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Argentina

2023

**VI Iberoamerican Conference on Supercritical Fluids,**  
Córdoba, Argentina, 2023.

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*“Touring the Supercritical Space”.*

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Universidad Nacional del Sur (Argentina)

*“The role of sub- and supercritical fluids in the processing of cannabis/hemp”.*

**Jerry King**

Arkansas University (USA)

*“Advances on the use of sustainable solvents for pharmaceutical and biomedical applications”.*

**Ana Rita Duarte**

Universidade Nova de Lisboa (Portugal)

*“Supercritical Fluid Technology for Food Processing”.*

**Julián Martínez**

UNICAMP (Brazil)

## Keynotes

*“Supercritical fluids technology and sustainability: some opportunities, many challenges”.*

**Speaker:** Gustavo Bolaños (Universidad del Valle, Colombia)

*“Hydrothermal extractions-reactions for circular bioeconomy”.*

**Speaker:** Danilo Cantero (Universidad de Valladolid, España)

*“Simulation of heat transfer effects on the supercritical CO<sub>2</sub> extraction at a two-vessel industrial plant”.*

**Speaker:** Felipe Toledo (Pontificia Universidad Católica de Chile)

*“Integrated and sustainable pressurized fluid processes for biorefinery of plant and animal by-products”.*

**Speaker:** Marleny Saldaña (University of Alberta, Canada)

*“Important aspects and challenges for the supercritical extraction processes in industry”.*

**Speaker:** Pedro Ivo Nunes (Singularity, Brazil)

*“Processing of hemp seed and cannabis flowers - a New Zealand perspective”.*

**Speaker:** Owen Catchpole (Callaghan Innovation, New Zealand)

*“Ultra-high pressure processes - Design and examples”.*

**Speaker:** Zeljko Knez (University of Maribor, Slovenia)

*“Development of an online integrated method for analyzing bioactive compounds: Pressurized Liquid Extraction coupled with High-Performance Liquid Chromatography”.*

**Speaker:** Juliane Viganó (Universidade Federal de Sao Carlos, Brazil)

*“Come into a new era of purification”.*

**Speaker:** Assia Kone (SFE Process, France)

*“Complex fluid phase behavior in binary and ternary systems, including the critical region”.*

**Speaker:** Cor Peters (Colorado School of Mines, USA)

*“ScCO<sub>2</sub>-impregnation of clove extract in polycarbonate, poly(L-lactic acid) and their blends”.*

**Speaker:** Mathilde Champeau (Universidade Federal ABC, Brazil)

*“Selection of green extraction solvents using the Hansen solubility parameters approach”.*

**Speaker:** Andrea Sánchez-Camargo (Universidad de los Andes, Colombia)



## Oral Communications

**008** – “*Simultaneous extraction of macauba oil and active compounds from olive leaves using pressurized propane.*” J. M. Jaski, C. E. Barão, C. da Silva, L. Cardozo-Filhoa, and V. F. Cabral.

**Speaker:** Vladimir Cabral, Universidade Estadual de Maringá

**009** – “*Development of  $\beta$ -sitosterol-loaded nanocapsules obtained by supercritical fluid extraction of emulsion process for potential use in functional foods.*” D. Cerro, C. Streitt, A. Rojas, J. Romero, and A. Torres.

**Speaker:** Daniela Cerro, University of Santiago de Chile

**010** – “*Concentration of oxygenated terpenes in orange essential orange by supercritical fluid adsorption.*” V. Saldanha Carvalho, J. Viganó, L. H. Fasolin, and J. Martínez.

**Speaker:** Victor Saldanha Carvalho, UNICAMP

**021** – “*Supercritical CO<sub>2</sub> and melt-extrusion to produce enhanced PLGA scaffolds.*” I. Gracia, F. Carrascosa, J.M. García, M.J. Ramos, J.F. Rodríguez, and M.T. García.

**Speaker:** Ignacio Gracia, University of Castilla-La Mancha

**023** – “*High-pressure sequential extractions using aqueous solutions of deep eutectic solvents (DES): a sustainable process with Green Certificate.*” L. Benvenuttia, A. A. Ferreira Zielinski, and S. R. Salvador Ferreira.

**Speaker:** Laís Benvenuttia, Federal University of Santa Catarina

**034** – “*Kappaphycus alvarezzi biorefinery: PLE and SFE applications for phenolics and carragenan recovery and aerogel drying.*” A. R. Rudke, C. J. De Andrade, and S. R. S. Ferreira.

