Improving Probabilistic Gas Hazard Assessment through HPC: Unveiling VIGIL-2.0, an automatic Python workflow for probabilistic gas dispersion modelling

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Solid Earth and Geohazards in the Exascale Era

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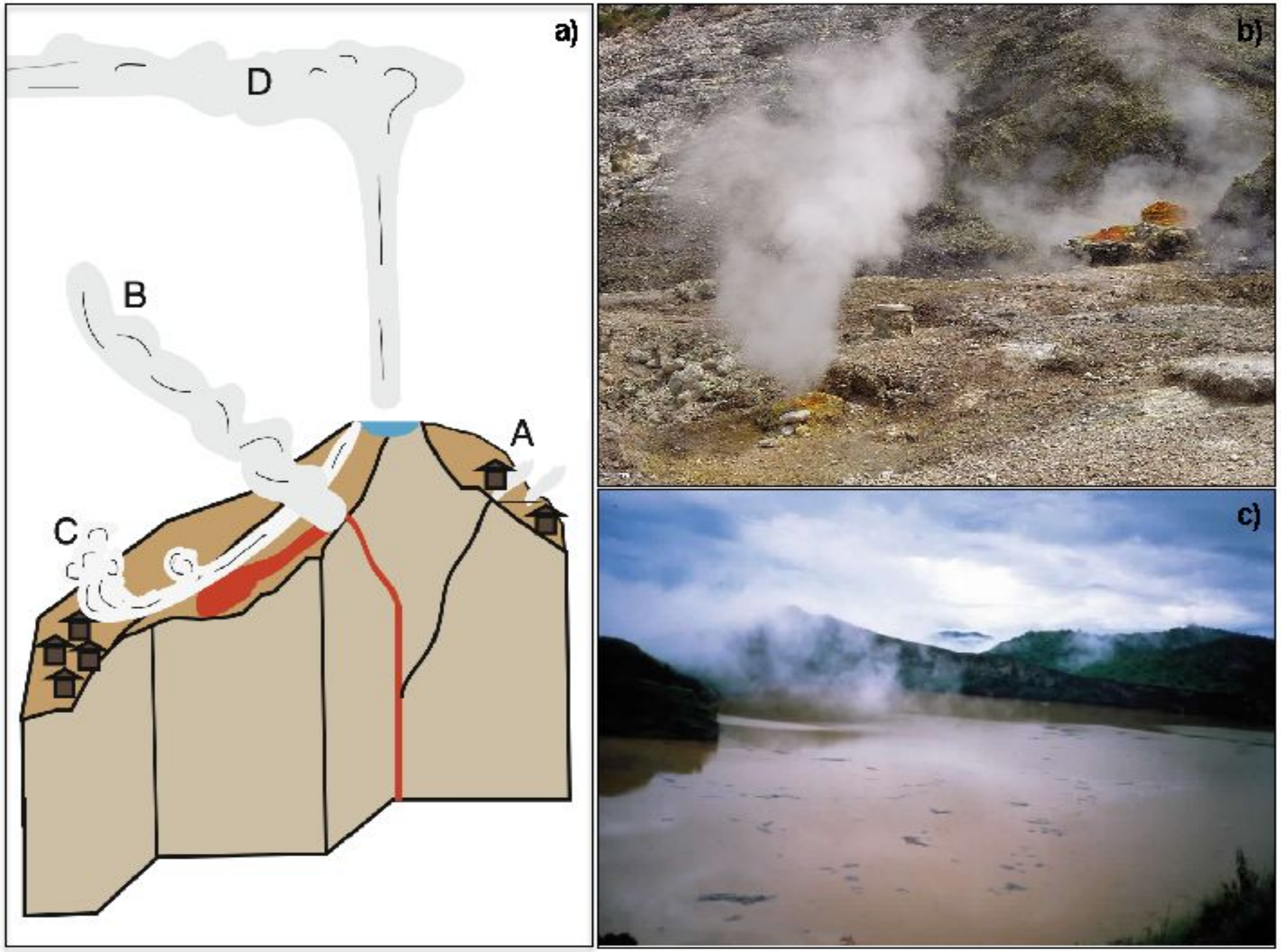
Gas dispersal hazard

- Gas dispersal is mainly controlled by the emission properties (flow rate, extent, temperature, density), meteorological conditions, and the terrain features;

