Introduction to CHIMERE: from Meteorology to Air Quality

Lecture 9

Ph.D., Senior lecturer Madina Tursumbayeva

Department of Meteorology and Hydrology

Lecture Objective and Learning Outcomes

Lecture objective

To introduce chemistry-transport modelling with CHIMERE: the processes it represents, its coupling with WRF, its input and output, and the limits of an air quality simulation.

Learning outcomes

By the end of this lecture, students will be able to:

1. explain why air quality modelling needs both a meteorological and a chemistry-transport model;
2. name the processes in the balance of a pollutant and the meteorological fields each of them needs;
3. distinguish offline from online coupling, and the direct from the indirect aerosol effect;
4. describe how emissions and aerosols (composition, size bins) are represented in CHIMERE;
5. read CHIMERE NetCDF output and name the main limits of an air quality simulation.

From Meteorology to Air Quality

WRF alone

- Wind, temperature, boundary layer, clouds
- Knows nothing about emissions, chemistry or deposition

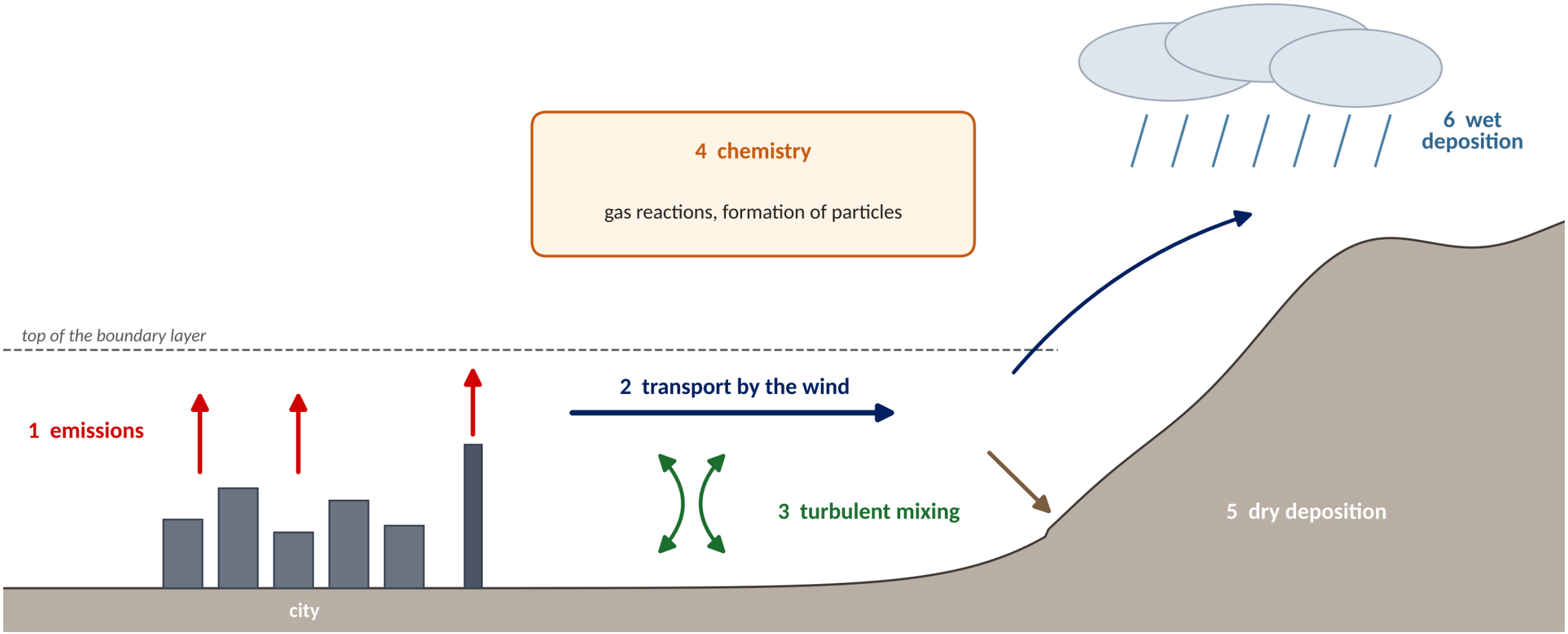
A pollution model alone

- Cannot work without wind, turbulence, temperature, sunlight and rain

Air quality needs two models working together

Meteorological model (WRF) + chemistry-transport model (CHIMERE)

