Central European Summer Time

Monday 5 July

01:30	9:00	10:30	Welcome period		
00:30	10:30	11:00	Welcome address		
		Chair:	Christophe		
00:45	11:00	11:45	**Keynote Speaker - François Nicol, Veolia Research** (recorded and available in replay)		
00:30	11:45	12:15	Ice breaker		
01:30	12:15	13:45	Break		
		Chair:	JC		
00:45	13:45	14:30	**Keynote Speaker - Antoon Ten Kate, Nouryon** (recorded and available in replay)		
			Session 1A	**Session 1B - IUT**	**Session 1C**
		Chair:			
			MS applied	**Electrolytes - Applications**	**Models**
00:20	14:35	14:55	**15 - A. Rahbari**, Delft Univ. of Technology Solubility of water in hydrogen at high pressures: A molecular simulation study	**133 - M. Williams-Wynn**, Univ. of KwaZulu-Natal, South Africa The distribution coefficients of Nd3+ between HNO3 and HDEHP	**18 - S. Hirohama**, Aveva, United-Kingdom Test of Inclusive gE Formula for Holderbaum-Gmehling Mixing Rule (PSRK) to Use NRTL together with Quadratic Mixing Rule with Temperature Dependent kji
00:20	14:55	15:15	**97 - E. Bourasseau**, CEA, France Thermodynamic properties study of MOX nuclear fuel using molecular simulation methods	**286 - J. Coutinho**, Univ. of Aveiro, Portugal The Impact of the Counterion in the Performance of Ionic Hydrotropes	**23 - R. Privat**, Univ. of Lorraine, France New insight on EoS/gE mixing rules for cubic equations of state: proposition of a unified approach
00:20	15:15	15:35	**115 - P. Petris,** Culgi BV, The Netherlands From COSMO to advanced molecular simulations	**333 - C. Lamas**, Univ. Complutense of Madrid, Spain Freezing point depression for different salty aqueous solutions using the Madrid-2019 model and the direct coexistence method	**219 - E. Moine**, Prosim, France Application of a comprehensive methodology for benchmarking a thermodynamic model

00:20	15:35	15:55	Break - The exhibitors welcome you on their booth		
			Session 2A	**Session 2B - IUT**	**Session 2C**
		Chair:			
			Interfaces	**Electrolytes - Theory**	**Models**
00:20	15:55	16:15	**64 - S. Stephan**, Lab. of Engineering Thermodynamics, Germany Enrichment of components at vapor-liquid interfaces: molecular modeling and prediction from macrosopic data	**139 - L. André**, BRGM, France Thermodynamics of saline aqueous solutions	**239 - N. von Solms**, Technical Univ. of Denmark New Association Schemes for Tri-Ethylene Glycol (TEG)
00:20	16:15	16:35	**122 - A. Mejia**, Univ. de Concepcion, Spain Experimental determination, theoretical modeling and molecular dynamics simulation of interfacial properties of CH4 + n-alkane binary mixtures	**350. A. Gonzales de Castilla**, Institute of Thermal Separation Processes, Germany : A modified closest approach parameter for the Pitzer-Debye-Hückel term to address underscreening in 1:1 electrolytes with low dielectric constants	**282 - J. N. Jaubert**, Univ. of Lorraine, France Search for the optimum values of the (u,w) parameters involved in cubic equation of state - discussion on the impact of a volume translation
00:20	16:35	16:55	**132 - S. Tiwari**, Indian Institute of Technology, Kampur, India Insight into the mechanism of nanoparticle induced suppression of detergency: experiments, modelling and simulations	**141 - X. Liang**, Technical Univ. of Denmark On the parameters used in the Debye-Hückel theory	**324 - C. S. Agger**, Calsep, Denmark Modified method of characteristics for generating EOR oil recovery curves
00:10	16:55	17:05	Break - The exhibitors welcome you on their booth		
01:00	**17:05**	**18:05**	**Student activity: Meet your hero** **The exhibitors welcome you on their booth**		

Tuesday 6 July

			announce		
		Chair:			
00:45	**10:00**	**10:45**	**Keynote Speaker - Joachim Gross, Univ. Stuttgart - Sponsored by Entropy** (recorded and available in replay)		
00:30	10:45	11:15	**3 min pitches for Helmut Knapp best poster awards - sponsored by CNRS**		
00:15	10:45	11:00	Break - The exhibitors welcome you on their booth		
			Session 3A	**Session 3B - IUT**	**Session 3C**
		Chairs:			

