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Concentration Trajectory Route of Air pollution with an Integrated Lagrangian Model (C-TRAIL Model v1.0) Derived from CMAQ v5.2

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Introduction:

- Long-range transport (LRT) of pollutants
- Chemical composition of outflow over a region can significantly affect air quality of the downwind.
- Conventional methods
  - Trajectory analysis: HYSPLIT, FLEXTRA
    (Choi et al., 2014; Lee et al., 2019; Oh et al., 2015; Pu et al., 2015, Lee et al., 2011, 2013)
  - Chemical-transport models: CMAQ
    (Bertschi and Jaffe, 2005; Carroll et al., 2008; Gratz et al., 2015; Price et al., 2004; Sadeghi et al., 2020; Weiss-Penzias et al., 2004)
  - Satellite retrievals and air quality stations
    (Chen et al., 2014; Chuang et al., 2008, 2018; Souri et al., 2016; Wang et al., 2010; Xu et al., 2019; Zhang et al., 2019)

Introduction:

1. Eulerian models (CMAQ) cannot clearly show the source-receptor linkage of polluted areas
2. Back-trajectory analysis (HYSPLIT) unable to detect that originated air mass is polluted or non-polluted.

Proposed solution:

- ❖ To implement a Lagrangian advection scheme into a Eulerian CTM.
- ❖ By implementing Trajectory Grid (TG) method into CMAQ we get Concentration Trajectory Route of Air pollution with the Integrated Lagrangian (C-TRAIL v1.0) model.

Methodology: Description of the TG approach

The TG method rewrites the advection equation for concentration as follows:

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + \mathrm{v} \cdot \nabla C = -(\nabla \cdot \mathrm{v})C$$

C: the concentration of species in velocity field v.

$\frac{dC}{dt}$: full derivative of concentration with respect to time.

$-(\nabla \cdot \mathrm{v})C$: the term containing velocity divergence.

Methodology: Description of the TG approach

Pros

- Conserves the mass, sign, and shape of the concentration profile.
- Differentiating among advection equations for each species is no longer necessary.
- Removes the associated numerical errors with the discretization of the advection equation.
- The trajectory will be three-dimensional and as accurate as the input for wind velocity and direction.

Cons

- Interpolation errors occur during the diffusion step, but they are typically considerably smaller than Eulerian advection errors.
- Management of Lagrangian points (packets) introduces new errors.