What a Chemistry-Transport Model Calculates



At every time step and in every grid cell the model adds up these six contributions

The Balance of a Pollutant

change of concentration = emissions ± transport ± mixing ± chemistry − deposition

Transport

needs the wind

Mixing

needs turbulence and the boundary layer

Chemistry

needs temperature, humidity and radiation

Wet deposition

needs clouds and precipitation

- The continuity equation, solved for every gas and every type and size of particle
- An air quality simulation can never be better than its meteorology

What Is CHIMERE?

A regional chemistry-transport model

- Developed in France (Laboratoire de Météorologie Dynamique and partner institutes)
- Under continuous development since 1999
- Open-source software
- From a hemisphere down to a city (grid of about 1 km)
- Version in our study: v2023r1 (Menut et al., 2024)

Research

Processes, sources, transport

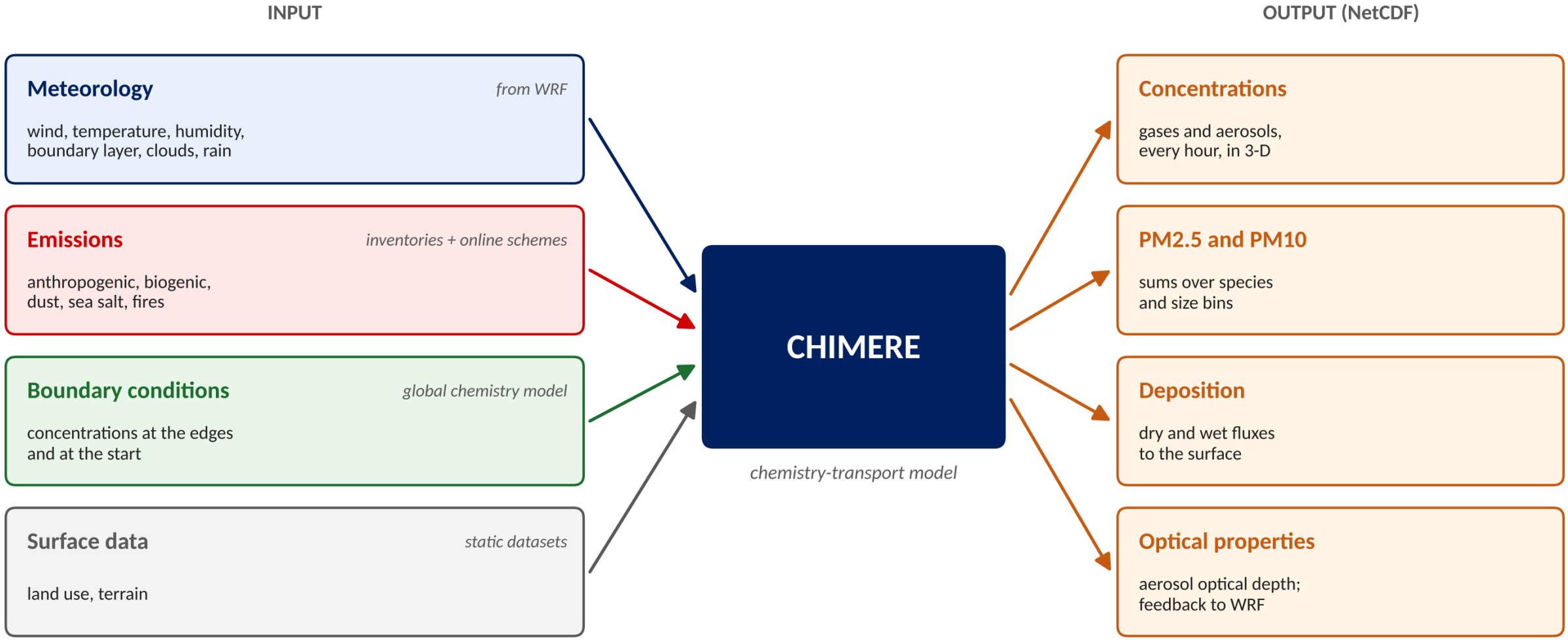
Forecast

Daily air quality forecasts, including the European CAMS ensemble

Scenarios

What if emissions change?