**Speaker:** Cristiano J. De Andrade, Federal University of Santa Catarina

**039** – “*Antioxidant extracts from olive pomace by compressed fluid extraction technologies: comparison between SFE and PLE.*” C. Dauber, M. Romero, A. Gámbaro, E. Ibáñez, and I. Vieitez.

**Speaker:** Cecilia Dauber, Universidad de la República

**046** – “*Effect of operational variables on the development of PLA/PBAT active foams using supercritical fluids.*” P. Rivera, A. Torres, J. Romero, F. Rodríguez, and M. J. Galotto.

**Speaker:** Alejandra Torres, University of Santiago de Chile

**048** – “Supercritical CO<sub>2</sub> assisted impregnation of pink pepper essential oil in gelatin-siloxane gels for biomedical applications.” U. Silva do Nascimento, B. Guzzo da Silva, and L. Passos Maia-Obi.

**Speaker:** Ligia Maia-Obi, Federal University of ABC

**050** – “Catalytic synthesis of ethyl levulinate aided by supercritical carbon dioxide.” Authors: M. E. Zakrzewska, A. B. Paninho, A. R. C. Duarte, and A. V. M. Nunes.

**Speaker:** Malgorzata Zakrzewska, NOVA School of Science and Technology

**051** – “Evaluation of the lipid fraction of tucumã-do-Amazonas (*Astrocaryum aculeatum*) almond extracts obtained by SFE.” L. M. S. Carvalho, R. Grimaldi, and J. Martínez.

**Speaker:** Luciedry Carvalho, UNICAMP

**053** – “Supercritical extraction from *Citrus reticulata* Blanco with carbon dioxide.” M. G. de F. Batista, M. B. Kolichieski, F. A. Pedersen Voll, and M. L. Corazza.

**Speaker:** Marcelle Batista, Federal University of Paraná

**056** – “Influence of phase behavior on enzymatic esterification of residual oils using propane as solvent: experimental study and thermodynamic modeling.” B. M. Nogueira, F. W. Tavares, and P. M. Ndiaye.

**Speaker:** Bruno Nogueira, Universidade Federal do Rio de Janeiro

**057** – “Effect of supercritical CO<sub>2</sub> extraction as pretreatment to obtain c-phycoyanin from spirulina (*Arthrospira maxima*).” J. A. López-Limón, M. A. Rios-Corripio, G. Romero-de la Vega, A. S. Hernández-Cázares, J. V. Hidalgo-Contreras, and R. del A. Mellado-Pumarino.

**Speaker:** Juana Lopez-Limón, Universidad Iberoamericana Puebla

**060** – “Extraction of neutral oil and polyphenolic fractions of spent coffee grounds: single step and sequential extractions with compressed fluids.” M. Nolasco Araujo, N. do Carmo Diniz, F. Hamerski, G. Varela Garcia Lesak, J. C. de Carvalho, and M. L. Corazza.

**Speaker:** Marcos Corazza, Federal University of Para

**062** – “Interfacial description of binary systems containing CO<sub>2</sub>, n-butanol and H<sub>2</sub>O.” R. Villablanca-Ahues, R. Nagl, T. Zeiner, and P. Jaeger.

**Speaker:** Rafael Villablanca – Ahues, Technische Univetsität Clausthal

**065** – “*Extraction of volatile oils from aromatic Ecuadorian plants.*” L. I. Jaramillo, E. Vera, J. Boujila, and S. Camy.

**Speaker:** Lorena Jaramillo, Escuela Politécnica Nacional / Université de Toulouse.

**069** – “*Nutraceutical delivery via SC-CO<sub>2</sub>: Lentil protein and pectin based aerogels to encapsulate  $\beta$ -carotene.*” S. Mekala and M. D. A. Saldaña.

**Speaker:** Srujana Mekala, University of Alberta

**073** – “*Ionic gelation assisted by compressed fluids (IGACF): a new process for microencapsulation of bioactives in chitosan.*” C. Pardo-Castaño and G. Bolaños.

**Speaker:** Camilo Pardo Castaño, Universidad del Valle

**077** – “*CO<sub>2</sub> + ethanol assisted impregnation of chitosan microparticles with curcumin.*” P. H. F. Tondo, R. M. F. Vargas, and E. Cassel.