			Mesophases	Electrolyte - Industry	SAFT
00:20	11:00	11:20	**154 - T. Lindeboom**, Imperial College, United-Kingdom Self-assembly of the mesophases of aqueous monoglycerides using coarse-grained SAFT force fields	**91 - B. Maribo-Mogensen**, Hafnium Labs, Denmark To infinite dilution and beyond – perspectives on predictive electrolyte models	**14 - B. D. Marchal**, Exxon Mobil A doubly associated reference perturbation theory for water
00:20	11:20	11:40	**50 - G. Perez-Sanchez**, Ciceco, Portugal Unravelling the Phase Behaviour of Imidazolium-based Ionic Liquid Aqueous Solutions through Coarse-Grain Molecular Dynamics Simulations	**352 - A. Bansal,** Aveva, USA Process modeling of electrolyte systems using equation-oriented framework in AVEVA™ Process Simulation	**32 - K. Langenbach**, Lab. of Engineering Thermodynamics, Germany Thermodynamic and dielectric properties from an equation of state
00:20	11:40	12:00		**260 - S. Kuitunen**, Neste Neste's view on needs for electrolyte thermodynamics	**54 - L. F. Vega**, Khalifa Univ. of Abu-Dhabi, U.A.E Extension of soft-SAFT EoS to polar fluids: Comparison with molecular simulations and application to experimental systems
02:00	12:00	14:00	**POSTER SESSION 1** **The exhibitors welcome you on their booth**		
			Session 4A	**Session 4B**	**Session 4C**
		Chairs:	**IFT / confinement**	**IUT**	**SAFT**
00:20	14:00	14:20	**89 - R. Nagl,** Graz Univ. of technology, Austria Interfacial Properties in ternary and quaternary Systems		**120 - T. van Westen,** Univ. of Stuttgart, Germany Accurate first-order perturbation theory for fluids: uf-Theory
00:20	14:20	14:40	**51 - I. Polishuk**, Israel About interrelation between PVT and phase equilibria in the systems of Ionic Liquids		**128 - J.Cripwell**, Stellenbosch Univ. Dipolar SAFT-γ Mie: extension to secondary groups and isomers
00:20	14:40	15:00	**164 - A. Mio**, Univ. of Trieste, Italy Investigation of friction force trends at the nanoscale using computation approach		**71 - M. Kohns**, Imperial College, United-Kingdom Modelling aqueous solutions of strong and weak electrolytes using the SAFT-γ Mie equation of state
00:20	15:00	15:20	Break The exhibitors welcome you on their booth	**Round table discussion on Industrial Use of Electrolyte Thermodynamics.**	Break The exhibitors welcome you on their booth

				The debate will cover 3 questions: 1. What modeling approach do you use when confronted with an electrolyte problem? 2. How to parameterize a model in the absence of data 3. How to create collaboration on an industrially important issue	
		Chairs:	**Session 5A**		**Session 5C**
			Confined fluids		**SAFT**
00:20	15:20	15:40	**295 - H. Adidharma**, Univ. of Wyoming, U.S.A. New isochoric method to measure the phase transitions of binary mixtures confined in nanopores		**112 - M. Kiesel**, Imperial College of London Structural Properties of Ionic Surfactants using a SAFT-γ Mie Force Field in Molecular Simulation
00:20	15:40	16:00	**70 - I. G. Economou,** Institut of Nanoscience & Nanotechnology, Greece Mesoscale Modelling of Fischer-Tropsch Product Mixtures Confined in Graphene Meso-Pores		**364 - P. Rehner**, Univ. of Stuttgart, Germany A model for non-ionic surfactants based on inhomogeneous PC-SAFT
00:20	16:00	16:20	**322 - P. Habibi**, Delft Univ. of technology, The Netherlands A DFT study of the hydrogen storage capabilities of 2D honeycomb borophene oxide		**309 - E. J. M. Filipe**, Univ. of Lisboa, Portugal Complete surface tension characterization of fluorinated alcohols and their mixtures with hydrogenated alcohols: experimental, soft-SAFT-DGT modeling and MD simulations
02:00	16:20	18:20	**Working Party meeting / Job forum** **The exhibitors welcome you on their booth**		