Input and Output of CHIMERE



The output is NetCDF: the tools of Lectures 4–7 apply directly

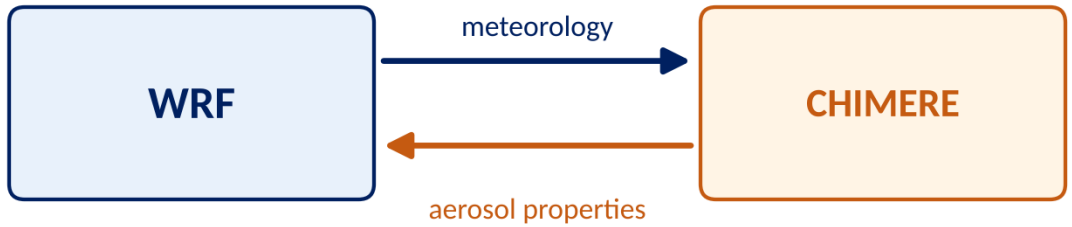
Offline and Online Coupling with WRF

Offline



WRF runs first; CHIMERE reads its output.
Pollution cannot change the weather.

Online

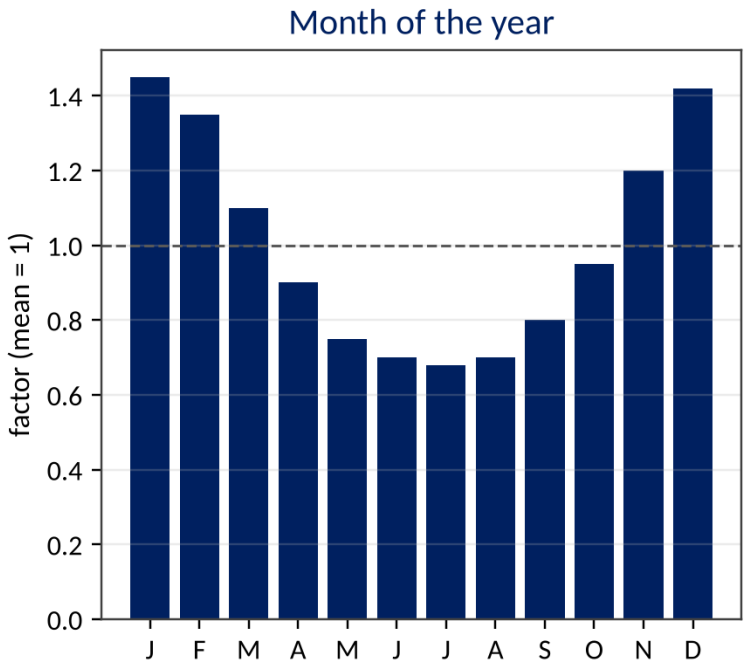


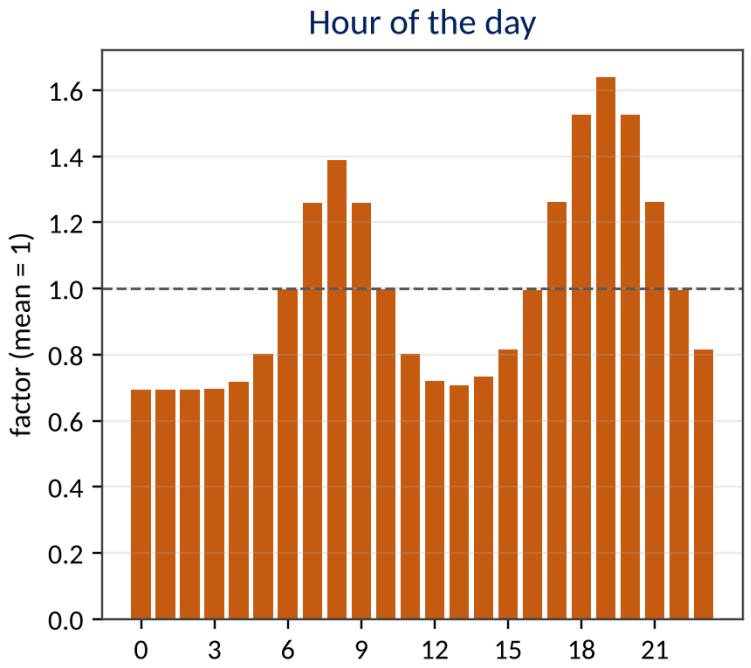
coupler OASIS3-MCT, every physical time step