**Speaker:** Eduardo Cassel, Pontifícia Universidade Católica do Rio Grande do Sul

**090** – “*Comparison of emerging extraction techniques for recovering phenolic compounds from avocado byproducts using a Natural Deep Eutectic Solvent based on chloride choline and lactic acid.*” J. F. Grisales-Mejía, V. Cedeño-Fierro, J. Pala Ortega, H. G. Torres-Castañed, M. M. Andrade-Mahecha, H. A. Martínez-Correa, G. Álvarez-Rivera, J. A. Mendiola, A. Cifuentes, and E. Ibañez.

**Speaker:** Juan F. Grisales-Mejía, Universidad Nacional de Colombia

**091** – “*Extraction and evaluation of peach (*Prunus persica*) seed oil obtained by supercritical CO<sub>2</sub> extraction.*” F. Huayta, H. Pajan, H. Obregón, J. Sedano, J. Paul Rosales, J. Argumé, and J. Palacios.

**Speaker:** Fredy Huayta, Pontificia Universidad Católica del Perú

**108** – “*Supercritical CO<sub>2</sub> extraction of oil from soldier fly larva meal (*Hermetia illucens* L) – yield and antioxidant activity.*” V. A. Cruz and A. L. De Oliveira.

**Speaker:** Vanessa Cruz, University of São Paulo

**110** – “*New Deep Eutectic Solvents based on hyperbranched polyglycerols and superbases for CO<sub>2</sub> absorption.*” G. Silveira dos S., D. Miranda de S. C., and R. C. Bazito.

**Speaker:** Gabriel Silveira Dos S., Institute of Chemistry University of São Paulo

**118** – “*Chitosan-TPP based aerogels for tissue engineering applications.*” C. S. A. Bento, J. P. Ruivo, H. C. de Sousa, A. M. A. Días, and M.E. M. Braga.

**Speaker:** Cristiana Bento, University of Coimbra

**119** – *“High pressure packed column for fractionation of low volatile and viscous mixtures. Conceptual design of glycerol acetates refinement with scCO<sub>2</sub>.”* M. Fortunatti Montoya, F. Sanchez, P. Hegel, and S. Pereda.

**Speaker:** Mariana Fortunatti Montoya, PLAPIQUI-UNS-CONICET

**121** – *“Extraction of bioactive compounds from *Scaptotrigona depelis* pollen using supercritical carbon dioxide.”* A. Gomes da Silva, E. Gama Ortiz Menezes, and R. Nunes de Carvalho Junior.

**Speaker:** Adriane Gomes da Silva, Universidade Federal do Pará

**125** – *“Production of homogeneous biofuel mixtures by supercritical transesterification: experimental results, process simulation and life cycle assessment.”* L. Molina and V. F. Marulanda.

**Speaker:** Victor Marulanda, Universidad de La Salle

**128** – *“Supercritical carbon dioxide processing of maritime pine (*Pinus pinaster*): sorption study.”* J. Leocádio, L. Fonseca, M. E.M. Braga, and H. C. Sousa.

**Speaker:** João Leocádio, University of Coimbra

**135** – *“Phase boundaries and copolymerization of acrylic acid + butyl methacrylate + carbon dioxide under high-pressure single-fluid initiation.”* R. S. Meleán Brito, J. E. Tasque, M. C. Strumia, F. Mattea, J. M. Giussic, and J. M. Milanesio.

**Speaker:** Juan M. Milanesio, IPQA-UNC-CONICET

**143** – *“Supercritical CO<sub>2</sub>-assisted impregnation of PLA films with R-carvone. I: Effect of processing on thermal and crystallinity properties.”* P. P. Miranda, N. A. Gañan, R. E. Martini, and M. L. Goñi.

**Speaker:** María Laura Goñi, IPQA-UNC-CONICET

## Poster Presentations

**001** – *“Phase behavior of ethanolic Passion Fruit (*Passiflora edulis* sp.) bagasse extract in supercritical CO<sub>2</sub>”.*

E. J. Santos de Araujo, A. J. Oliveira Braga, P. Matar Ndiaye, and J. Martínez

**002** – *“Ultrasound-assisted Pressurized Liquid Extraction from Tucumã-do-Amazonas Almonds (*Astrocaryum aculeatum*) Defatted with Supercritical CO<sub>2</sub>”.*

