Fluids for Extraction and Energy production

Research group **FEE** - Fluids for Extraction and Energy production

Leader: Yohann Coulier(https://iccf.uca.fr/annuaire/m-yohann-coulier)

Research Topics

The development of technologies for the capture of CO2 is a major research front, requiring thermodynamic knowledge on solubility, selectivity and diffusion of gases in absorbing media. The originality of the group's research on CO2 absorption is the measurement of energetic quantities, which are crucial for the steps of regeneration of the absorbent: too strong a binding of CO2 makes the capture process hardly reversible. The challenge resides in the search for the optimum compromise, reconciling the highest possible CO22load with an energetically (and economically) acceptable regeneration of the absorbent. The group's studies of gas sorption calorimetry contribute to characterize and develop new absorbent media for industrial capture and also for geological sequestration. Thermodynamic models are formulated in order to describe the physical and chemical equilibria in these multi-component systems containing ions, gaseous and liquid species.

The geological storage of CO2 is then a very logical complement to the group activities. Indeed, when CO2 is separated from industrial effluents, it must be either used or stored in secure storage areas. One of the solutions is the geological storage in deep aquifers. The knowledge of geological, geochemical and thermodynamic properties is fundamental to avoid serious environmental problems (brutal spill of a large amount of gas for example). In this context, the study of variations in physicochemical (pH,...) and thermodynamic properties (enthalpies of dissolution of gas, solubility,...) of the medium in presence of dissolved gas is fundamental. Experimental studies realized in the laboratory at conditions close to storage sites conditions (high temperatures and high pressures) will be fundamental for the development or adjustment of rigorous thermodynamic models describing those environments, in order to predict the behavior of the sites in the presence of dissolved gases.

Finally, if the CCS (carbon capture and storage) is a major pathway for reducing greenhouse gas emissions of fixed sources using fossil fuels, it is important to contribute to the development of "clean" processes for energy production, for example using biomass. The Group has started recently a thermodynamic study of molecules associated with the bio-conversion, in collaboration with Ecole des Mines of Fontainebleau (CEP

/TEP). This work, which is essential in the design and development of new processes is currently poorly studied and documented.

News(https://iccf.uca.fr/english-version/research/thermodynamics/gas-absorption-mechanisms/news)

Competences

Researches in the field of capture and storage of CO2 combine original experimental methods and thermodynamic model uses.

THERMODYNAMIC AND PHYSICO-CHEMICAL PROPERTIES STUDIED:

- Volumic masses, molar, excess, standard volumes...
- Solution enthalpies of Gas in solution, coupled with indirect determination of gas solubility limits
- liquid-liquid mixing enthalpies
- Protonation enthalpies
- Specific heat capacities, excess, standard heat capacities...
- Liquid-liquid or liquid-gas phase separation temperature
- Phase diagrams
- pKa, equilibrium constants...

EXPERIMENTAL METHODES AVAILABLE:

Volumetry

Vibrating tube densimetersto work from -20°C to 400°C pressure up to 400 bars.

Calorimetry

Micro-calorimeters with fluxmetric detection for liquid-liquid or liquide-gas mixing.
MicroDSC for the determination of phase transitions with low energy and heat capacities, up to 200°C.
Picker type calorimeter with power compensation for heat capacities up to 400°C and 400 bars.

Phase equilibria

Phase equilibria cell for visualisation of LL and LV phase separation up to 125°C and 400 bars.

Potentiometry

automatic titrator for aqueous solutions (glass electrode) up to 70°C

MODELISATION GROUP CONTRIBUTION (UNIFAC)

- Local composition (NRTL, UNIQUAC...)
- Activity coefficients and fugacity models
- Molecular simulation (force field, prediction of properties derived from Gibbs Energy)

Programs

RUNNING PROGRAMS :

- 2016 - 2019 : ANR/NSERC International program France-Canada : SiModEx

To understand the CO2 capture processes : combination or reactive molecular simulation , thermodynamic models and experimental data.