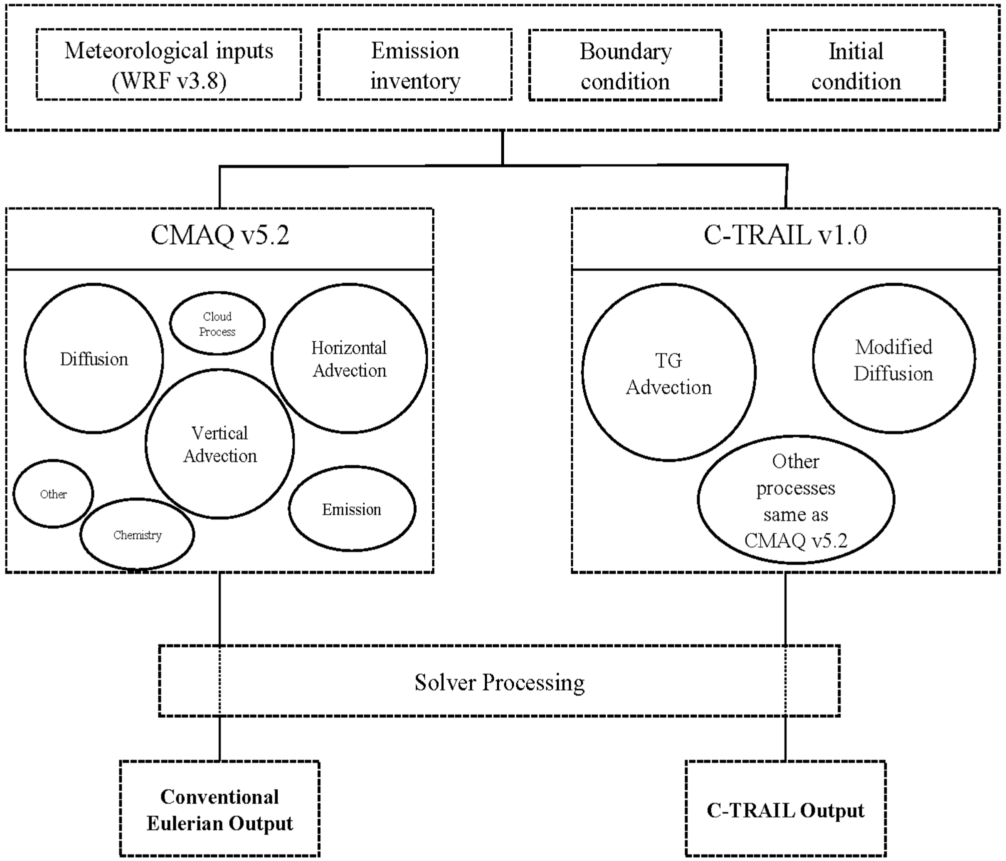

Figure 1: Schematic of conventional CMAQ versus C-TRAIL

1. Initialization

Packets are generated based on the IC and BC in grid cells.

Each packet receives an ID, x, y, z.

Time-step selection is based on the condition that a packet may not travel more than ¾ of the distance between all opposite faces of a grid cell.

2. Packet Management

The number of packets in each grid cell must not exceed five.

If exceeded: Remove the extra packets.

The concentration of remaining packets will be the average of all available packets.

Each grid cell must not be empty.

If empty: Add an extra packet.

The concentration of the added packet will be similar to that of the closest packet.

The properties of the packets are controlled through all time steps.

3. Advection

The three-dimensional advection equation is solved to update the location of packets.

4. Diffusion

The implicit Eulerian diffusion equation is solved to obtain an average over the number of packets in each grid cell.

By considering each packet the center of the cell and the cell average as neighboring cells, the diffusion equation is solved for each packet using the predictor-corrector method.

Horizontal diffusion requires extra sub-grid diffusion for pair-wise diffusion.

5. Emission

The emission fluxes of various species (similar to CMAQ) are added to each packet through vertical diffusion.

6. Output Generation

Based on Lambert's projection, the x, y, and z of each packet are converted into longitude, latitude, and altitude.

C-TRAIL is generated during every output time step (1 hour).

Figure 2: Algorithm of the C-TRAIL model

Setup of the Model

- CMAQ model version 5.2
- Horizontal grid resolution of 27-km
- 2010 MIX emission inventory (Li et al., 2017) at a 0.25-degree spatial resolution.
- CB05 emission mechanism
- 2011 Clean Air Policy Support System emission high-resolution (1-km) inventory for Korea
- WRF model v3.8