M. de P. Kraüss Ferreira, L. M. S. Carvalho, and J. Martínez

**003** – *“Supercritical CO<sub>2</sub> fractionation of passion fruit by-products extract using zeolite 13-X to concentrate phytosterols and squalene.”*

L.C. dos Santos, R. B. Silva, E. Scopel, T. Hatami, C. Rezende, and J. Martínez

**004** – *“Production of vitamin C-vitamin B3 cocrystals by the gaseous antisolvent (GAS) technique.”*

C. A. Balbinot Filho, J. L. Dias, E. A. Rebelatto, S. R. S. Ferreira, and M. Lanza

**005** – *“Effect of temperature and solvent composition on the pressurized liquid extraction of phenolic compounds from spent hop.”*

A. M. B. Oliveira, J. Viganó, and J. Martínez

**006** – *“Supercritical impregnation of phenolic compounds of passion fruit (*Passiflora edulis* sp.) bagasse extract in corn starch aerogels: effect of operation mode.”*

E. J. Santos de Araujo and J. Martínez

**007** – *“Pressurized liquid extraction of phenolic compounds from pequi almond (*Caryocar brasiliense* Camb.)”.*

I. F. Morenoa and J. Martínez

**011** – *“Recovery of bioactive compounds from sesame cake by combined high-pressure methods.”*

M. A. de Avila Souza, A. R. Rudke, and S. R. Salvador Ferreira

**012** – *“Optimization of pressurized liquid extraction used to recover flavonoids present in testa shell from *Anacardium Occidentale*.”*

L. J. da Silva, E. Sousa de Brito, and S. R. Salvador Ferreira

**014** – *“Supercritical CO<sub>2</sub> extraction of essential oil from guarana (*Paullinia cupana*) peel.”*

R. P. F. de Melo, R.C. Moreira, J. L. Bicas, N. C. Bastos, A. L. Atroch, T. P. De Souza and J. Martínez

**015** – *“Fractionation of  $\alpha$ -terpineol and limonene by supercritical fluid adsorption.”*

R. P. F. de Melo, B. B. Kienast, L. C. dos Santos, R. C. Moreira, J. L. Bicas, and J. Martínez

**016** – *“Supercritical fluid extraction of alkaloids from *Cestrum* plants.”*

F. D. Sanches and J. Martínez

**017** – *“Effects of temperature and molar ratio between acetic anhydride and  $\alpha$ -terpineol on terpinyl acetate production in SC-CO<sub>2</sub>.”*

R. C. Moreira, R. P. F. de Melo, J. Martínez, and J. L. Bicas

- 018** – *“Recovery of phenolic compounds of the Melão-de-São-Caetano (M. charantia) peel by high-pressure extraction methods.”*  
M. C. de Sousa, A. R. Rudke, and S. R. S. Ferreira
- 019** – *“Chlorella vulgaris fractionation by green sequential extractions: the potential of (bio)surfactant modifiers.”*  
G. G. González, S. R. Salvador, and C. J. De Andrade
- 020** – *“Influence of chemical composition on the properties and foamability with supercritical CO<sub>2</sub> in thermoplastic polythiourethanes.”*  
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- 022** – *“Assessment of pressurized solvents extractions from grape pomace residues.”*  
V. S. Carvalho, L. C. Freitas, and M. L. Corazza
- 024** – *“Supercritical fluid technology as a tool to valorize bacuri fruit (Platonia insignis Mart.) shell.”*  
L. Cantão Freitas, F. C. Seabra Pires, T. Costa de Araújo, and R. Nunes de Carvalho Junior
- 025** – *“Pressurized propane extraction of umari (Poraqueiba sericea Tul.) oil: extraction kinetics and fatty acid composition.”*  
L. Cantão Freitas, V. Souza Carvalho, M. L. Corazza, and M. L. Massona
- 027** – *“High Pressure Liquid Impregnation of Barbatimão Stryphnodendron adstringens (Mart.) Coville bark extracts in biopolymeric membranes.”*  
P. C. Veggi, L. F. Campos, L. E. do Carmo, J. Viganó, L. P. Mazur, and L. H. I. Mei
- 028** – *“Pressurized liquid extractions of proteins and biocompounds with antioxidant activity from banana inflorescence (Musa acuminata cv. Cavendish).”*  
G. E. Motta, G. A. Valencia, and S. R. Salvador Ferreira
- 029** – *“A model sugar cane waste biorefinery based on sub and supercritical water processing: a LCA case study.”*  
V. F. Marulanda
- 030** – *“Gurguéia nut (Dipteryx lacunifera Ducke) cake as a source for obtaining extracts rich in bioactives using pressurized liquid extraction.”*  
G. Polmanna, P. H. Santos, R. Alves Morais, S. R. Salvador Ferreira, and J. M. Block
- 031** – *“Scaling up of the Extraction of Dill Essential Oil.”*  
M. Franco and M. D.A. Saldaña
- 032** – *“Pressurized liquid extraction as a promise method to obtain protein from broken black bean cotyledon.”*  
R. Fialho Teixeira, L. Benvenuto, D. de Oliveira, and A. A. Ferreira Zielinski
- 033** – *“Supercritical fluid extraction of oil from Mauritia flexuosa pulp: a comparison with traditional extraction techniques.”*  
M. P. Carrillo-Bautista, L. L. Orduz-Díaz, J. E. C. Cardona-Jaramillo, and G. Bolaños
- 035** – *“Peach seed cake (Prunus persica): a comparative study of different extraction methods for the recovery of protein fraction.”*  
C. R. M. Rudke, T. M. S. Torres, A. A. F. Zielinski, and S. R. S. Ferreira

