URL: Electronic link)

2016 **Interview with Dr. Luís Fernando Mercier Franco** (URL: Electronic link)

2016 **Interview with Prof. Ioannis G. Economou** (URL: Electronic link)

2017 **Welcome to the YouThermo Channel** (URL: Electronic link)

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2017 **Interview with Dr. Rafael de Pelegrini Soares** (URL: Electronic link)

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2017 **Carbon dioxide flow using a compressibility chart** (URL: Electronic link)

2017 **Interview with Dr. Luc N. Véchot** (URL: Electronic link)

2017 **Boas vindas ao ano letivo de 2017** (URL: Electronic link)

2017 **Interview with Dr. Douglas Junior Nicolin** (URL: Electronic link)

2017 **Explicando diagramas pressão-entalpia** (URL: Electronic link)

2017 **Compressão isentrópica com a equação de estado de Soave-Redlich-Kwong** (URL: Electronic link)

2017 **Compressão isentrópica** (URL: Electronic link)

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2017 **Compressão isentrópica em um diagrama pressão-entalpia** (URL: Electronic link)

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2017 **Interview with Professor Jean-Charles de Hemptinne** (URL: Electronic link)

2017 **Escoamento de dióxido de carbono usando o fator de compressibilidade** (URL: Electronic link)

2017 **Thermath: the tool that built XSEOS** (URL: Electronic link)

2017 **Interview with Dr. Mirella Simões Santos** (URL: Electronic link)

2017 **XSEOS no CBTERMO 2017** (URL: Electronic link)

2017 **On being a female Engineering student, with Drs. Ghada Salama and Sara K. Hillman** (URL: Electronic link)

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2017 **Normal boiling temperature of n-hexane using the Peng-Robinson equation of state** (URL: Electronic link)

2017 **Ajuste do parâmetro de interação binária da equação de estado de Peng-Robinson** (URL: Electronic link)

2017 **Fitting the binary interaction parameter of the Peng-Robinson equation of state** (URL: Electronic link)

2017 **Solubilidade de ácido palmítico em etanol** (URL: Electronic link)

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2018 **Curso de XSEOS (XSEOS course in Spanish), Córdoba, Argentina - 1 y 2 de marzo de 2018** (URL: Electronic link)

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2018 **EQUIFASE 2018: Applications of thermodynamics to process safety and to supersonic fluid separators** (URL: Electronic link)

2018 **EQUIFASE 2018: Round table - Teaching Thermodynamics for Chemical Engineering in the XXI Century** (URL: Electronic link)

2018 **Book review: Compositional grading in oil and gas reservoirs** (URL: Electronic link)

2018 **Welcome to the YouThermo Channel (2018 edition** (URL: Electronic link)

2018 **Explicando diagramas Txy** (URL: Electronic link)

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2018 **It's cool! Part I. Heat effects in water+sodium chloride solutions** (URL: Electronic link)

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2016 **Flash calculations with specified entropy and stagnation enthalpy**, Elsevier AudioSlides for Fluid Phase Equilibria, published online on 9 November 2016. (URL: Electronic link)

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