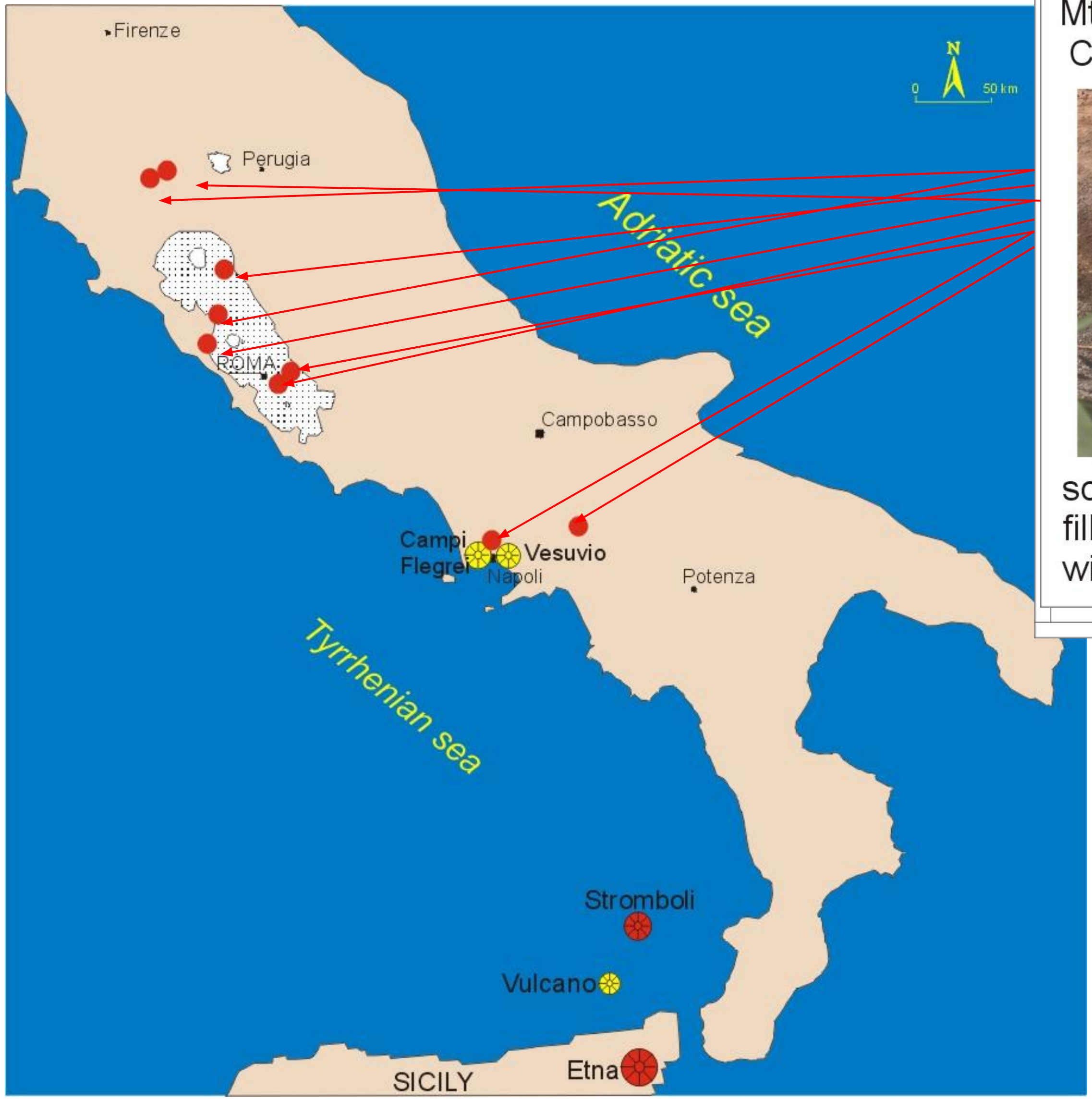
- Volcanic gases may be passively transported by wind (e.g. diffuse degassing, fumaroles) or dispersed as gravity flows (e.g., flows of cold CO_2-rich gases following a phreatic or limnic eruptions;

- Long-term exposure to high concentration of different gas species dispersed in the atmosphere (e.g., CO_2, H_2S, SO_2) can be a threat for humans, for animals and the surrounding environment.



from Dioguardi et al. (2022)

❑ Gas dispersal hazard: examples



Mt. Amiata (Siena): strong diffuse CO_2 emission

some people died inside a karstic 'dolina' filled by CO_2. The area is a lethal trap for wild animals.

Natural dense CO_2 emissions in Central Italy

The CO_2 emissions in Italy represent a danger for humans and animals. The mitigation of this risk can be obtained with a better knowledge of the natural phenomena.

Gas dispersal hazard: examples

Limnic eruptions in Africa

On 26 August 1986 a very large CO_2 volume emitted from Nyos lake in Camerun killing ca. **1700 people** and **3500 animals**.
Two years later a similar event occurred at Monoum lake, in Camerun, and **37 people** died.

