Programme de la Journée Scientifique 2022
du Labex CaPPA
Jeudi 10 mars 2022
Amphithéâtre Pascal
Cité Scientifique, IMT Nord Europe
Villeneuve d'Ascq

8:30-9:00  Accueil - Café
9:00-9:25  Introduction – Point d'avancement du projet CaPPA.
9:30-10:45 Synthèse des activités scientifiques 2021 (1ère partie) *
  9:30-9:55  WP6 : "Box modelling of the atmospheric chlorine chemistry", Zainab Srour
  9:55-10:20 WP5 : "Impact of fuel composition on primary and secondary aeronautic emissions: gaseous and particulate chemical characterization at molecular level", Raphael Barrellon-Vernay
  10:20-10:45 WP4 : "Improved characterization of volcanic SO$_2$ emissions and plume dispersion using inverse modelling assimilating TROPOMI, OMPS and IASI observations into an Eulerian chemistry-transport model", Abhinna K. Behera
10:45-11:00 Pause
11:00-11:30 Poster flash (liste en page 3)
11:30-12:15 Session Poster
12:15-13:00 Buffet
13:00-13:45 Café - Posters
13:45-15:00 Synthèse des activités scientifiques 2021 (2ème partie) *
  13:45-14:10  WP1 : "Nighttime atmospheric degradation of biomass burning compounds: the fate of methylated furan compounds", Fatima Al Ali
  14:10-14:35 WP2 : "Synergic retrieval of atmospheric properties using visible and thermal infrared spectrum", Marcos Herreras-Giralda
  14:35-15:00 WP3 : "Aerosol optical and chemical properties at the ATOLL site", Alejandra Velazquez-Garcia
15:15-16:00 Conférence Plénière (visio) – Andreas Zuend, Mac Gill University
« Modeling of aerosol hygroscopicity, phase separation and cloud droplet activation »**
https://univ-lille.fr.zoom.us/j/92147275016?pwd=N29pbzB1ODFWYUhBRkFFejFjIzbfNWQT09
16:00-16:30 Posters - Café
16:30  Clôture de la journée

* Découpage par WP : bilan 2021 par les WPs leaders (5’), présentation scientifique (15’), questions (5’)
** Résumé en page 2 de ce programme
Modeling of aerosol hygroscopicity, phase separation and cloud droplet activation

Abstract:

The water uptake characteristic (hygroscopicity) of atmospheric aerosols is among several key properties controlled by chemical composition. The hygroscopicity is relevant for particle size, cloud droplet activation, and interactions with radiation. The equilibrium state of a particle is affected by nonideal thermodynamic mixing within its condensed phases and the simultaneous partitioning of semivolatile organic and inorganic species. The occurrence of liquid–liquid phase separation in mixed organic–inorganic particles can affect the aerosol mass concentration, phase viscosities, and particle surface properties. Thermodynamic and dynamic models of these processes attempt to provide predictions for use in detailed single-particle models as well as large-scale atmospheric models. However, a trade-off exists between the level of affordable chemical complexity, available information, and computational costs. In this seminar, we will introduce a relatively detailed framework based on the AIOMFAC model as well as a reduced-complexity organic aerosol model, which offers the ability to process input information typically available in large-scale air quality models and/or data from field studies. We will discuss applications of these models toward a predictive understanding of aerosol hygroscopicity, gas–particle partitioning, and cloud droplet activation.
Liste des posters:

P1 : "Synergy of Mie-Raman-fluorescence lidar and Radiometer measurements for aerosol hygroscopicity studies"
Robin Miri

P2 : "Biowaste volatile organic compounds emissions and potential for particle formation"
Kwathar M. Haider

P3 : "Millimeter-wave spectroscopy of methylfuran isomers: local vs global treatment of the internal rotation"
Jonas Bruckhuisen

P4 : "Cavity-enhanced Faraday rotation measurement for OH monitoring"
Minh Nhut Ngo

P5 : "Differentiating indoor and outdoor individual exposure to particles: methodology and first results"
Jérôme Chesneau

P6 : "Mixing State of Atmospheric Particles during Pollution Events in an Urban and Industrialized Area"
Soulemane Ngagine

P7 : "Predictive simulations of core electron binding energies of halogenated species interacting with solvent environment from relativistic quantum embedding calculations"
Richard O. Opoku

P8 : "Assessing MP2 frozen natural orbitals in relativistic correlated electronic structure calculation"
Xiang Yuan

P9 : "Absolute absorption cross section of the C_2H_5O_2 radical and kinetic of its self-reaction : Rate constant and branching ratio"
Cuihong Zhang

P10 : "OH-initiated atmospheric degradation of 2,3,4,5-chlorophenol insecticide"
Hisham K. Al Rawas

P11 : "OH-initiated atmospheric degradation of phosmet insecticide"
Reem Al Mawla

P12 : "Reactivity of OH with CH3I in the presence of H2O"
Sonia Taamalli

P13 : "Reactivity of H atoms with halogenated polycyclic aromatics hydrocarbons"
Nesrine Bekkal

P14 : "Kinetic study of heterogeneous reactions on oleic acid clusters using a QM/MM approach"
Akilan Rajaman

P15 : "Unexpected phase behavior of complex particles containing ammonium sulfate, glycolic acid and oligomer: Study at the single particle scale"
Mikel Sader

P16 : "Polluen" : le pollen à l'ère de l'anthropocène
Marie Choël