- 2015 - 2016 : joint research programm with CTP Fontainebleau
- 2013 - 2016 : ANR blanc International France-Canada : DACOOTA project

"Demixing Amines for CO2 capture: Thermodynamic and Spectroscopic Approach"

- 2014 - 2017 : ANR SEED : SIGARRR Simulations de l'Impact des Gaz Annexes (SOx, NyOx, O2) co-injectés avec le CO2 lors de son stockage géologique) sur la Réactivité des Roches-Réservoirs
- 2014 - 2016 : ADEME : LIS - VALORCO

Research Program for the reduction of CO2 emissions called LIS for « Low Impact Steelmaking »; two main research axes : reduction of CO2 with gaz recycling in high-furnace (« TGRBF ») and valorisation of CO2 (« Valorco »)

People

PERMANENT MEMBERS

M. Jean-Michel ANDANSON (https://iccf.uca.fr/annuaire/m-jean-michel-andanson)

MME Karine BALLERAT BUSSEROLLES (https://iccf.uca.fr/annuaire/karine-ballerat)

M. Yohann COULIER (https://iccf.uca.fr/annuaire/m-yohann-coulier)

M. Jean-Yves COXAM (https://iccf.uca.fr/annuaire/m-jean-yves-coxam)

Laurence RODIER (https://iccf.uca.fr/annuaire/laurence-rodier)

PHD STUDENTS

Nom	Position	Support	Dates
Olympe Longeras	PhD student	UCA	october 2017 - ..
Fernando Hevia de los Mozos	PhD student (spain)	short term stays	sept-dec. 2017 et sept-dec. 2018

STUDENTS/POST-DOC/VISITING SCIENTISTS/CDD

Nom	Position	Support	Dates
Yohann Coulier	Researcher	ANR SiModEx	May 2018 - August 2018
Juzaimi, Nurhazwani	Master of Science in Advanced Chemical Engineering	AAP Emergence, i-Site CAP2025, Coll. Imperial College, Londres	July 2018
Yiyan ZHENG	Elève Ingénieur, cycle Ingénieur Civil	Stage de fin d'étude, coll. ICCF-CTP-Calnesis	Juillet 2018
Giovanni Ramdani	Master II	AAP Emergence, i-Site CAP2025	janvier - Juillet 2018
Ryan Wilkins	Master's Student of Guelph, stage	ANR SiModEx	1 Mai 2018 - 27 Juillet 2018
Johan Vigier	Master I	ANR SiModEx	Avril - Juillet 2018

STUDENTS/POST-DOC

Name	Level	Financial Support	date
Yohann Coulier	CDD Researcher	ANR DACOOTA, ANR SiModEx	apr. 2016 - ...
Alexander Lowe	PhD student	ANR DACOOTA	oct. 2013 - ...
Barbara Liborio	PhD student	ANR SIGARRR	feb. 2014 - ...
Elena Baboi	PhD student	ANR SiModEx	May 2016 - ...

Clément Rico	Master I	ANR SiModEx, CALNESIS	April - July 2016

OLD CONTRACT AND POST-DOCT

Nom	Position	Financial Support	Dates	Actual Position
Alejandro Moreau	Researcher	Ademe Inv. Avenir VALORCO	février 2015 - février 2016	Imperial College, London
Javier Mesones Mora	Researcher	Ademe Inv. Avenir VALORCO	septembre 2014 - Aout 2015	URSA (resp. Quality)
Alexandre Moury	Undergrad Student L1	UBP	july 2014	
Eva CZAJKOWSKA	Undergrad Student (poland)	Univ. of Gdansk	july 2014	
Mickael Simond(http://iccf.univ-bpclermont.fr/spip.php?article410)	Engineer, CDD	CNRS	nov. 2013-feb 2014	President, CALNESIS

PAST PHDS

Name	Defence date	Financial Support	Actual Position
Mickael Simond(http://iccf.univ-bpclermont.fr/spip.php?article410)	27/11 /2013	MESR	Engineer, CDD, ICCF
Yohann Coulier	16 december 2011	FUI ACACIA	Post-Doc at University of Guelph, Guelph, ON, Canada
Dimitrios Almantariotis	27 may 2011	ADEME	
Hugues Arcis	15	MENSR	Post-Doc at University of

	december 2008		Guelph, Guelph, ON, Canada

[Pictures from the group](https://iccf.uca.fr/english-version/research/thermodynamics/gas-absorption-mechanisms/pictures-from-the-group)