Gas Estimates at Lake Nyos

Potential CO_2 accumulation	1.45 km^3
CO_2 accumulation in May 1987	0.38 km^3
CO_2 released in 1986	0.68 km^3 (fino a 1 km^3)

(Kling, 1989)

❑ Long-term Probabilistic Gas Hazard Assessment

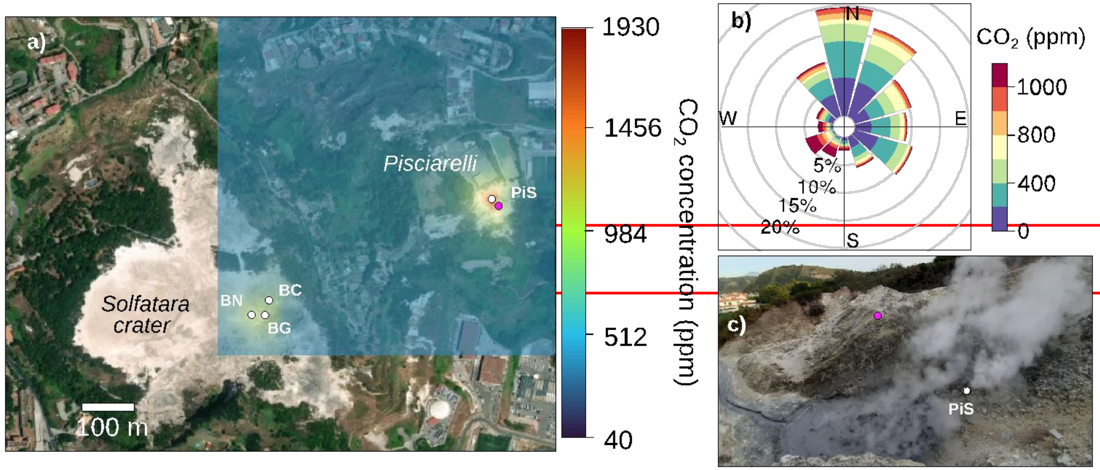
In this context, the natural variability associated to the natural phenomena needs to be explored to provide **robust probabilistic gas dispersion hazard assessments** which are based on running physical models to explore the full range of uncertainty in the input parameters and boundary conditions, allowing an aware application of simulation tools, such as VIGIL, for quantifying the volcanic hazard.

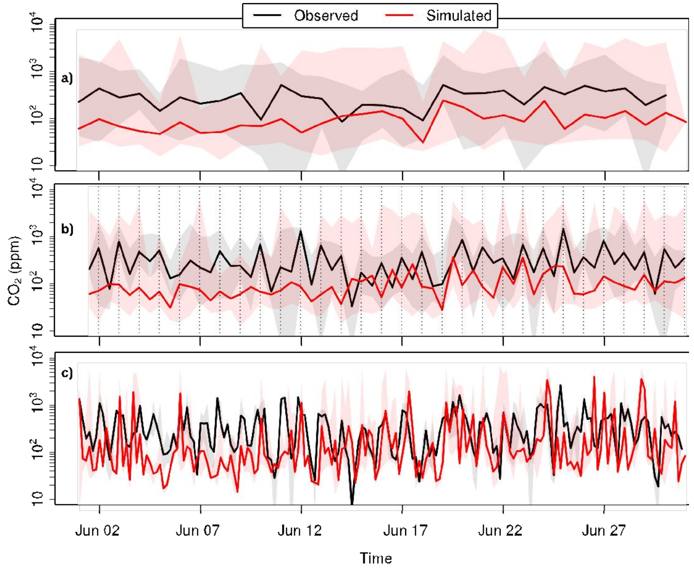
Using VIGIL workflow, we aim to:

- ❑ **Calibrating gas fluxes** using atmospheric concentration measurements, through the solution of an inverse problem with an ensemble approach;
- ❑ **Testing the accuracy of the numerical modelling** in providing realistic results at investigated areas by the statistical reproduction of the observed gas concentrations (i.e., CO_2 , H_2S);
- ❑ **Identifying hazardous gas dispersal scenarios** (e.g. for limnic eruptions);
- ❑ **Evaluation of the long-term hazard for human and animal lives posed by CO_2 and other gases.**

Examples of model validation & indirect estimate of gas fluxes

La Solfatara crater (Campi Flegrei, Italy)