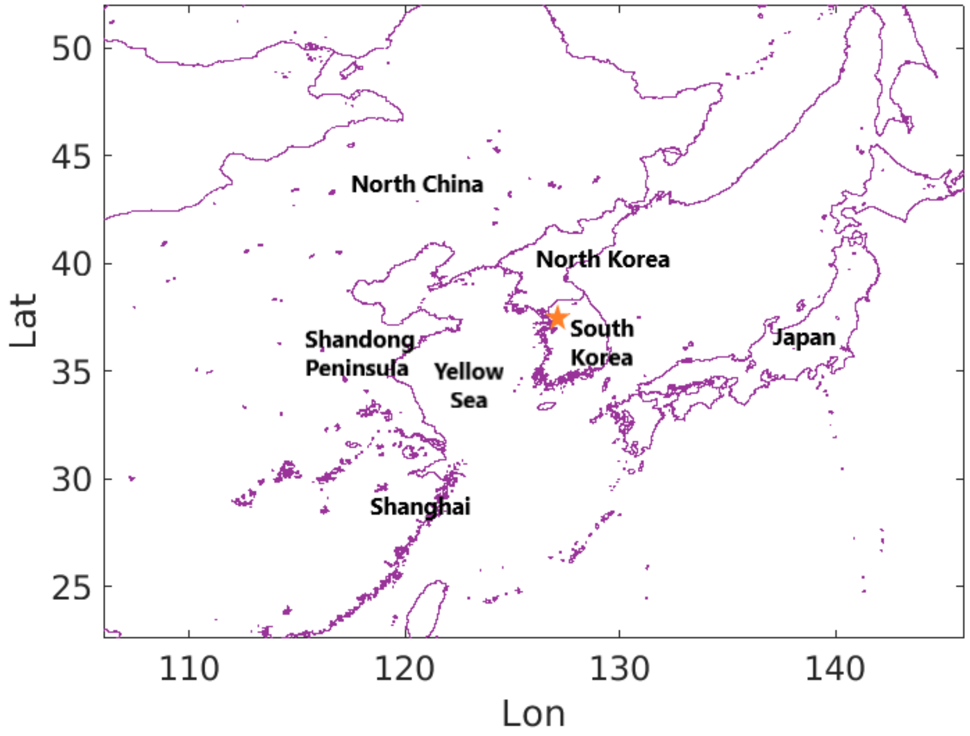

Figure 3: Domain of the study; the orange star indicates the Seoul Metropolitan Area (SMA)

CMAQ results

Major findings:

- During the Dynamic Weather Period (May10-16): a mixed response from the LRT of CO and local emissions occurred. Interpretation of the LRT effect by conventional methods was hard.
- During the Stagnant Period (May 17-22): extremely low wind speed and the stagnant air, the latter of which eliminated the impact of LRT.
- During Extreme Pollution Period (May 25-28): the anticyclone over the Yellow Sea contributed to the transport of more CO from China to the Korean Peninsula.

