[Arial Bold; 10,5pt.] Example
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CARATk, a new toolkit for radionuclides atmospheric transport simulation for the CHIMERE model

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INTRODUCTION AND MAIN RESULTS

We present our work on the CHIMERE Assisting Radioactive Analysis Toolkit (CARATk), a new toolkit for the CHIMERE chemistry transport model. It will permit simulation of transport, chemistry and physical processes of radionuclides in the atmosphere. Our poster will focus on two main points in our development of CARATk.

Firstly, we compared the performances of CHIMERE and of the Lagrangian model FLEXPART, in the context of the ^{106}Ru pollution detected in 2017 over the Northern Hemisphere.

Secondly, we will elaborate on what is CARATk particularly on what is its aim. We will present uses of CHIMERE with CARATk in the context of the Fukushima accident to illustrate some of its capabilities, limitations and prospects for future developments.

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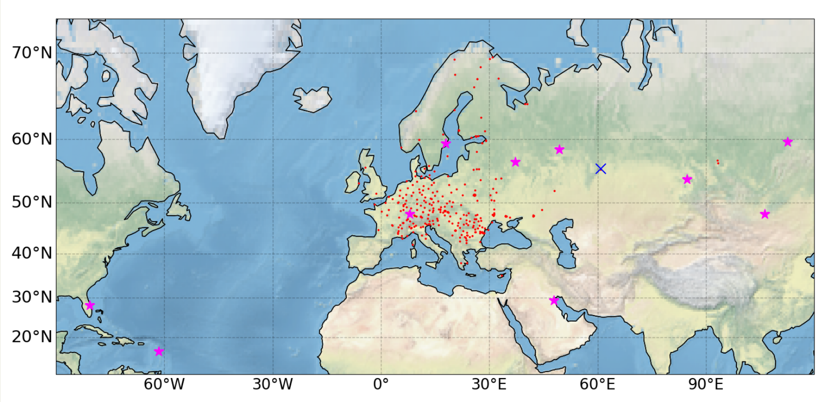
Long range transport validation of CHIMERE

Two types of model are usually used to describe atmospheric transport of pollutants: Lagrangian and Eulerian models. Compared to Lagrangian models, Eulerian models tend to present a numerical diffusion that can deteriorate their precision (Eastham and Jacob, 2016; Zhuang et al., 2018).

Before adding new mechanisms to CHIMERE an Eulerian chemistry transport model, we propose to evaluate if its numerical diffusion does not impede too much its performances. We chose to compare CHIMERE to FLEXPART in the context of the ^{106}Ru pollution detected in 2017 over the Northern Hemisphere (see map of stations that detected the pollution below and for which we had access to data).



Simulations with both models were performed with parameters as close as possible in CHIMERE and FLEXPART.

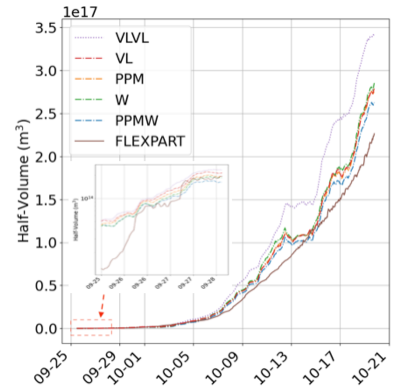
Publication : Léo Adenis et al.
"Lagrangian and Eulerian modelling of 106Ru atmospheric transport in 2017 over northern hemisphere", Journal of Environmental Radioactivity, Volume 275, 2024, 107416, ISSN 0265-931X, https://doi.org/10.1016/j.jenvrad.2024.107416.

Mitigating numerical diffusion in CHIMERE

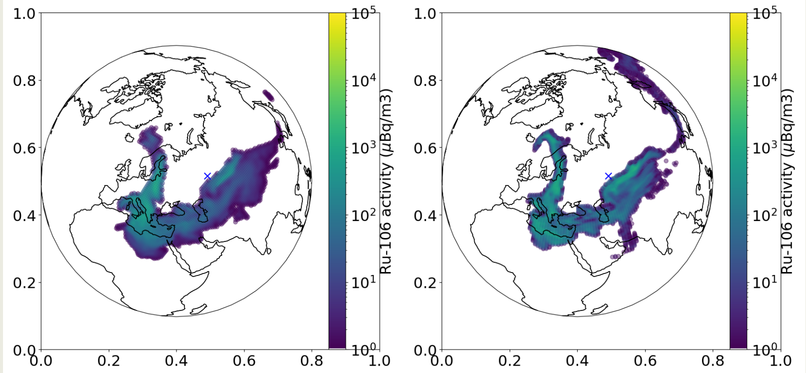
In CHIMERE multiple numerical schemes for transport are available. We tested them to evaluate if numerical diffusion could be under control. The table below is summarizing the scheme we tested.