Wednesday 7 July

min	10:00				
		Chair:			
00:45	10:00	10:45	**EFCE Michael Michelsen award lecture 2020 - Gabriele Sadowski, TU Dortmund**		
00:10	10:45	10:55	Sponsored by Elsevier - (recorded and available in replay)		
00:15	10:45	11:00	Break - The exhibitors welcome you on their booth		
		Chairs:			
			Session 6A **Molecular design**	**Session 6B** **Electrolyte - Theory**	**Session 6C** **SAFT**

00:20	11:00	11:20	**19 - J. Ilja Siepmann**, Univ. of Minnesota, U.S.A High-Throughput Simulations and Machine Learning for Adsorption in Nanoporous Materials: Applications to Storage and Separations	**49 - O. Bernard**, CNRS, France Thermodynamic properties of polyelectrolytes and associating electrolytes in solution	**99 - M. Fischlschweiger,** Graz Univ. of technology, Austria Modeling of Diffusion in Highly-Crosslinked Epoxy Resins with Maxwell-Stefan Approach and PC-SAFT
00:20	11:20	11:40	**165 - M. Fermeglia,** Univ. of Trieste, Italy How molecular simulations can inform business decisions in different industrial sectors: the composelector example	**370 - S. Hassanjani Saravi,** Princeton Univ. U.S.A Activity coefficients and relative permittivity of aqueous electrolytes from molecular simulations	**114 - J. Eller**, Univ. of Stuttgart, Germany Adsorption in heterogeneous porous media using classical density functional theory based on the PC-SAFT equation of state
00:20	11:40	12:00	**327 - T. Specht,** Lab. of Engineering Thermodynamics, Germany Quantitative fingerprinting and thermodynamic modeling of poorly specified mixtures with NMR spectroscopy and machine learning	**323 - J.P. Simonin**, CNRS, France About the "Born" term used in thermodynamic models for electrolytes	**170 - A.Reinhardt**, KIT, Germany Interfacial properties of water + long-chain molecules
02:00	12:00	14:00	**POSTER SESSION 2** **The exhibitors welcome you on their booth**		
			Session 7A	**Session 7B**	**Session 7C**
		Chairs:			
			Molecular design	**Electrolyte EOS**	**SAFT**
00:20	14:00	14:20	**27 - R. J. Sadus,** Swinburne Univ. of technology, Australia Ab initio potentials for thermophysical properties	**372 - P. J. Walker,** Imperial College of London Importance of the relative static permittivity in electrolytic SAFT-VR Mie equations of state	**113 - C. G. Alba,** Univ. of Ramon Llull, Spain Study of the Solubility of 4th Generation Refrigerant R513a with Compatible Lubricants and their Performance in Refrigeration Cycles using Polar Soft-SAFT
00:20	14:20	14:40	**29 - C. Lemarchand**, CEA, France An anisotropic coarse-grained model for polybutadiene	**291 - S. Kournopoulos,** Imperial College of London SAFT-γ Mie models for aqueous organic electrolytes: simulation benchmarks and development of a model for carboxylate salts	**213 - D. Jovell,** Univ. of Ramon Llull, Spain Characterization of the Absorption of F-Gases in new Fluorinated Ionic Liquids and Deep Eutectic Solvents with Soft-SAFT
00:20	14:40	15:00	**301 - C. Mc Cabe**, Vanderbilt Univ. of Nashville, USA Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter Systems	**345 - L. Cassayre,** CNRS, France A thermodynamic model representing solid-liquid equilibria in the VOSO4-H2SO4-H2O system based on water activity and solubility measurements	**248 - F. J. Blas**, Univ. de Huelva, Spain Interfacial properties of coarse-grained models of greenhouse gases, refrigerants, and long alkanes from density functional theory and computer simulation
00:20	15:00	15:20	Break - The exhibitors welcome you on their booth		