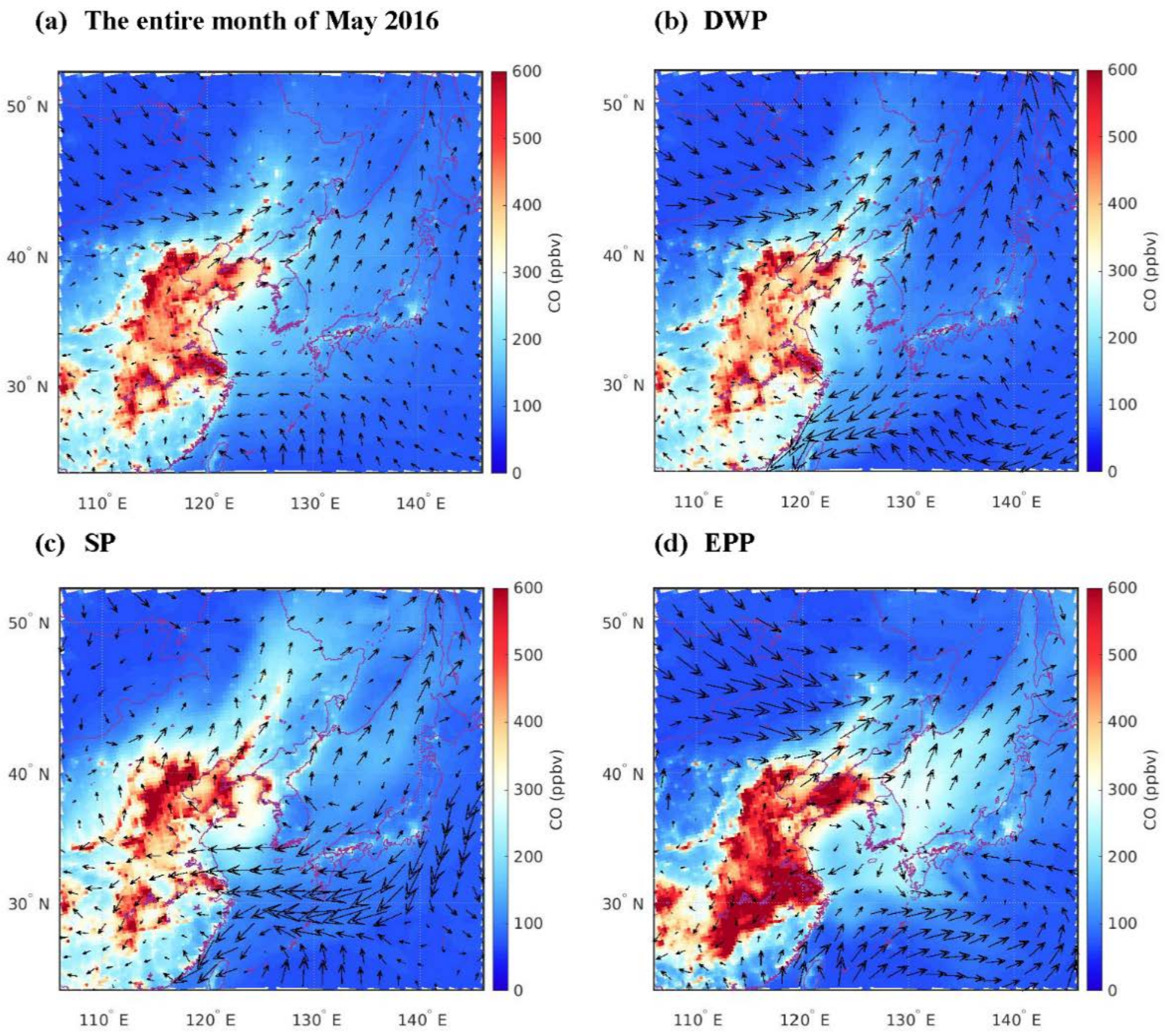

Figure 5: Model CO concentrations and wind patterns over the surface

Analysis of C-TRAIL

Benefits from C-TRAIL results:

- Study the changes in the concentrations of selected species along their paths,
- Investigate evidence for the amount of pollution in originated air masses,
- Study the reason behind the oscillation of concentrations, and
- Examine the linkage of oscillations to both sources and sinks along the path.