Advection schemes used in our simulation using CHIMERE.

Simulation Label	Horizontal advection	Vertical advection
VLVL	Van Leer (Van Leer, 1977)	Van Leer (Van Leer, 1977)
VL	Van Leer (Van Leer, 1977)	Deprés-Lagoutière (Després and Lagoutière, 1999)
PPM	Piecewise Parabolic Method (Colella and Woodward, 1984)	Deprès-Lagoutiére (Després and Lagoutière, 1999)
W	Walcek (Walcek, 2000)	Deprés-Lagoutière (Després and Lagoutière, 1999)
PPMW	PPM+W (Mailler et al., 2023b)	Deprés-Lagoutière (Després and Lagoutière, 1999)



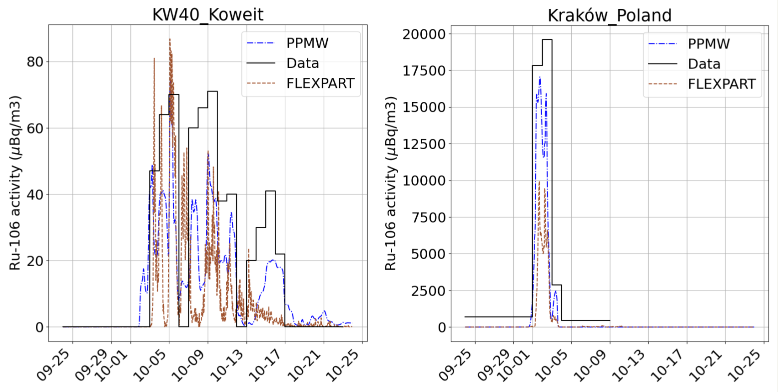
Numerical diffusion was evaluated with the notion of half-volume, the smallest volume that contains at least half the mass of tracer (Lachatre et al. 2020). Results shown on the left indicate that numerical diffusion was reduced.



Snapshots of the simulations, CHIMERE on the left, FLEXPART on the right.

FLEXPART and CHIMERE performances

We compared FLEXPART performances to CHIMERE's by comparing both to all the measurements we had access to. Qualitatively simulations and data are presented at two stations below.



Quantitatively we went with the confusion matrix way and computed some key indicators to evaluate performances globally with all measurements (below).

Example of confusion matrix between a simulation (SIM) and Measurements.

		Measured	
		Yes	No
SIM	Yes	TP	FP
	No	FN	TN

Confusion matrices for FLEXPART, PPMW, PPM, W, VL and VLVL simulations.

		Measured			Measured			Measured	
	FLEX	Yes	No	*PPMW*	Yes	No	*PPM*	Yes	No
Model	Yes	345	286	Yes	341	108	Yes	342	116
	No	169	540	No	173	718	No	172	710
	W	Yes	No	*VL*	Yes	No	*VLVL*	Yes	No
Model	Yes	349	150	Yes	335	104	Yes	335	102
	No	165	676	No	179	722	No	179	724

In our study, overall CHIMERE performed better

Performances indicators for all simulations. Bold is for best performances in the tested models and italic is for the worst, random no-skill model excluded.

Label	Bias	Sensitivity	Specificity	Precision	NPV	Accuracy	Baccuracy	MCC
VLVL	*0.850*	*0.652*	**0.877**	**0.767**	0.802	**0.790**	0.764	0.548
VL	0.854	*0.652*	0.874	0.763	0.801	0.789	0.763	0.545
PPM	0.891	0.665	0.860	0.747	0.805	0.785	0.762	0.538
W	**0.971**	**0.679**	0.818	0.699	0.804	0.765	0.749	0.500
PPMW	0.874	0.663	0.869	0.759	**0.806**	**0.790**	**0.766**	**0.549**
FLEXPART	1.228	0.671	*0.654*	*0.547*	*0.762*	*0.660*	*0.662*	*0.317*
RANDOM	1.000	0.384	0.616	0.384	0.616	0.527	0.500	0.000