**036** – *“Recovering bioactive compounds from pineapple waste: a comparison between pressurized liquid and supercritical fluid extractions.”*

F. A. Maia and L. H. Fasolin

**037** – *“Integration of alternative solvents for enhanced stability of dill (*Anethum graveolens* L.) aroma volatile compounds.”*

J. Vladoic, S. Jokic, K. Aladic, I. Jerkovic, and A. R. Duarte

**038** – *“Naringin processed by gas antisolvent technique.”*

P. V. Oliveira, J. L. Dias, G.P. S. Aguiar, K. Z. Kuhn, O. Sanaiotto, A. C. Provinelli, C. F. Daniel, A. Bortoluzzi, A. M. Siebel, L. A. Lerin, C. Trapella, L. G. Müller, and J. V. Oliveira

**040** – *“Recovery of phenolic compounds from pink pepper fruits.”*

E. A. Rebelatto, L. Vitali, A. R. Rudke, K. S. Andrade, and S. R. S. Ferreira

**041** – *“Sequential extraction of tocopherols and carotenoids from *Butia capitata* fruits using supercritical carbon dioxide and pressurized fluids.”*

G. S. Lourenço Pereira, P. Tonon de Souza, S. Fraga, and K. Araujo Sampaio

**043** – *“Recovery of extracts rich in phenolic compounds from buriirana pulp (*Mauritella armata*) using high-pressure extraction processes.”*

R. Alves Morais, E. A. Rebelatto, S. R. Salvador Ferreira, and J. M. Block

**044** – *“Production of vitamin C-vitamin B3 cocrystals by the gaseous antisolvent (GAS) technique.”*

C. A. Balbinot Filho, J. L. Dias, E. A. Rebelatto, S. R. S. Ferreira, and M. Lanza

**045** – *“High-pressure phase equilibrium data for carbon dioxide + 2-methyltetrahydrofuran-3-one and carbon dioxide + 2-methyltetrahydrofuran-3-one + glucose systems.”*

E. L. S. Barros, E. A. Rebelatto, D. A. Mayer, and J. V. Oliveira

**047** – *“Obtaining and characterization of quinoa starch (*Chenopodium quinoa* Willd.) defatted by supercritical fluids for its application as biopolymer.”*

Y. Aliaga and L. Olivera-Montenegro

**049** – *“Gelatin-Siloxane xerogel and cryogel loaded with ibuprofen by supercritical CO<sub>2</sub> assisted impregnation.”*

U. Silva do Nascimento and L. Passos Maia-Obi

**052** – *“Sequential supercritical extraction of extract of *L. rivularis* stems using CO<sub>2</sub> and ethanol-modified CO<sub>2</sub>”.*

C. Marillán and E. Uquiche

**054** – *“Enzymatic copolymerization of  $\omega$ -pentadecalactone and globalide in supercritical carbon dioxide.”*

R. D. Santos, E. A. Rebelatto, D. A. Mayer, and J. V. de Oliveira

**055** – *“Supercritical fluid extraction of coffee oils for sunscreen formulations.”*

N. Trullo, I. Mejía and G. Bolaños

**058** – *“Gelatin-Siloxane aerogels by supercritical drying.”*

B. Andrade de Campos and L. Passos Maia-Obi

- 059** – *“Value-added products from wheat straw using pressurized water + ethanol mixtures.”*  
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## Calculation of critical endpoints and phase diagrams of highly asymmetrical binary mixtures