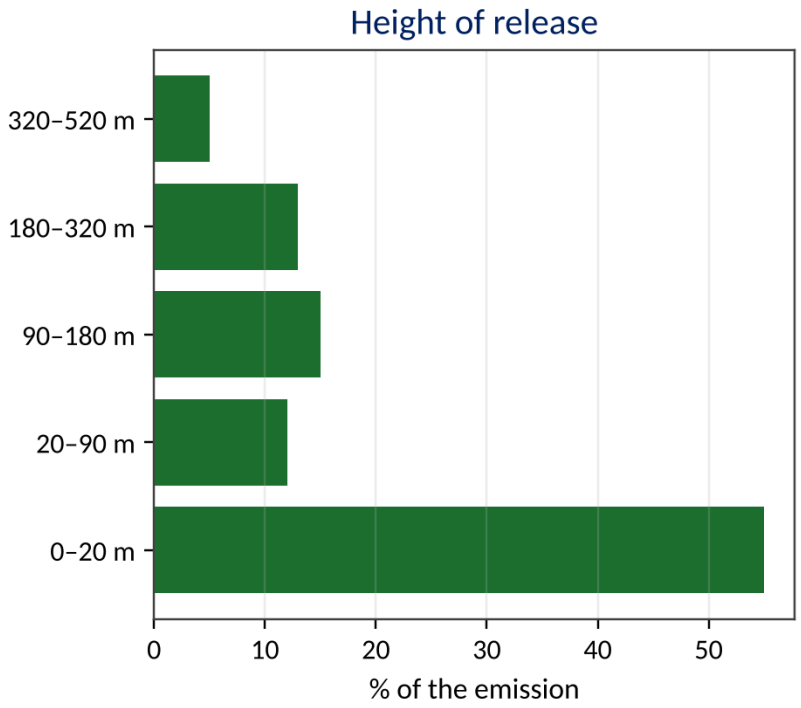
Both models run together.
Aerosols change radiation (direct effect)
and clouds (indirect effect).

- Direct effect: aerosols scatter and absorb sunlight. Indirect effect: aerosols change clouds
- Our Almaty study: online coupling (Menut et al., 2021)

Emissions: from an Inventory to the Model



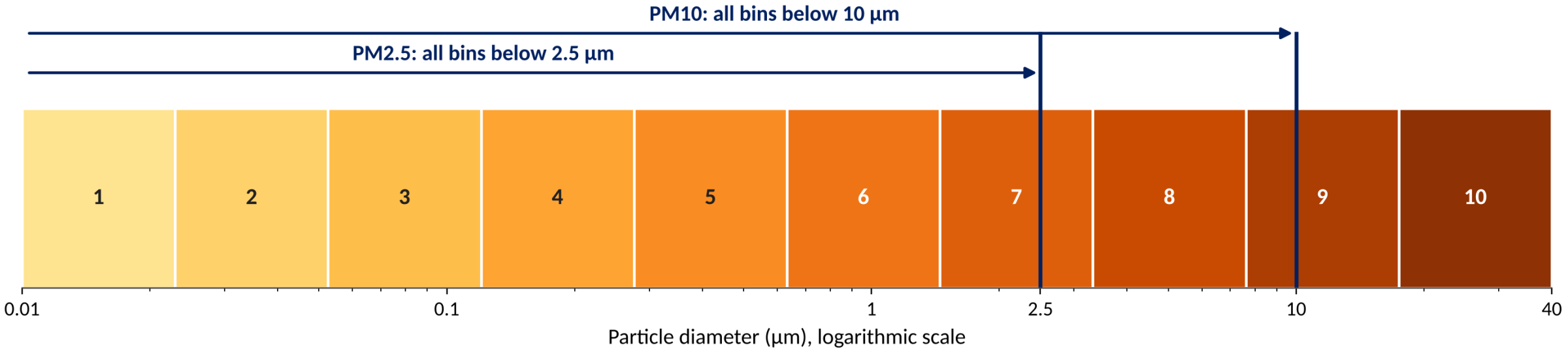




- Inventory: an annual total per grid cell → distributed by month, hour and height of release
- Our study: BC from the global CAMS inventory (about 10 km), adjusted to the concentrations measured in Almaty