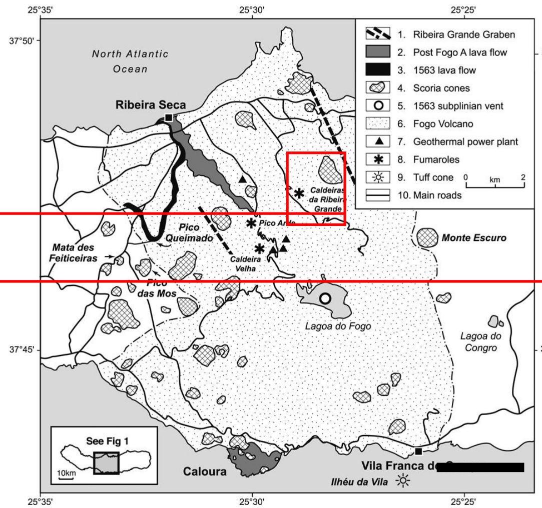


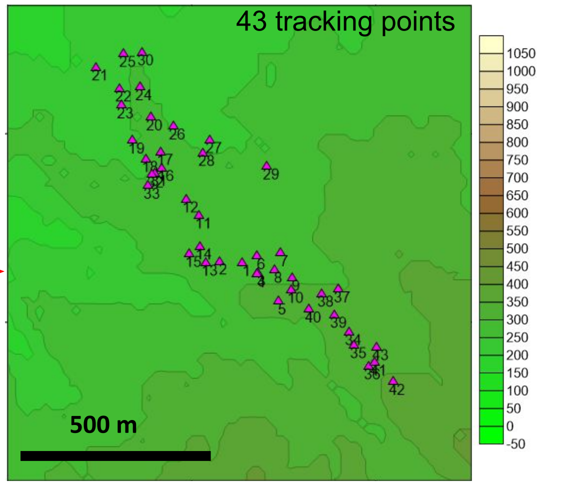


Model validation to reproduce the CO_2 concentration data in June 2020;
Comparison of observed and simulated data within 3 time-averaging windows provides a good correlation for daily averages at 5% significance level.

from Massaro et al. (2022)

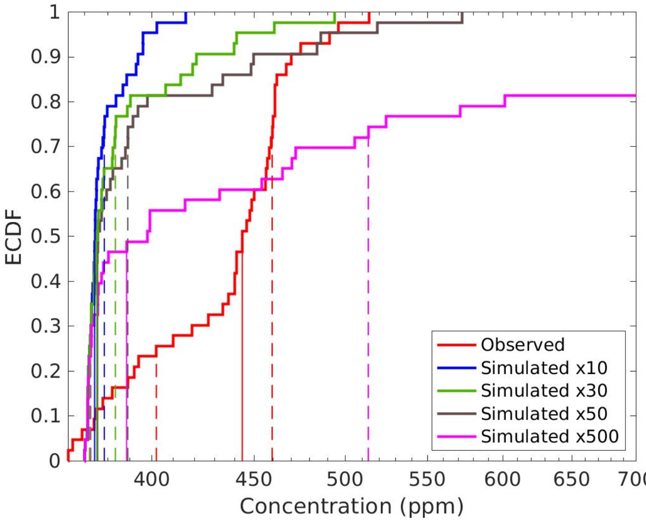
Caldeiras da Ribeira Grande (S. Miguel, Azores)





Model validation to reproduce CO_2 concentrations in July-August 2021;

Statistical tests to find out the best scaling factor able to estimate the unknown fumarolic contribution and reproduce the observed diffusive one.



from Viveiros et al. (2023)

❑ Modelling strategies

Gas dispersal can be modelled by solving the standard conservation equations for mass, momentum, and energy (Navier-Stokes equations) for the pollutant and the air phases. This approach is **computationally expensive**, particularly when probabilistic simulations are needed for hazard quantification studies. It is possible to simplify the equations by making some assumptions and focusing on specific scenarios/applications.

Heavy-gas scenario

Gas density at the source is higher than the surrounding environment.
Gas collapses and flows as a density current **mainly controlled by the topography**.
Entrainment of external air also occurs, contributing to the reduction of the density contrast

MODELLING APPROACH: shallow-water conservation equations
Solver: TWODEE-2 (Folch et al. 2009)

Light-gas scenario

Gas density at the source is comparable to the surrounding environment.
The gas dispersal is **mainly controlled by wind advection and atmospheric turbulence** (diffusion)
Entrainment of external air also plays a role in mixing and diluting

MODELLING APPROACH: advection-diffusion equations
Solver: DISGAS (Costa and Macedonio, 2016)

❑ VIGIL: *probabilistic VolcanIc Gas dIspersion modeLling*

It is a Python workflow able to manage the full gas dispersal simulation (using **TWODEE-2** for heavy-gas and **DISGAS** for light-gas) in two modes: **forecast** and **reanalysis.**

The meteorological conditions in the computational domain over the terrain (provided with a DEM) are simulated using the **diagnostic wind model DIAGNO** (Douglas et al., 1990) starting from observations/model data in at least one point of the domain. Three possible weather data sources:

- Automatically retrieved **ECMWF ERA5** reanalyses, or **NOAA GFS** forecasts
- Manually-provided weather station data

Main outputs:

- **Single simulation**, continuous (long-lived emission) simulations or N probabilistic simulations;
- **Probabilistic simulations** can be run in parallel by varying meteorological data and source conditions;
- Outputs are combined to obtain ECDF (Empirical Cumulative Density Functions) and **persistence maps**;
- **Plots of gas concentration** (optional gas species conversion), with the possibility to interrogate the ECDF outputs to obtain plots at specific exceedance probabilities;
- **Tracking points** feature to plot time series of gas concentration and hazard curves at specific locations