			Session 8A	Session 8B	Session 8C
		Chairs:			
			Molecular design	**Electrolytes - Molecular Simulation**	**SAFT**
00:20	15:20	15:40	**37 - F. Jirasek**, Univ. of California, Irvine, USA Prediction of Activity Coefficients with Machine Learning	**204 - C. Nieto-Draghi,** IFPEN, France Coarse-graining simulation of the thermodynamic and mechanical behaviour of semi-permeable membranes used in redox flow batteries	**40 - O. Wilmhelsen**, Norwegian Univ. of Science & Technology SAFT for quantum fluid mixtures and the hydrogen society: present state-of-the-art and fundamental challenges
00:20	15:40	16:00	**134 - A. Alhadid,** Technical Univ. of Münich, Germany Design of Deep Eutectic Solvents: Selecting Constituents Based on Molecular Structure	**232 - P. T. Cummings,** Vanderbilt Univ. of Nashville, USA Molecular Modeling of Supercapacitors	**339 - N. Novak,** NCSR, Greece Modeling of water-hydrocarbon phase equilibria with the SAFT-VR Mie equation of state
00:20	16:00	16:20	**355 - P. Krokidas**, Nat. Center for Scientific Research, Greece Physics-driven machine learning model for the design of highly selectivy zeolitic-imidazolate frameworks	**307 - W. R. Smith,** Univ. of Guelph, Canada Molecular Simulation of Reactive Electrolyte Solutions and Applications to CO2 Capture	**116 - T. Lafitte**, Siemens PSE, U.K The use of SAFT-y Mie EoS in industrial process modelling applications
02:00	16:20	18:20	**Job forum** **The exhibitors welcome you on their booth**		

Thursday 8 July

			Session 9A	Session 9B	Session 9C
		Chairs:			
			Experimental	**Innovative processes**	**SAFT**
00:20	9:30	9:50	**274 - D. Tuma**, Fed. Inst. for Materials Research & Testing, Germany Carbon dioxide solubility in the ionic liquid 1-Hexyl-3-methylimidazolium hexafluorophosphate	**194 - A. B. Pereiro,** Univ. Nova of Lisboa, Portugal Mitigation of the environmental impact of fluorinated gases using key enabling technologies	**93 - S. Dohrn,** TU Dortmund Univ. lab of thermodynamics, Germany Understanding solvent-induced phase separation during spray drying of pharmaceutical formulations using PC-SAFT
00:20	9:50	10:10	**30 - F. Zaidin**, Petronas, Malaysia The solubility of CO2 + H2S mixtures in water, NaCl and mixed salts aqueous solution at 373.15 K to 423.15 K and pressure up to 25 MPa. experimental and modelling	**3 - F. Montel,** Univ. of Pau, France Compositional Gradient in a thermal field	**208 - M. Wehbe**, Imperial College of London Prediction of phase diagrams and ph-solubility profiles of active pharmaceutical ingredients using the SAFT-y Mie group contribution approach

00:20	10:10	10:30	167. **V. Dumouilla**, Roquette, France : Raman spectroscopy to model and characterize physicochemical properties of aqueous solutions of carbohydrates and polyols	**181 - G. M. Kontogeorgis**, Tech. Univ. of Denmark Industrial Requirements for Thermodynamic and Transport Properties - 2020	**300 - P. A. Korchak**, St-Petersburg State Univ., Russia ePC-SAFT modeling of l-tryptophan partitioning in aqueous biphasic systems with amino acid alkylimidazolium ionic liquids
00:20	10:30	10:50	**388 - R. Dohrn,** Bayer A.G, Germany Good reporting practice - essential for all who measure or use experimental data		**7 - C. Held**, TU Dortmund Univ. lab. of thermodynamics, Germany Predicting the solubility of electrolytes in water-poor media with ePC-SAFT
00:20	10:50	11:10	Break - The exhibitors welcome you on their booth		
00:20	**11:10**	**11:30**	**EFCE Junior researcher Excellence award - Sponsored by Prosim**		
00:10	11:30	11:40	(recorded and available in replay)		
00:10	11:40	11:50	**Announcement + Helmut Knapp best poster awards**		
02:00	11:50	13:50	**POSTER SESSION 3** **The exhibitors welcome you on their booth**		
			Session 10A	**Session 10B**	**Session 10C**
		Chairs:			
			Hydrates	**Non-equilibrium**	**SAFT**
00:20	13:50	14:10	**280 - O. Toure**, Roquette Frères, France From quantum chemistry to the simulation of complex aqueous solutions including electrolytes and carbohydrates	**118 - V. Gerbaud**, Univ. of Toulouse, France Extremal principles in non-equilibrium thermodynamics	**243 - W. G. Chapman,** Rice Univ. of Houston, USA Self-assembly and phase behavior of mixed patchy colloids with any bonding site geometry: theory and simulation
00:20	14:10	14:30	**160 - Saeideh Babaee**, Univ. of KwaZulu-Natal, South Africa Gas Hydrate Concentration Measurements on Sucrose Solutions Using a New Pilot Test Rig	**197 - Tim Zeiner,** Graz Univ. of technology, Austria Computational fluid dynamics of ternary extraction systems	**157 - A. Siddiqi**, Univ. of Bath, UK Water effect in the reverse micellar formation of docusate in cyclohexane. A coarse-grained molecular dynamic approach
00:20	14:30	14:50	**359 - M.A. Marcelino Neto,** Federal Univ. of technology, Brazil Experimental study and thermodynamic modelling of carbon dioxide and methane hydrates in the presence of isopropanol	**80 - A. Dehlouz,** Univ. of Lorraine, France Can we efficiently predict fluid viscosity data by combining an equation of state with the entropy-scaling concept?	
00:20	14:50	15:10	Break - The exhibitors welcome you on their booth		