Profiles are illustrative, not the ones used in the study

Aerosols: Composition and Size



By composition

Black carbon, organic matter, sulphate, nitrate, ammonium, mineral dust, sea salt

By size: sectional approach

10 bins between 0.01 and 40 µm in our study;
PM2.5 = the sum of all species in the bins below 2.5 µm

Chemistry, Deposition and Black Carbon

Chemistry

- Gas-phase chemical mechanism
- Inorganic gases ⇒ particles
- Secondary organic aerosol

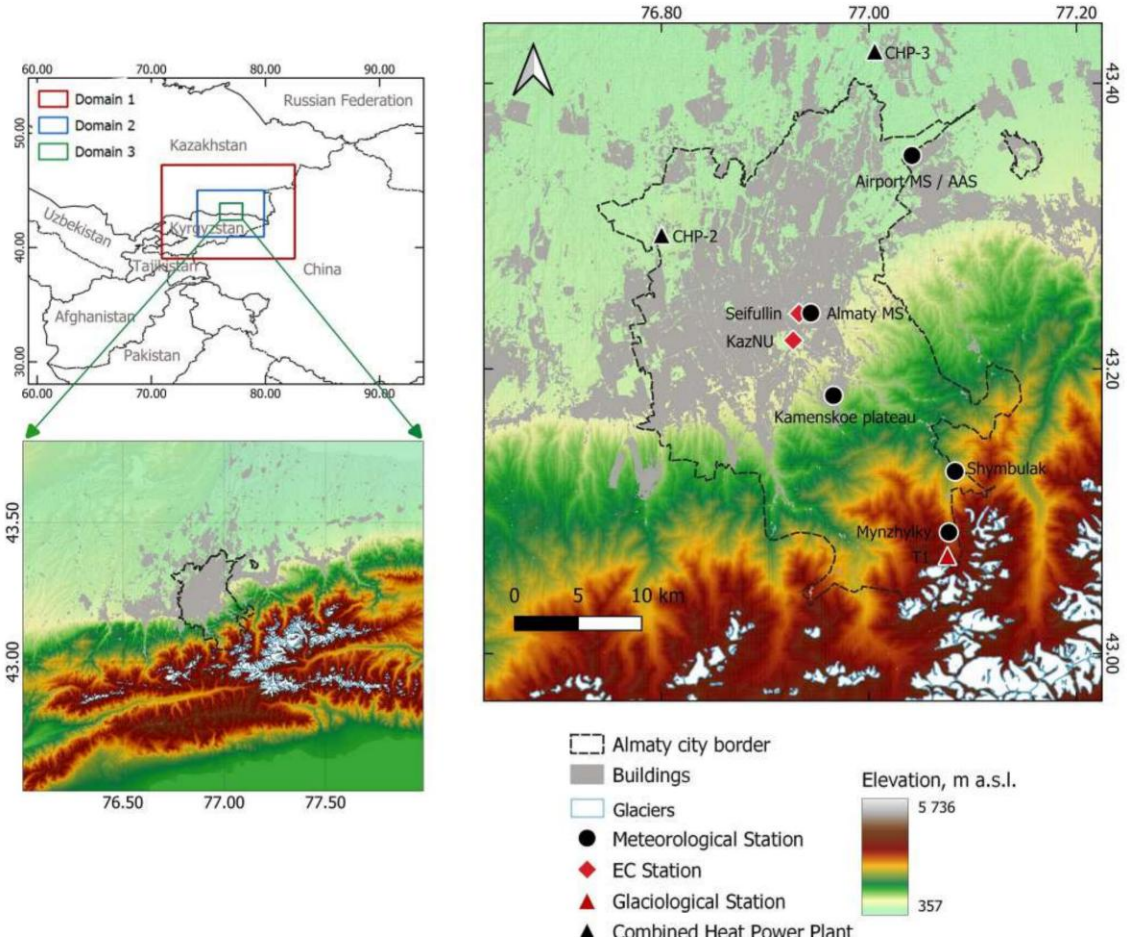
Deposition

- Dry: contact with ground, vegetation, snow
- Wet: clouds, rain and snow
- For gases and for every particle size