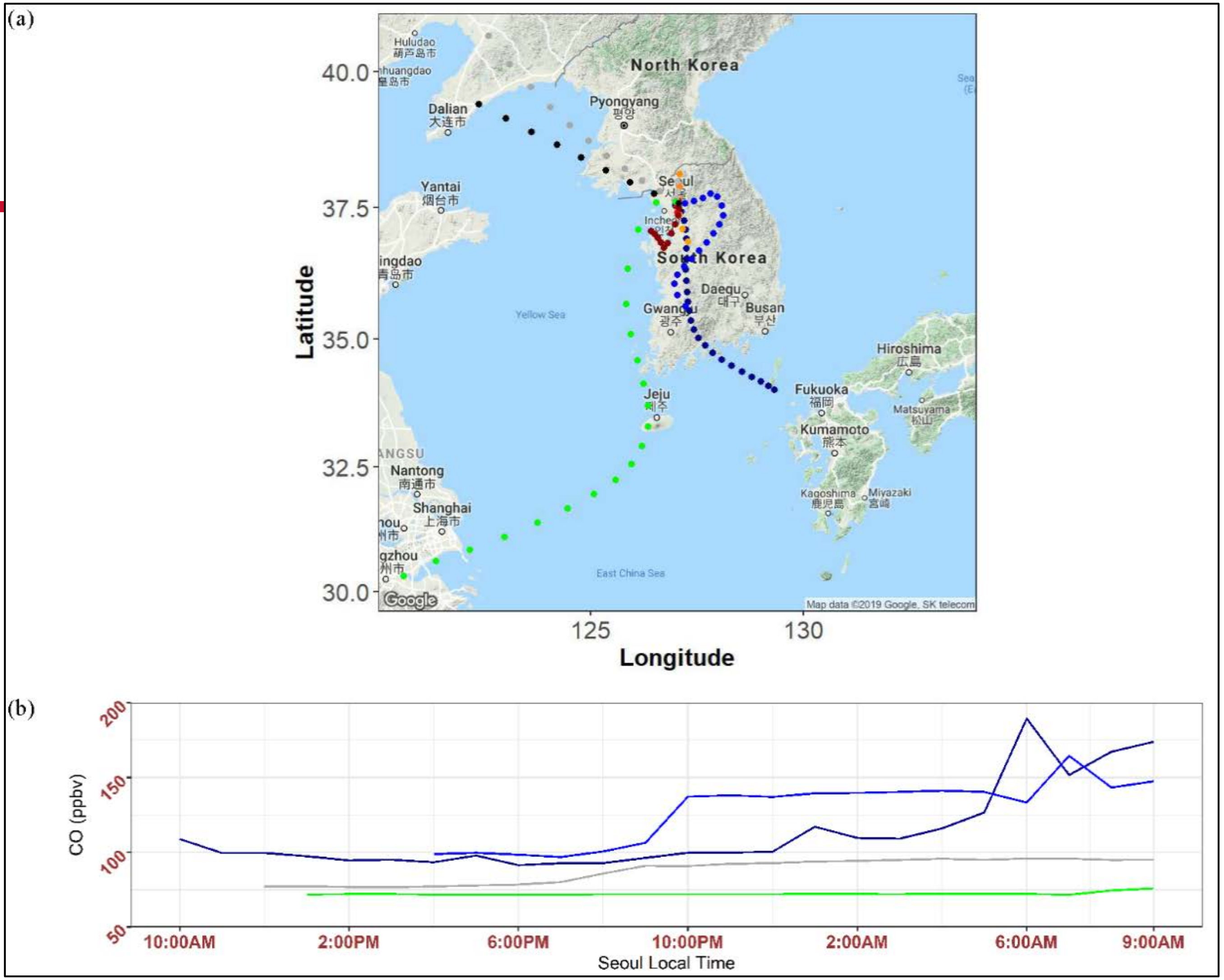

Figure 6: C-TRAIL output for June 4, 2016: (a) the trajectory of packets reaching Seoul at 9:00 AM local time (b) changes in the CO concentrations of four aged packets moving toward Seoul from source points

C-TRAIL output for the entire month of May 2016

- High variability in concentrations with a median of around 150 ppbv and a maximum as high as 500 ppbv.
- Packets originated far from the receptor (i.e., eastern, northern, and south-eastern China).
- Distances also showed more variation during this time, which could be explained by the different paths of the trajectories.
- Higher concentrations of CO of local trajectories resulting from surface on-road emissions.