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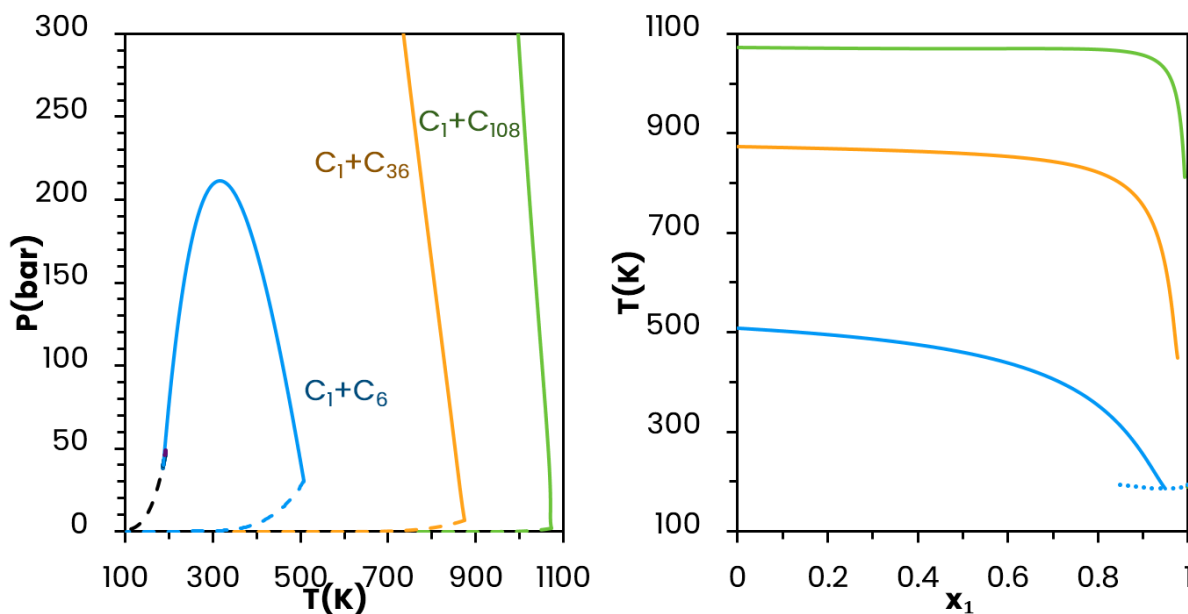
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### GRAPHICAL ABSTRACT



### ABSTRACT

The determination of monovariant lines like critical and three-phase equilibrium curves in phase diagrams of binary mixtures plays a fundamental role in analyzing potential process conditions and assessing the qualitative and quantitative capabilities of thermodynamic models. In this regard, the automatic generation of global phase equilibrium diagrams (GPED) has become an invaluable analytical tool, enabling intelligent solutions to highly complex and nonlinear mathematical problems. In particular, it was mainly the software GPEC (Global Phase Equilibrium Calculations) and the publications describing its computation strategies and methods that made it possible for a large international community of researchers to use GPED's as frequent tools in the application of equations of state to different problems.

However, the original GPEC algorithm face challenges in resolving highly asymmetric mixtures, such as gases ( $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{CO}_2$ ,  $\text{N}_2$ ) in combination with heavy paraffins, vegetable oils, or even polymers, as well as electrolytic aqueous systems. These challenges manifest in convergence problems and floating point overflow. More specifically, the UCEP or “ $k$  point” located quite close to the pure gas critical point (phase behavior of type III or IV) frequently fails to be properly found and converged in this type of systems due to the low concentration of the solute in the critical phase.

In this study, we present an innovative calculation methodology to address these challenges in highly asymmetric binary systems. Our approach builds upon the extension of existing algorithms, aiming to achieve an automatic generation of GPED that does not require manual intervention. The approach is based on the formulation of other phase equilibrium problems dealing with nearly pure phases. As a case study, we apply our methodology to analyze phase equilibrium transitions in industrially relevant systems, such as  $\text{CO}_2$  with heavy alkanes.

*Keywords:* asymmetrical binary mixtures, critical lines, critical end points, LLV, EOS