Black carbon: a tracer of transport

- Primary particle: emitted directly, not formed in the atmosphere
- Chemically almost inert
- Controlled only by emissions, transport, mixing and deposition

The WRF-CHIMERE Configuration of Our Study



Source: Tursumbayeva et al. (2026), Meteorological Applications, 33, e70183

WRF v4.3 + CHIMERE v2023r1, online

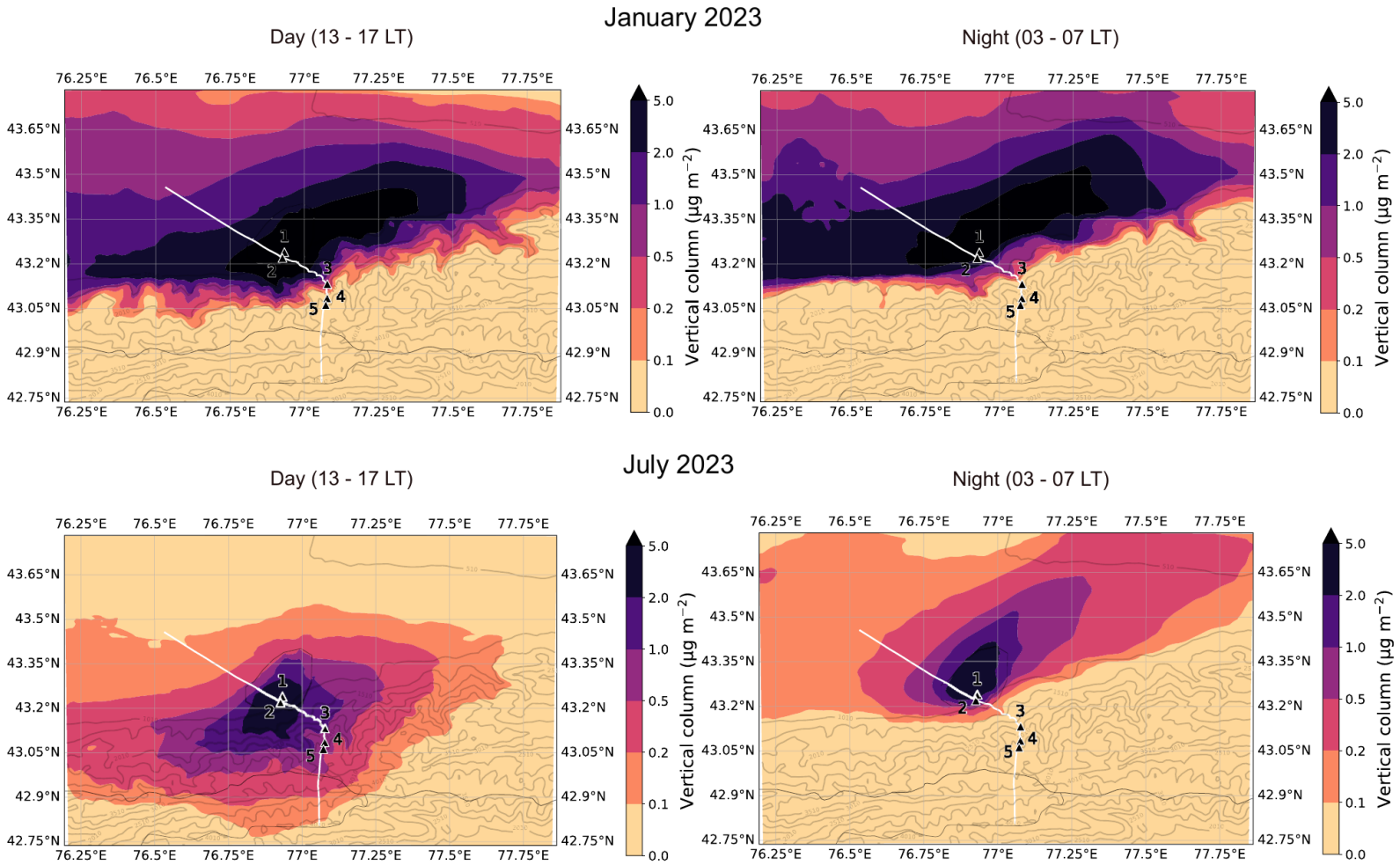
- Three nested domains: 9, 3 and 1 km; 50 levels
- Meteorological input: CFSv2 reanalysis
- Chemical boundary conditions: global model climatology
- BC emissions: CAMS inventory, kept only in the Almaty area (semi-idealised)
- 10 aerosol size bins
- January and July 2023