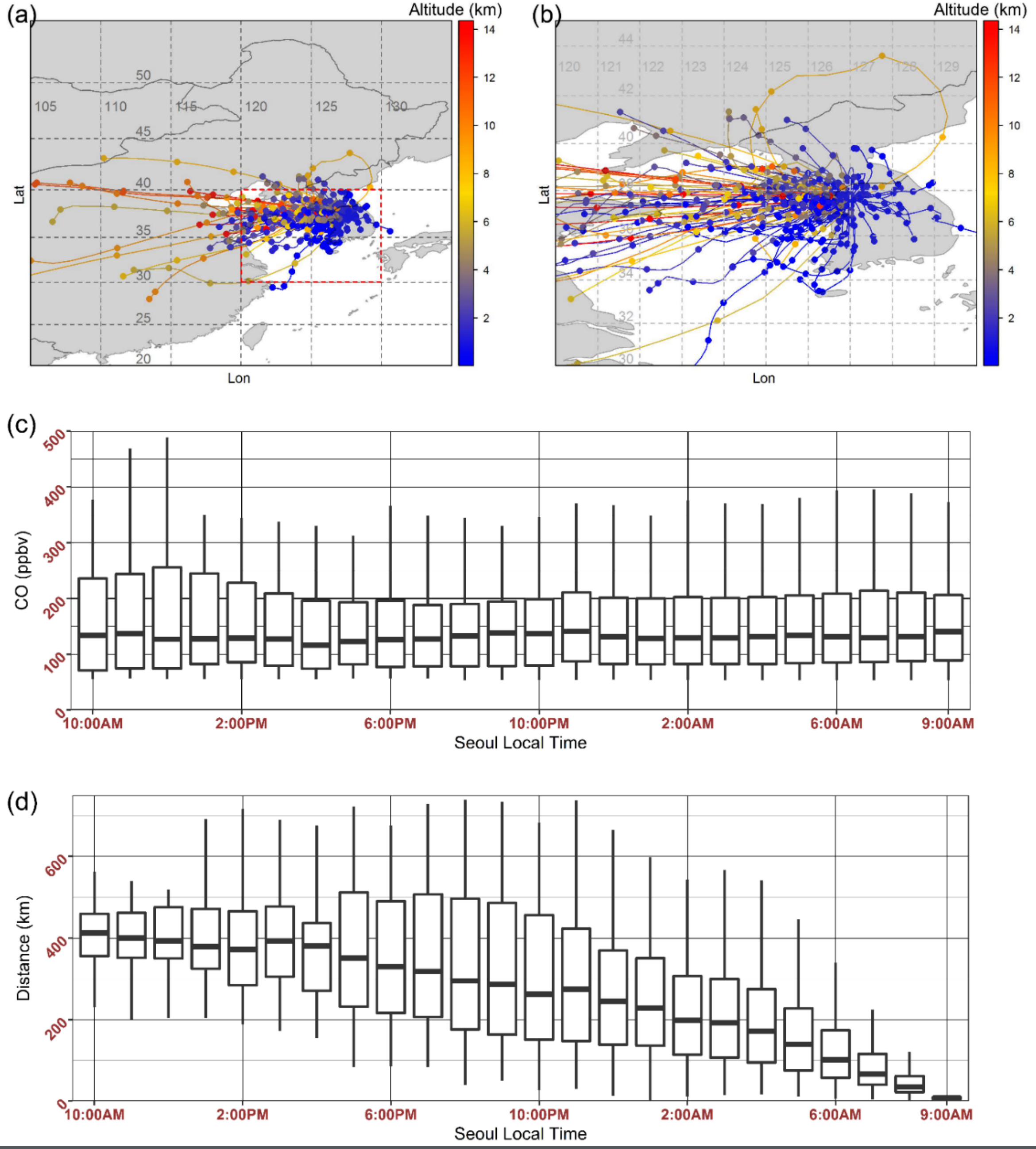

Figure 7: C-TRAIL output for the entire month of May 2016

C-TRAIL output for the dynamic weather period (DWP)

- Mixed response of trajectories from both local and long-range transport.
- Few packets contained high concentrations of CO (close to 300 ppbv), but the majority consisted of low concentrations (around 100 ppbv).
- Distances as long as 500 km (over the Shandong Peninsula).
- Polluted trajectories, which originated in the Shandong Peninsula, were from the near-surface.