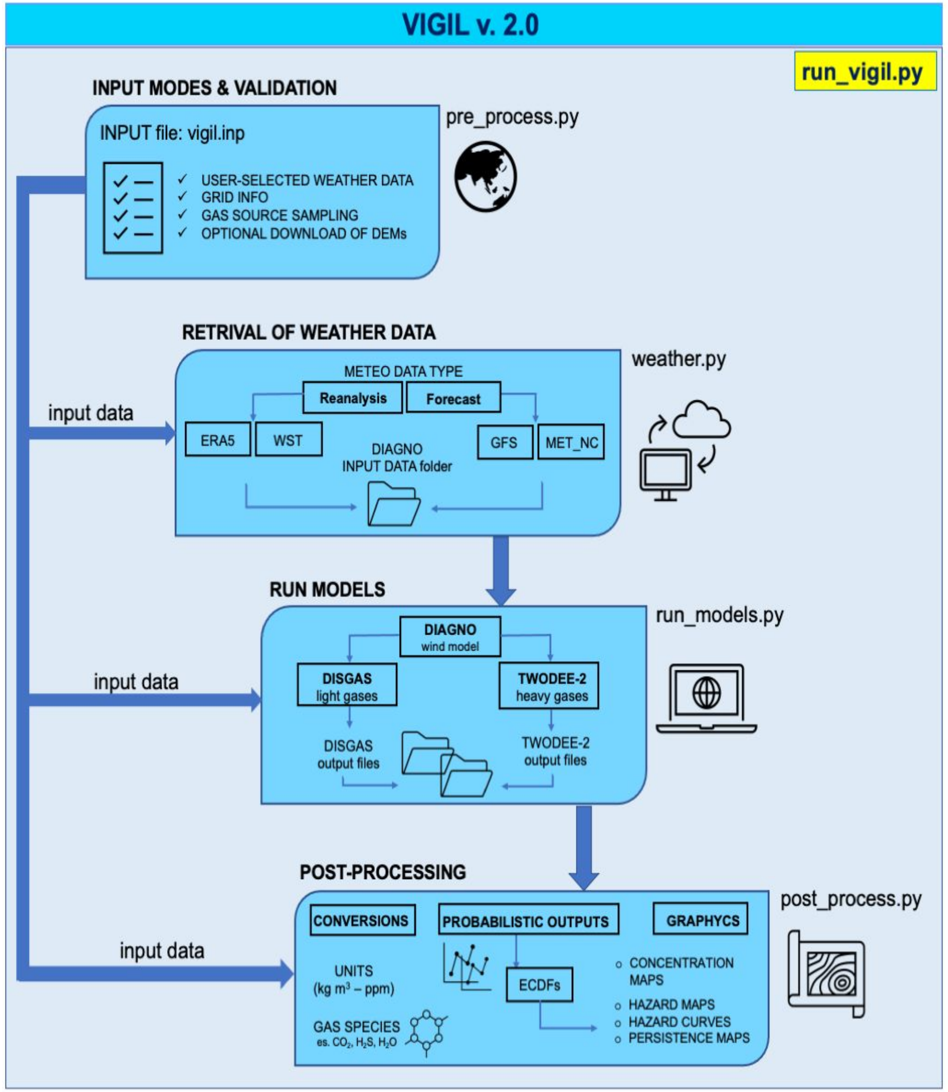
The VIGIL-2.0 improvements

A new version of VIGIL is under construction. The VIGIL-2.0 version (in development) includes:

- Integration of all the workflow in a single run script, without loosing the modularity of the first version. That means that the previous modules can be executed by applying small changes.
- Implementation of a new input file, where all the variables can be recorded for a project.
- Input data validation

Additionally, new features will be added in the future such as

- PyCOMPSs orchestration (workflow and resources management)
- Containerization (portability)