Working with CHIMERE Output

```
import xarray as xr

# CHIMERE output file (the name is an example)
ds = xr.open_dataset("out.2023010100_24_ALMATY.nc")
print(ds)           # read the header first

pm = ds["PM25"]                        # µg m-3
pm_sfc  = pm.isel(bottom_top=0)     # lowest level
pm_mean = pm_sfc.mean("Time")

pm_mean.plot()
```

- NetCDF, as in WRF: the same tools
- Variable names differ: read the header
- Particles: µg m^{-3}. Gases: ppb
- Then maps, profiles, cross-sections, validation

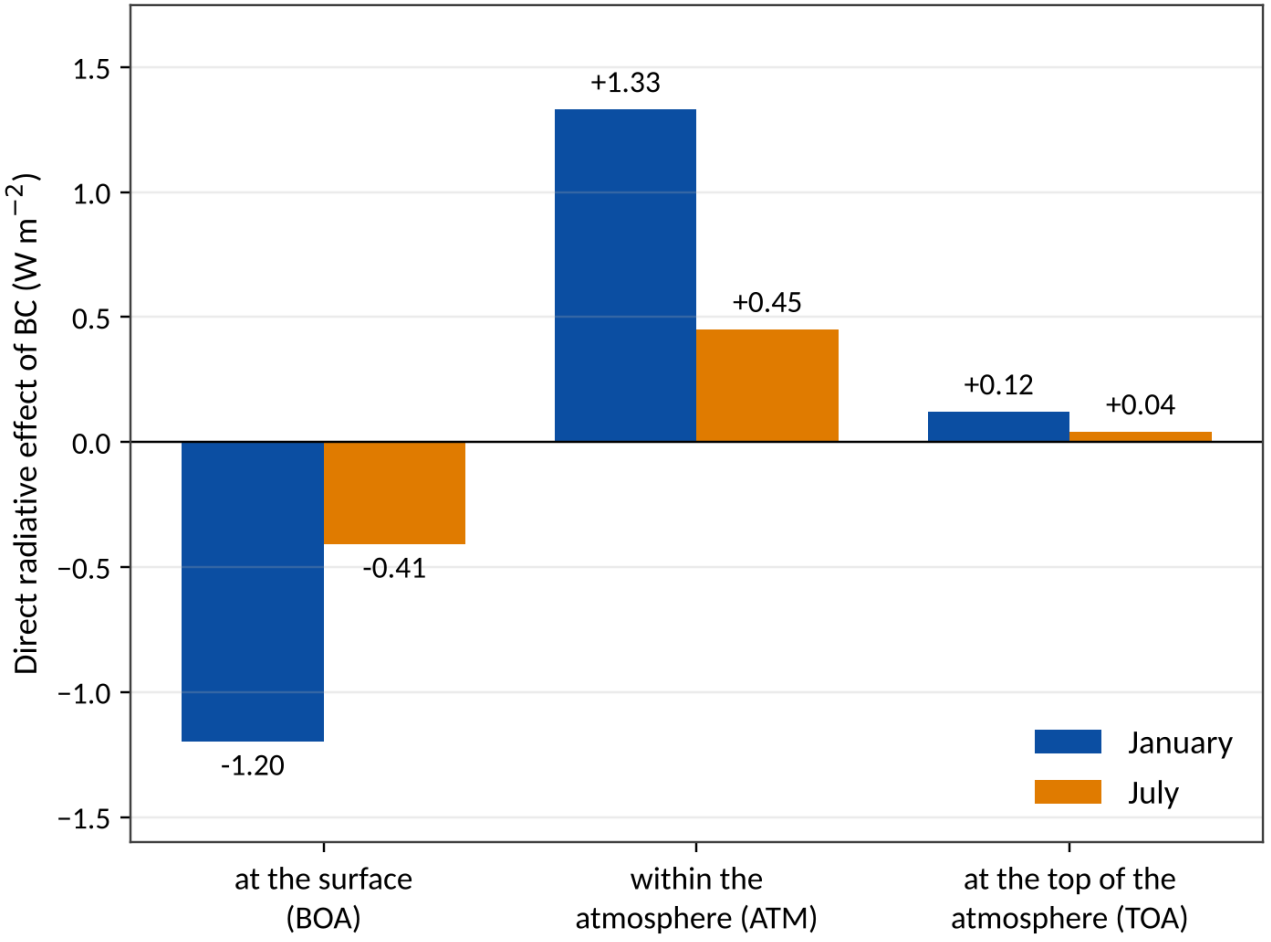
Research Example: Reading the Maps as Processes