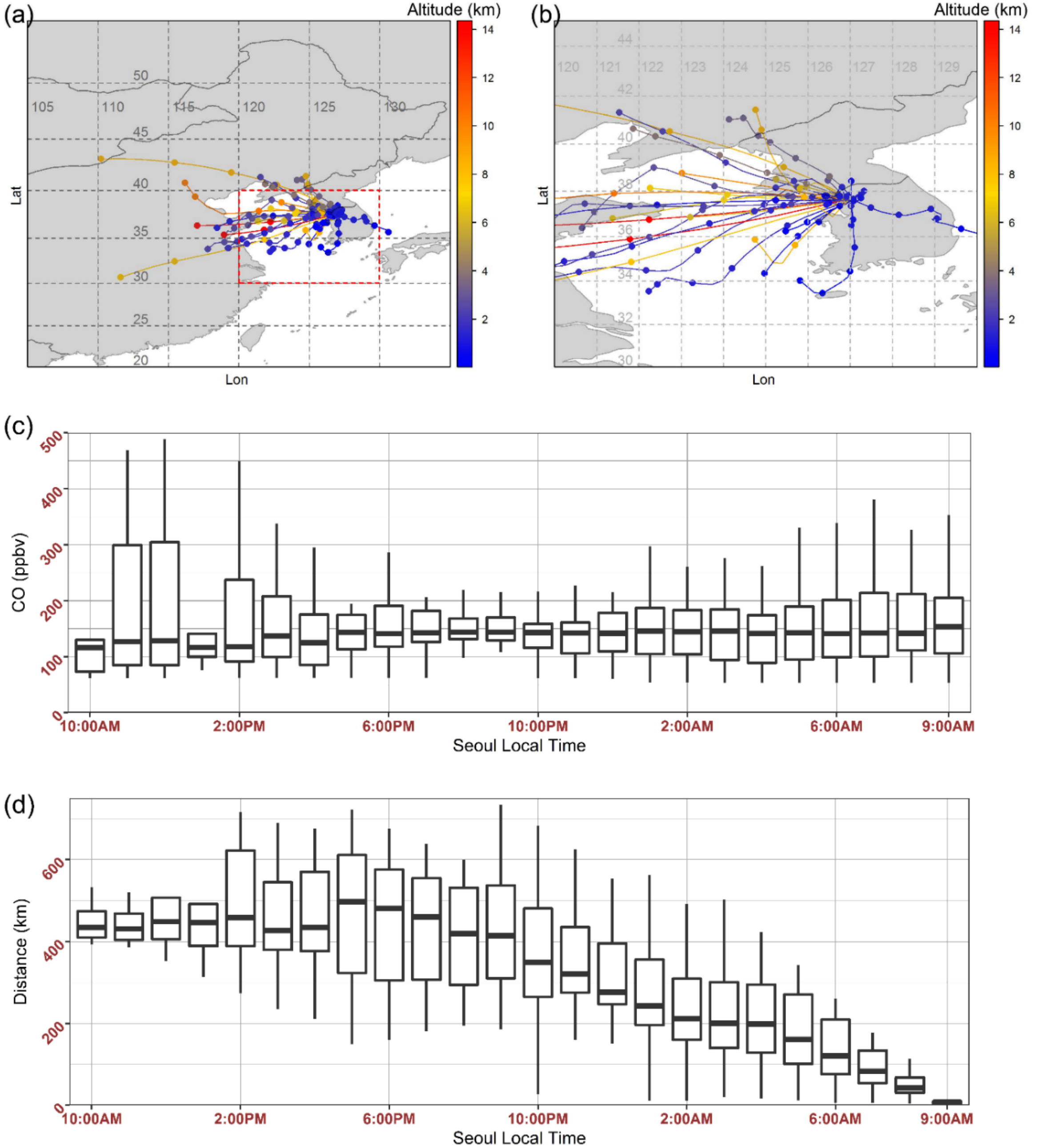

Figure 8: C-TRAIL output for the dynamic weather period (DWP) for Seoul as the receptor

C-TRAIL output for the stagnant period (SP)

- All of the trajectories are local.
- High-pressure system over the Korean Peninsula during this time period, which was responsible for very low wind speeds
- Diffusion, played a significant role in CO concentration values at the receptor location.