The VIGIL-2.0 workflow

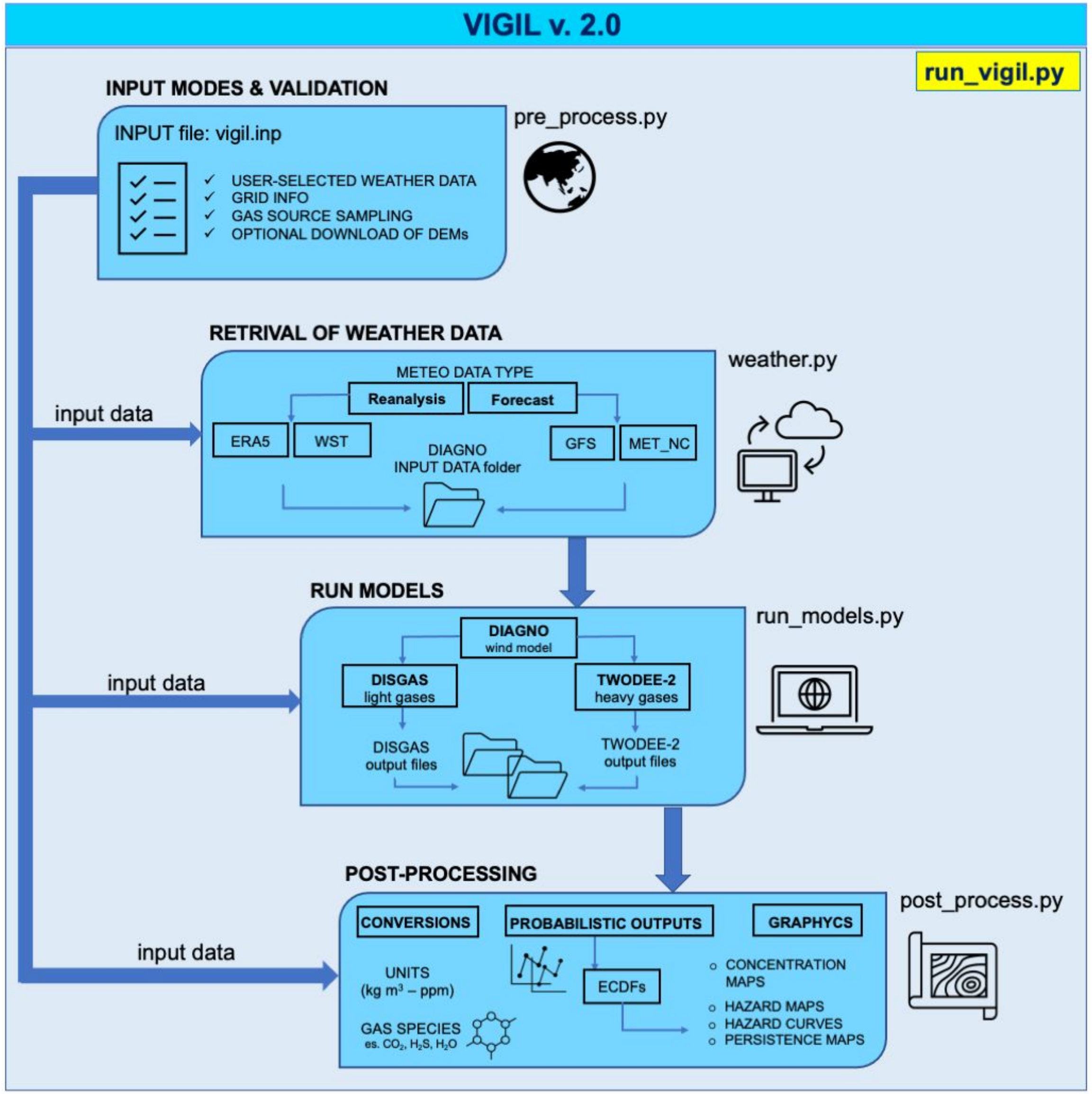
VIGIL-2.0 is launched through **run_vigil.py** which sequentially allows to run four scripts:

- **pre_process.py**: it provides the pre-process (input modes and validation) through a single input file. An optional automatic download of the Digital Elevation Model can be also provided through OpenTopographyAPI. It prepares the file needed to run DIAGNO, DISGAS or TWODEE-2, for each day of the selected simulations.

- **weather.py**: it prepares the weather data by either retrieving reanalysis data from the ECMWF ERA5 database;

- **run_models.py**: it runs DIAGNO and successively DISGAS or TWODEE-2 using a deterministic or probabilistic approach;