			Session 11A	Session 11B	Session 11C
		Chairs:			
			Hydrates	**Diffusion**	**Models**
00:20	15:10	15:30	**121 - A. K. Sum,** Colorado School of Mines, USA The Applied Thermodynamics of Water as Gas Hydrates: from Molecules to Phase Equilibria	**349 - H. M. Polat,** Total, France Predicting the transport properties of acid-gases in aqueous MEA solutions using molecular simulations	**374 - T. Zhao**, Imperial College of London *Ab initio* development of generalized Lennard-Jones (Mie) force fields for predictions of thermodynamic properties in advanced molecular-based saft equations of state
00:20	15:30	15:50	**144 - B. Bouillot,** Mines St Etienne, France Phase equilibrium for sea/waste water treatment and carbon capture with clathrate hydrates	**357 - M. S. Santo**s, Univ. of Queensland, Australia Finite-size effects on the diffusion coefficients from molecular dynamics simulations in crystal-like structures	**143 - S. Müller**, Hamburg Univ. of technology, Germany Including additional first-principles information into the COSMO-RS-ES model: a study on the local polarizability
00:20	15:50	16:10	**63 - P. Ahlström**, Univ. of Boras, Sweden Predicting crystal structures and gas adsorption in organic clathrates	**108 - M. Minelli,** Univ. of Bologna, Italy A thermodynamic approach for gas sorption in high free volume at cryogenic temperatures	**88 - C. Mayer,** Graz Univ. of technology, Austria Excess Gibbs-energy models based on discrete modeling of dice-like molecules
00:30	**16:10**	**16:40**	Break		
01:00	16:40	17:40	**Cultural event**		

Friday 9 July

		Chair:			
00:45	10:00	10:45	**Keynote Speaker - Kamil Paduszinsky, Warsaw Univ. of Technology** (recorded and available in replay)		
00:15	10:45	11:00	Break - The exhibitors welcome you on their booth		
			Session 12A	**Session 12B**	**Session 12C**
		Chairs:			
			Solvent CO2	**BioReactors**	**Algo**
00:20	11:00	11:20	**6 - G. Sadowski**, TU Dortmund Univ., Germany Solvent blends for an increased solubility of sour gases in amine solutions	**340 - F. A. Sanchez**, Univ. Nacional del Sur, Argentina Phase equilibrium engineering in biorefinery reactive systems: n-alkanol acetylation	**86 - F. de Azevedo Medeiros,** Tech. Univ. of Denmark RAND-based Geochemical Calculation Algorithms for CO2 Sequestration