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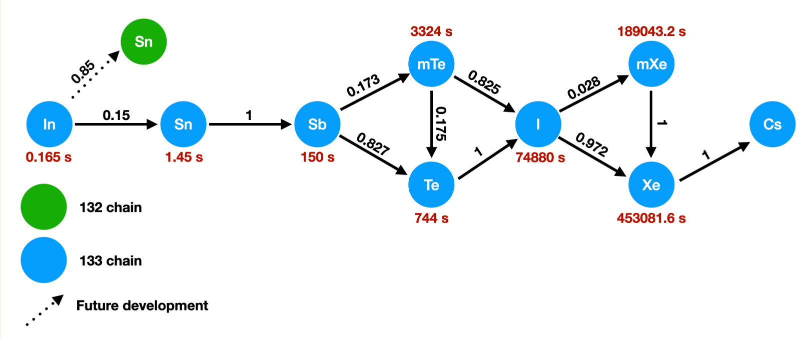
What is CARATk

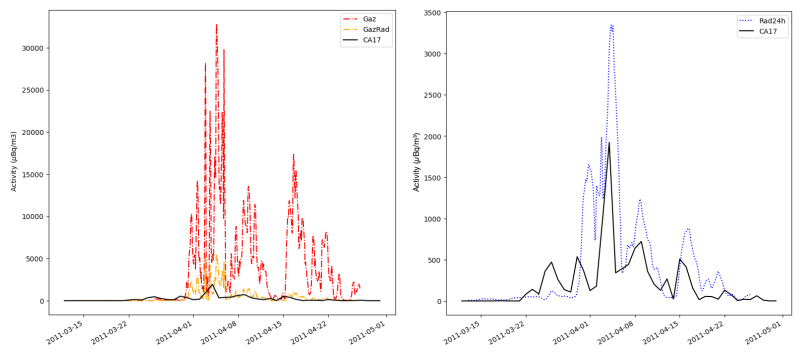
Our objectives when developing CARATk is to propose a series of numerical tools to help take advantages of the flexibility of CHIMERE chemistry engine to better represent radionuclides when modelling a radioactive atmospheric pollution event. To that end, CARATk will be composed of a database with physical and chemical parameters needed to model radionuclides in CHIMERE. At the very least it will contain their half-lives and branching factor in their decay chains (graphic representation example of chain 133 below).



This database will be enriched with new parameters as we need it. CARATk will also propose pre- and post-processing scripts to prepare the necessary input files for CHIMERE and extract simulated radionuclides of interest in the results files of CHIMERE simulations.

Modeling Fukushima accident with CARATk

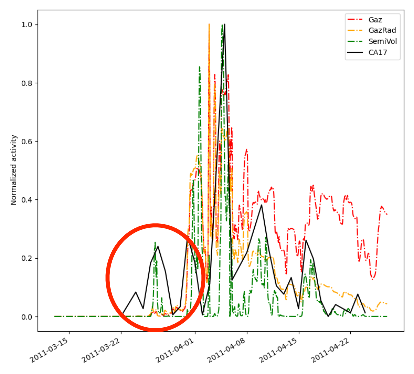
The first mechanisms we tested with CARATk were the basics of radioactive decay and filiation for gas tracers in CHIMERE. We decided to simulate the accident at Fukushima as it presented many measurements and a complex release source term (G. Katata et al. 2015 and ASNR). Below are presented comparisons of two simulated tracers (representing iodine 133) with CHIMERE with the measurements done at the CA17 station of the IMS (in black). Left present two CHIMERE simulations: in red a simulation of a simple gas tracer in CHIMERE and in orange a tracer prepared with CARATk. On the right, only the tracer from CARATk is presented so that results are more clearly shown in comparison of the measurements.



As expected a better representation of the radioactive decay can produce simulations that are closer to the reality.

Prospects for CARATk

With CARATk we wanted to allow the simulations of transport of radioactive decay chains in the atmosphere with CHIMERE. With this first step and the verification that numerical diffusion is under control done, new prospects for our toolkit arise. Some in terms of post-processing with scripts to pursue radioactive decay in the deposition calculated by CHIMERE, for example. Some in pre-processing, CHIMERE offers a complex physico-chemistry engine that could allow us to even better represent radioactive elements. One of our latest tests involved being able to have a gas-particle equilibrium for a radioactive species (see bottom figure). Our future works will focus on those improvements for the next release of CARATk.



On the left, we show the normalized activity at the CA17 station to better highlight the first peak in every simulation. The red circle highlights our main interest in this first test. The first detected peak (data in black) might be better represented compared to our previous simulations (same legend as middle figure).