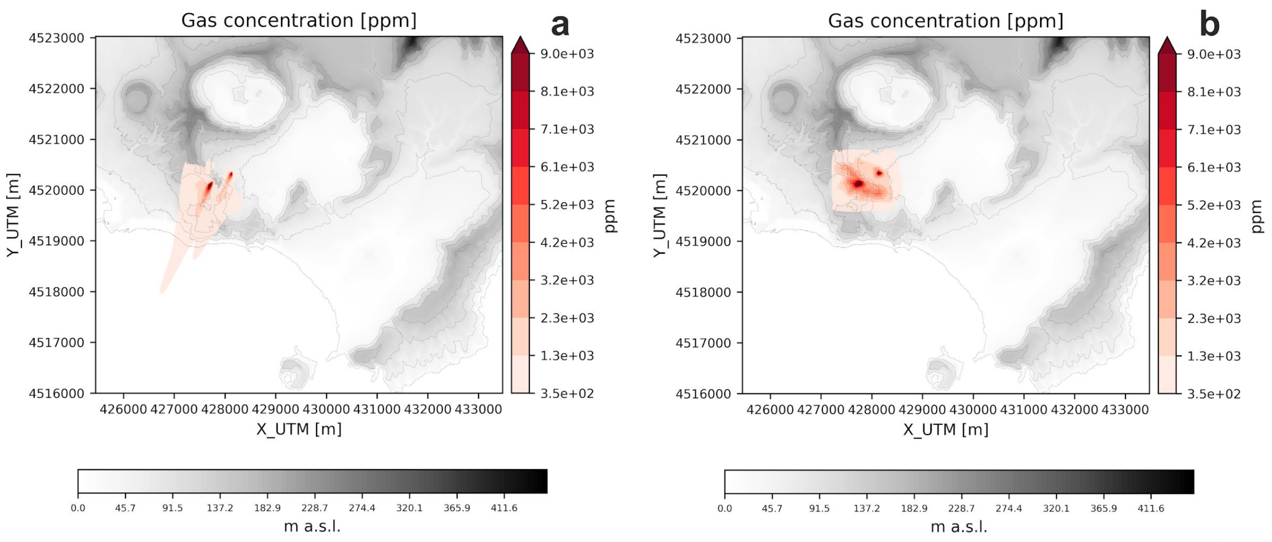
- **post_process.py**: it reads the DISGAS or TWODEE-2 outputs produced by run_models.py and converts the model outputs in concentration of other gas species based on the gas species properties.

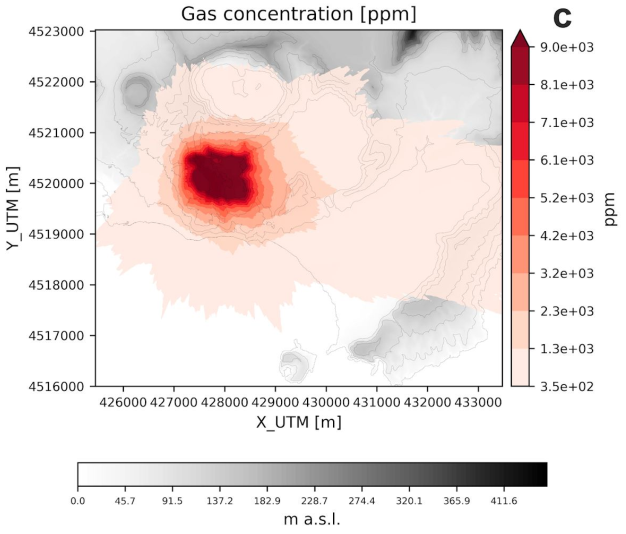


❑ Examples of graphical outputs (I)

Probabilistic concentration maps. CO_2 concentration (in ppm) is shown at 1.5 m above the ground after 24 hours from the emission start.

a) CO_2 concentration for one of the 100 days;
b) Long-term hazard map showing CO_2 concentration corresponding to the 50% exceedance probability of the whole simulation dataset;
c) Long-term hazard map showing CO_2 concentration corresponding to the 5% exceedance probability of the whole simulation dataset;





DISGAS application example: La Solfatara, Campi Flegrei (Italy)

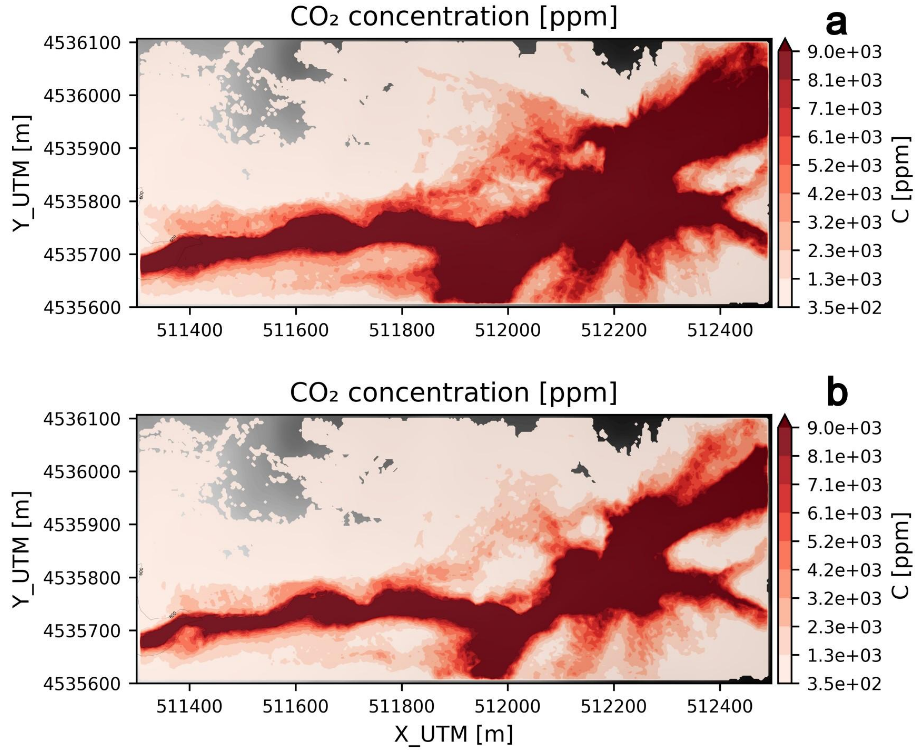
m a.s.l.