00:20	11:20	11:40	**138 - F. de Meyer**, Total, France Prediction of CO2/H2S/CH4 solubility in pure water and MDEA, and in an aqueous MDEA solution, using molecular simulations	**265 - R. I. Canales**, Univ. Catolica de Chile Thermodynamic study of the separation of guaiacol from solvents used in the bio-oil catalytic upgrade to fuels	**98 - D. Paterson,** Linde Engineering, Germany Volume based formulation for multiphase envelope calculation
00:20	11:40	12:00	**320 - F. Tzirakis,** Center for research & technology- hellas, Greece Assessment of phase change solvents used in CO2 capture	**188 - E. A. Macedo**, Univ. of Porto, Portugal Ethyl lactate-based ATPS for recovery of flavonoids	**218 - V. Koulocheris**, Nat. Technical Univ. of Athens, Greece Chemical and phase equilibria of mercury in natural gas with the UMR-PRU model
02:00	**12:00**	**14:00**	**POSTER SESSION 4** **The exhibitors welcome you on their booth**		
		Chair:			
00:45	14:00	14:45	**Keynote Speaker - Joann Brennecke, Univ. of Texas - Sponsorised by Chemical Engineering** (recorded and available in replay)		
00:00	14:45	14:45			
			Session 13A	**Session 13B**	**Session 13C**
		Chairs:			
			Solvent CO2	**Solvent Biomass**	**Process + applications**
00:20	14:45	15:05	**137 - D. Bahamon**, Khalifa Univ. of Abu Dhabi, UAE Molecular simulations of degraded products in aqueous amines for CO2 absorption	**192 - E. Boli,** Nat. Technical Univ. of Athens, Greece Extraction of bioactive compounds from olive leaves using alternative solvents: experiments and modelling	**209 - S. Al Ghafri**, Univ. of western Australia Advanced Improvements of Boil-Off-Gas (BOG) Modelling in LNG Fuel Tanks
00:20	15:05	15:25	**258 - E. Hernandez**, Univ. Autonoma de Madrid, Spain Ionic liquid-based catalysts for effective CO2 valorization to carbonates	**195 - J. Garcia-Cano**, Univ. of Alicante, Spain Aqueous two-phase systems with short-chain alcohols and different salts: low critical solution temperature and critical compositions	**81 - P. Stringari**, Mines ParisTech, France Toward an optimized design of the LNG production process: Measurement and modeling of the solubility limits of p-xylene in methane and methane + ethane mixtures at low temperature
00:20	15:25	15:45	**53 - I. I.I. Alkhatib**, Khalifa Univ. of Abu Dhabi, UAE An integrated approach using soft-SAFT with process modelling for the efficient screening of hybrid solvents for CO2 capture	**169 - A. Roth,** Karlsruhe Inst. of technology, Germany Thermodynamic Properties of Water + Polar Polymer + Salt Mixtures	**279 - S. Lasala,** Univ. of Lorraine, France The exploitation of reactive working fluids in a closed thermodynamic cycle. A breakthrough high-energy conversion system
00:20	15:45	16:05	Break - The exhibitors welcome you on their booth		
			Session 14A	**Session 14B**	**Session 14C**
		Chairs:			

			CO2 Process	API+	Safety
00:20	16:05	16:25	**72 - K. Nasrifar,** Sultan Qaboos Univ., Oman Carbon Dioxide Freeze-out from Vapor and Liquid Phases	**234 - I. Sales**, Univ. federal da Bahia, Brazil Improvement of artemisinin solubility using ionic liquids as hydrotropes	**373 - R. Claveau,** CEA, France Toward a physical description of energetic materials sensitivity
00:20	16:25	16:45	**183 - M. G. De Angelis**, Univ. of Bologna, Italy Measurement and modelling of sorption of CO2/CH4/C2H6 mixtures in a glassy polymeric membrane for gas separation	**271 - M. Popovic,** Techn. Univ. of Münich, Germany Thermodynamic characterization of viruses: enthalpy, entropy and Gibbs energy	**231 - P. Paricaud,** ENSTA ParisTech, France Using ab initio calculation to predict the thermochemical and safety properties of multicomponent systems
00:20	16:45	17:05	**240 - W. G. Chapman,** Rice Univ. of Houston, USA Understanding CO2 Enhanced Gas Recovery from Gas Competitive Adsorption in Shale Nanopores using Molecular Density Functional Theory	**337 A. Victorov,** Saint Petersburg State Univ., Russia Specific interactions in the model of mixed nonionic micelles: predicting aggregation behavior and details of structure	**342 - M. Maury,** CEA, France Comparison of approaches to determine lower flamability limits
00:05	17:05	17:10	**Beekast results**		
00:20	17:10	17:30	Closing remarks		