- Amount: emissions (more in winter)
- Shape of the plume: transport by the wind
- Vertical extent: mixing (shallow in winter, deep in summer)
- The model shows the processes together, and can separate them

Column black carbon, January (top) and July (bottom). Source: Tursumbayeva et al. (2026), Meteorological Applications, 33, e70183

A Numerical Experiment: Black Carbon and Radiation



Two runs of the coupled model

Run 1: BC has no effect on radiation

Run 2: online exchange switched on

- Difference = direct radiative effect of BC from Almaty
- Surface: shading (−1.2 W m^{-2} in January)
- Atmosphere: absorption, warming (+1.3 W m^{-2})
- Stability changed by less than 2 %

Mean over the urban area of Almaty, daytime, clear sky. Data: Tursumbayeva et al. (2026), Meteorological Applications, 33, e70183

Limits of an Air Quality Simulation

Emissions

Inventories are uncertain, especially for a city

Meteorology

Wind errors in complex terrain pass into transport

Observations

No BC measurements in the mountains for validation

Design of the experiment

One pollutant, one city, two months

Next steps: a local emission inventory, measurements at different altitudes, spring and autumn simulations

Summary

Key points

- Six processes: emissions, transport, mixing, chemistry, dry and wet deposition
- CHIMERE: an open-source regional chemistry-transport model
- Meteorology from WRF, offline or online; online allows feedback
- Particles: composition and size bins; PM2.5 is a sum
- NetCDF output: all the tools of this course apply

Next lecture

PM2.5 and meteorology

How the weather controls the concentration of fine particles

Thank you for your attention!

Self-Check Questions

1. Why can neither WRF nor a pollution model alone simulate air quality?
2. Which six processes change the concentration of a pollutant in a grid cell?
3. What is the difference between offline and online coupling?
4. How is an annual emission inventory turned into model input?
5. Why is black carbon a good tracer of transport?
6. What are the main sources of uncertainty in an air quality simulation?

References

1. Menut, L., Cholakian, A., Pennel, R., Siour, G., Mailler, S., Valari, M., Lugon, L., & Meurdesoif, Y. (2024). The CHIMERE chemistry-transport model v2023r1. Geoscientific Model Development, 17(14), 5431–5457. https://doi.org/10.5194/gmd-17-5431-2024
2. Menut, L., et al. (2021). The CHIMERE v2020r1 online chemistry-transport model. Geoscientific Model Development, 14(11), 6781–6811. https://doi.org/10.5194/gmd-14-6781-2021
3. Tursumbayeva, M., Ciarelli, G., Di Antonio, L., Bettineschi, M., Kissebayev, D., & Baimatova, N. (2026). Modelling the Black Carbon Variability and Dynamics in Almaty, Kazakhstan, During Winter and Summer Seasons. Meteorological Applications, 33, e70183. https://doi.org/10.1002/met.70183
4. CHIMERE model website: https://www.lmd.polytechnique.fr/chimere/
5. Skamarock, W. C., et al. (2019). A Description of the Advanced Research WRF Model Version 4. NCAR Technical Note NCAR/TN-556+STR. https://doi.org/10.5065/1dfh-6p97
6. Seinfeld, J. H., & Pandis, S. N. (2016). Atmospheric Chemistry and Physics: From Air Pollution to Climate Change (3rd ed.). Wiley.