

**J.J. Luetić**

**CVRRICVLVM VITÆ**

**NAME (transliteration)**

Juan José Luetich

**TITLE**

CHEMICAL THERMODYNAMICIST

Area of Physical Chemistry

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**BIRTH**

January 24th, 1964

Rosario, Argentina



Columbia, SC. February, 2000

## EDUCATION

- B.Sc., Chemical Engineering, Universidad Tecnológica Nacional, Argentina, 1995
- Ph.D., Chemical Engineering, Universidad Nacional del Litoral; thesis: *Five Contributions to Reactive Distillation Thermodynamics*; presented (with honours) on July 6th, 2001

## RESEARCH INTERESTS

- Thermodynamics of multiphase systems undergoing chemical reactions
- Equilibrium and non-equilibrium reactive distillation operations
- Effect of the change in thermodynamic parameters on the behaviour of distillation and absorption devices
- Modelling of highly non-ideal liquid mixtures
- Ab initio calculations of binary interaction parameters
- Simulations by means of Molecular Dynamics, Monte Carlo, and Cellular Automata techniques
- The use of electronic structure methods to calculate ideal gases properties
- Thermodynamics and kinetics of gas phase reactions
- Thermodynamics of isomerisation, dimerisation and polymerisation reactions
- Chemical thermodynamics of voltaic and fuel cells

## SKILLS

- Rule-based programming with *Mathematica*
- Procedural programming with FORTRAN and LISP
- Parallel computing with *Gaussian* (National Center for Supercomputing Applications, USA), NWChem (Department of Energy, USA), and GAMESS, CHARMM and EGOVII (Clementina, SeTCIP, Argentina)
- Ab Initio calculations with *Gaussian*, GAMESS and NWChem
- Molecular Dynamics simulations with Cyrius and HyperChem
- Monte Carlo simulations with HyperChem
- Unices: Linux (Slackware, Debian, RedHat, Mandrake, Caldera), Digital Unix, SCO Unix

## GRANTS

- International visiting student at the Department of Chemical Engineering of the University of South Carolina, 2000. Topics: *Parallel Computing of Thermodynamic Properties by means of Ab Initio Methods*, and *Molecular Dynamics Simulations for the Computation of Dielectric Constants*. Professor: Dr. Perla Balbuena
- FOMEC scholarship postgraduate student at UNL, 1999 to 2001. Project Director: Ing. Alberto Castro. Topic: *Reactive Distillation*. Director: Dr. Enrique Campanella. Co-director: Dr. Ricardo Grau
- Scholarship postgraduate student at INTEC, 1997 to 1998. Topic: *Extractive Distillation*. Director: Dr. Enrique Campanella
- FRR scholarship student at the Department of Organic Chemistry. Topic: *Synthesis of Polypeptides and other Macromolecules*, 1987 to 1988. Director: Academician Oscar Nemeç
- Scholarship student at the Laboratory of Organic Chemistry, FRR, UTN. Topic: *Synthesis of Azo-Colorants*, 1986 to 1987. Director: Academician Oscar Nemeç

## WORK EXPERIENCE

- Founding member of the Luventicus Academy of Sciences, 2001-2002
- External Postdoctoral Researcher at INTEC, Area of Chemical Reactors, 2001
- High School Teacher of Physics and Chemistry, Colegio Salesiano “San José”, Rosario, 1995 to 1999
- Consultant Engineer at the OFFSET Printing Plant (properties of water+alcohol+additives system; metallic inks rheology), Editorial Didascalía, Rosario, 1997 to 1998
- College level Teacher of Mathematics, Physics and Chemistry, Instituto “Lagrange”, Rosario, 1992 to 1999
- High School and College level Teacher of Mathematics, Physics and Chemistry, Centro de Estudios “Rosario”, 1983 to 1991

## POSTGRADUATE COURSES

- Thermodynamics
- Statistical Thermodynamics
- Thermodynamics of Non-Ideal Liquid Mixtures Separation
- Chemical Reactors Analysis
- Chemical Kinetics
- Energy Transfer
- Mass Transfer
- Fluid Mechanics
- Numerical Analysis of Partial Differential Equations

## SEMINARS

- Chemical Reactors Analysis, INTEC, 1998. *The Impact of the Change in Mass Transfer Parameters on the Calculated Size of a Reactive Absorption Device*. Referees: Dr. Orlando Alfano and Dr. Ricardo Grau
- Thermodynamics, INTEC, 1999. *Free and Bound Energies*. Referee: Dr. E. Campanella
- Chemical Kinetics, FIQ, 1999. *Polymerisation in a Benzene Flame: Molecular Mass Distribution*. Referee: Dr. Eduardo Miró
- Numerical Analysis of PDEs, FIQ, 1999. *A Method to Solve Hyperbolic Partial Differential Equations Using Mathematica*. Referee: Dr. Carlos Neumann

## MEETINGS

- Third National Meeting of Young Researchers, UNL, 1999. *The Composition Variables of Equilibrium Reactive (Multi-Phase) Systems*
- Fifth Meeting of the Argentinian Committee of Phase Diagrams, Buenos Aires, 2000. *Transformed Composition Variables and the Description of Phase Equilibrium in Reactive Systems*, co-worker: Dr. E. Campanella
- XII Argentinian Congress on Physical Chemistry, Neuquén, 2001. *The Use of Ab Initio Methods to Predict Vapor-Liquid Equilibrium of Reactive Systems*, co-workers: Dr. E. Campanella and Dr. P. Balbuena

## PAPERS

- *The Choice of Composition Variables in Multi-Phase Multi-Reaction Systems* (review)
- *Ab initio calculations of Gas Phase Esterification Equilibrium Constants*, co-worker: Dr. P. Balbuena
- *Standard Gibbs Free Energy of Esterification Reactions Calculated by a Combined Electronic Structure and Volume Integration Method: I. General Discussion around the Ethyl Acetate Case, II. The Alkyl Acetate Family, III. Kinetics in the Non-Condensed Phase, IV. Vapour and Liquid Phases: Two Related Open Systems*
- *Kinetics and Thermodynamics of Gas Phase Benzene Combustion*
- *Thermodynamic Equilibrium of the Compressed Liquid Esterification of Acetic Acid with Ethanol*, co-worker: Dr. R. Grau
- *A Model for VLE in Reactive Systems*
- *A Comparison of Reactive Absorption and Reactive Distillation Thermodynamics*
- *Thermodynamic Definition of Reactive Azeotrope* (review)
- *Equilibrium Constants and Residue Curve Maps*, co-worker: Dr. E. Campanella
- *An Alternative Definition of Fugacity* (educational journal article)
- *A Chemical Short Circuit* (magazine article)
- *Planet Paths and Chemical Equilibrium. An Excursion To Some Ideas of Adrien-Marie Legendre* (magazine article)

## OTHER INTERESTS

- Music: Play the piano—music of the neo-romantic period. Compose music for piano solo and string ensembles
- Anthropology: Indoeuropean studies—languages, institution history, mythology

To obtain more information about J.J. Luetich see the *Biographical Sketch*:  
<http://www.luventicus.org/personalpages/jjluetich.pdf>