Academic and Industrial Collaborations

ACADEMIC COLLABORATIONS

- Pr Nikolay Akinfiev, Geochemistry Laboratory, Institute of Geology of ORE deposits, Petrography et Mineralogy, (IGEM), Russian Academy of Sciences.
- Dr Christophe Coquelet, TEP Laboratory, Energetic and Process Center, Mines Paris Tech'
- Pr Peter Tremaine, Department of Chemistry, University of Guelph, Guelph, ON, Canada
- Pr Pierre Cézac, Thermic Energetic et Process, Université de Pau et des pays de l'Adour

INDUSTRIAL PARTNERS

- IFP Energies Nouvelles
- SETARAM
- Total
- Processium
- ExxonMobil Research and Engineering Company

Communication - Diffusion

Meeting participation of CO2 group:

2016

Oral communications

LIQUID-LIQUID PHASE SEPARATION FOR MIXTURES CONTAINING DISSOLVED GASES, APPLICATION TO CARBON CAPTURE PROGRAMS
K. Ballerat-Busserolles Coulier, A. Moreau, A. Lowe, J-Y. Coxam, 24th International Conference on Chemical Thermodynamics (ICCT-2016), 21-26 August 2016, Guilin, China

SOLID-LIQUID PHASE DIAGRAM OF UREA + CHOLINE CHLORIDE DEEP EUTECTIC SOLVENT AND IMPACT OF WATER ON THE MELTING TEMPERATURE
K. Ballerat-Busserolles, X. Meng, J-M. Andanson, P. Husson,24th International Conference on Chemical Thermodynamics (ICCT-2016), 21-26 August 2016, Guilin, China

CALORIMETRIC AND DENSIMETRIC MEASUREMENTS FOR MODELLING ELIMINATION OF CARBON DIOXIDE BY DISSOLUTION IN AQUEOUS SYSTEMS: DATA FOR GEOLOGICAL SEQUESTRATION
Barbara Liborio, Alejandro Moreau, Nicole Nénot, Karine Ballerat-Busserolles, Jean-Yves. Coxam,3rd international conference on thermophysical and mechanical properties of advanced materials (THERMAM), 1-3 September 2016, Izmir, Turkey

NEW AMINE BASED SOLVENTS FOR ACID GAS REMOVAL
Yohann COULIER, Elise EL AHMAR, Jean-Yves COXAM, Elise PROVOST , Didier DALMAZZONE, Patrice PARICAUD,Christophe COQUELET, Karine BALLERAT-BUSSEROLLES, 6th INTERNATIONAL ACID GAS INJECTION SYMPOSIUM (AGIS VI), 25-28 october 2016, Houston, TX, USA

LIQUID-LIQUID PHASE EQUILIBRIA OF DEMIXING AMINES FOR CARBON CAPTURE AND STORAGE
Alexander Lowe, Yohann Coulier, Karine Ballerat-Busserolles, Jean-Yves Coxam, 66th Canadian Chemical Engineering Conference, 16-19 october 2016, QUÉBEC CITY, QC, Canada

Posters

LIQUID-LIQUID EQUILIBRIUMS IN AQUEOUS SOLUTIONS OF DEMIXING AMINES LOADED WITH GAS FOR CO2 CAPTURE PROCESSES.
Yohann Coulier, Alexander R. Lowe, J-Y. Coxam, Karine Ballerat-Busserolles, 14th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), May 22-26, 2016, Porto, Portugal

2015

Communications orales

CALORIMETRY IN AQUEOUS SOLUTIONS OF DEMIXING AMINES FOR PROCESSES IN CO2 CAPTURE,
Karine Ballerat-Busserolles, Alexander R. Lowe, Yohann Coulier, J-Y. Coxam, 5th INTERNATIONAL ACID GAS INJECTION SYMPOSIUM (AGIS V), May 19th -22n

Publications(https://iccf.uca.fr/english-version/research/thermodynamics/gas-absorption-mechanisms/publications)

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