

## **MODELING MOLECULAR MARKERS OF ORGANIC AEROSOLS TO ASSESS GAS/PARTICLE PARTITIONING OF ORGANIC COMPOUNDS IN THE ATMOSPHERE**

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Atmospheric aerosols have an impact on air quality and climate. The organic component (OA, organic aerosols) represents a large part of aerosols. OA can be emitted directly (primary OA) or formed by the oxidation of volatile organic compounds into secondary organic aerosol precursors (SOA). Both primary and secondary sources can be of biogenic or anthropogenic origin.

Many complex phenomena contribute to the formation of OA (gas/particle partitioning of semi-volatile compounds influenced in particular by the effect of viscosity, complex and non-linear gaseous or aqueous chemistry, hydrophilic or hydrophobic properties of the compounds, oligomerization, etc.). Because of the lack of knowledge on these processes, Chemistry-Transport Models (such as the CHIMERE model co-developed by INERIS and CNRS) use simplified parameterizations that do not represent all these phenomena and tend to underestimate the formation of AOs. In addition, many studies point out a complex dependence of the formation of AO to the concentrations of radicals (HO<sub>2</sub>, RO<sub>2</sub>, OH), ozone, nitrogen oxides (NO<sub>x</sub>), but also to the concentrations of inorganic aerosols.

OA molecular markers are chemical compounds characteristic of the primary emission sources of AOs or of the processes by which AOs are formed from specific precursors. Incorporating such compounds into models can be used to study and improved the representation of AOs in models. We previously demonstrated, using such an approach, that models strongly underestimated the gas/particle partitioning of organic compounds and did not account for some AOS precursors ([Grazia Lanzafame thesis defended in 2019](#)).

The main objective of the thesis proposed here will be to improve the representation of AO, markers and more particularly gas/particle partitioning in the CHIMERE air quality model. Ultimately, this work will provide key elements on the formation processes of molecular markers in order to account for the potential use of their representation in the CHIMERE model for the purpose of tracing and assessing sources and precursors of AO.

In this context, recent studies show that the gas/particle partitioning could be strongly affected by the viscosity of AOs. Indeed, the viscosity could affect the dynamics of condensation/evaporation of organic compounds and could for example trap compounds within the particle. The gas/particle partitioning would then move away from the thermodynamic equilibrium, usually assumed in 3D modeling. However, approaches used currently in 3D modeling do not adequately take into account the low volatility of AOs as well

as the effect of viscosity which influences the condensation/evaporation processes of organic compounds. A new methodology has been developed to overcome these difficulties by generating reduced mechanisms from complex mechanisms (GENOA tool, Zhizhao Wang's thesis, defense planned in 2022).

The PhD student will have to:

- (1) Improve the reduced mechanisms of formation of various molecular markers of secondary AOs of biogenic and anthropogenic origin based on mechanisms available in the literature and the GENOA tool. The list of markers treated during Grazia Lanzafame's thesis will be extended to new compounds (notably markers of sesquiterpenes and spores or acid oxalic).
- (2) Implement these new mechanisms in the air quality model CHIMERE and the evaluation of the model results by comparison to in-situ measurements (INERIS data from Grazia Lanzafame and Deepchandra Srivastava's thesis, CARA program, Landex project).
- (3) Evaluate the effect of viscosity on the gas/particle partitioning of molecular markers.

### PROFIL

- Degree Master on chemistry or on modeling
- Strong skills in programming and modeling
- Knowledge in chemistry would also be welcomed
- Autonomy, scientific rigor, adaptability, communication and writing abilities.
- Good English level

**Ce poste est ouvert aux personnes en situation de handicap.**