from Dioguardi et al. (2022)

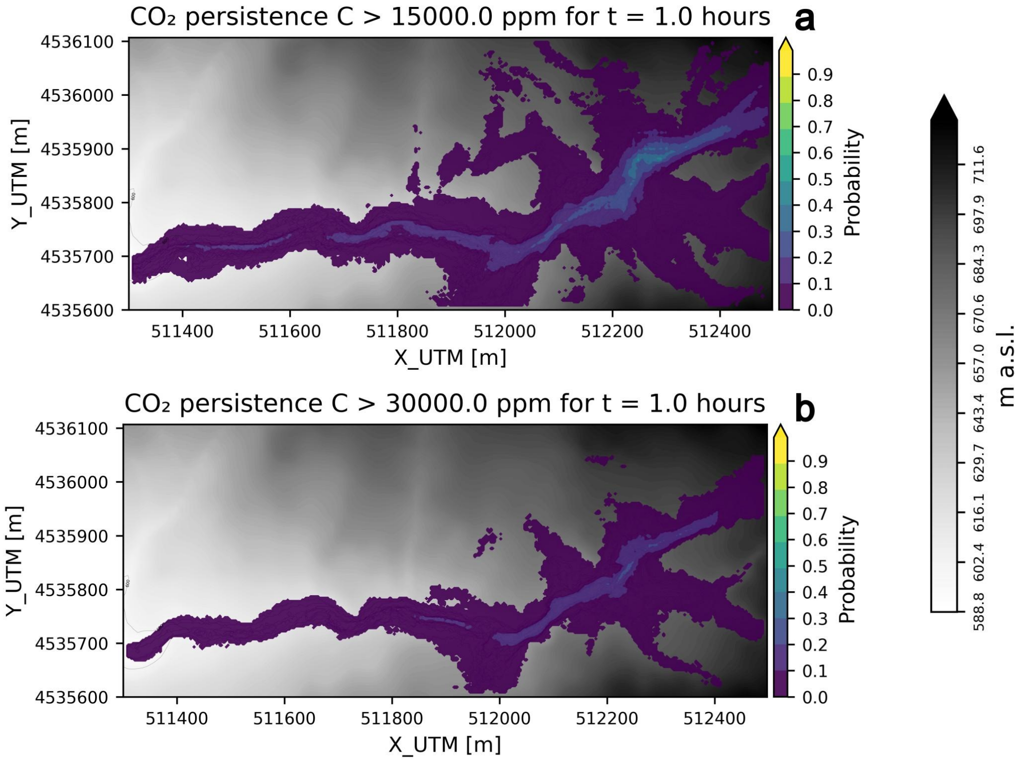
Examples of graphical outputs (II)

TWODEE-2 example: Mefite d’Ansanto (Italy)

from Dioguardi et al. (2022)



Long-term hazard maps of CO_2 concentration at (a) 0.5 m and (b) 2 m above the ground averaged over the whole duration of the simulation (4 hours) at an exceedance probability of 5%.



Persistence maps for CO_2, i.e. the probability to overcome a concentration threshold of (a) 15,000 ppm for 1 hour and (b) 30,000 ppm for 1 hour. Both maps refer to a height of 2 m above the ground.

❑ Conclusion and further development

- The probabilistic gas hazard assessment is based on computational models of volcanic gas dispersion which represent a valuable tool to forecast dangerous concentrations, study past events, cross-validate measurements of gas emission rates, making quantitative gas dispersal evaluations;

- In the enhancement of the code towards a higher-scale computing, we presented the ongoing improvements on VIGIL, a new tool to manage the gas dispersal simulation workflow for reanalyses, forecasts and hazard assessments, aimed to extend some code functionalities such as memory management, modularity revision, and full-ensemble uncertainty on gas dispersal scenarios (e.g., sampling techniques for gas fluxes and source locations);

- Optimizations in terms of tracking errors, redesignation of the input file are included in the new version VIGIL-2.0 in order to facilitate the users which could run it on laptops or large supercomputer, and to widen the spectrum of model applications from routinely operational forecast of volcanic gas to long-term hazard and/or risk assessments purposes.

- VIGIL is under development. The latest release will be soon available at: https://github.com/BritishGeologicalSurvey/VIGIL/releases/

Thank you !