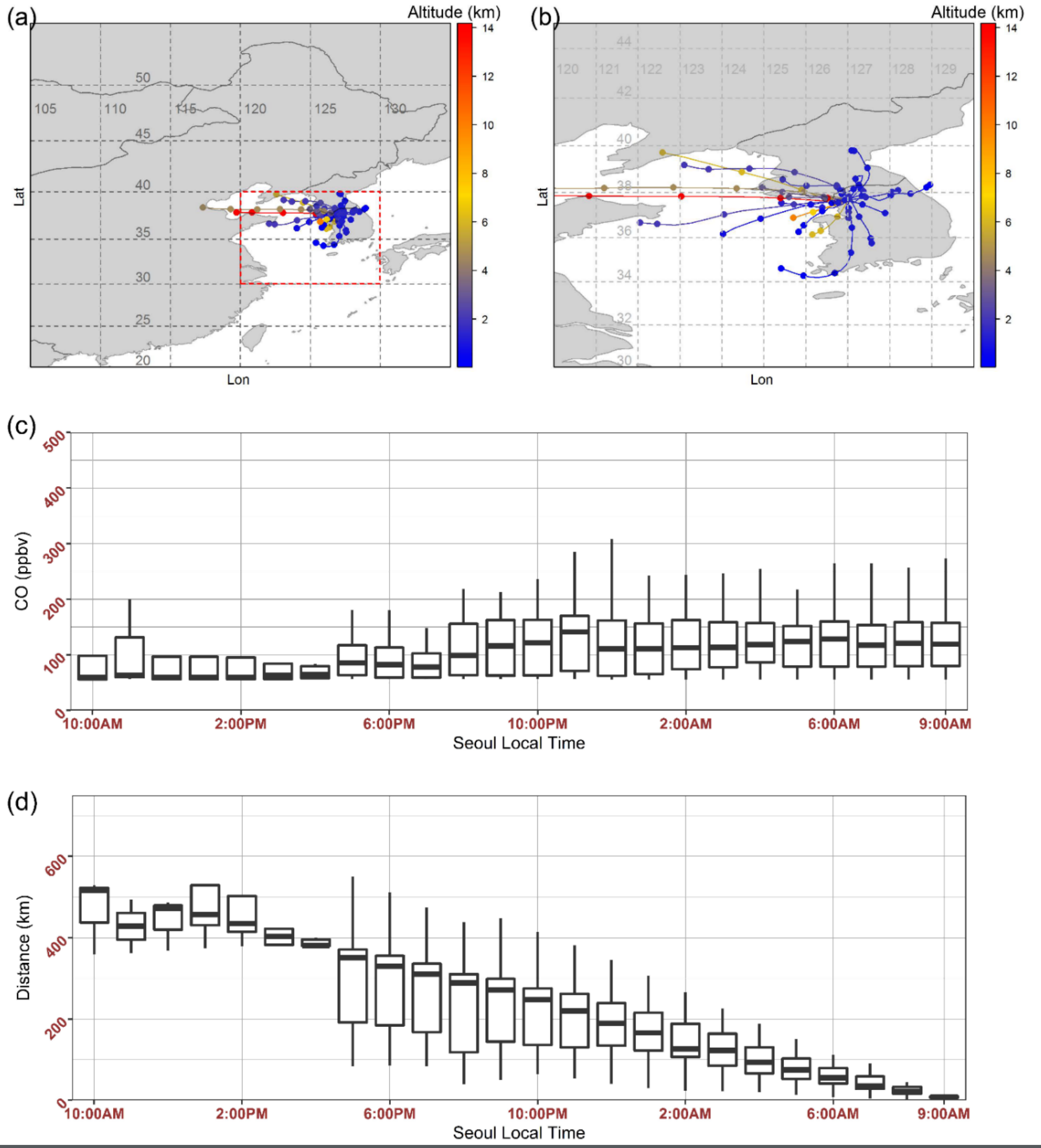

Figure 9: C-TRAIL output for the stagnant period (SP) for Seoul as the receptor

C-TRAIL output for the extreme pollution period (EPP)

- High concentrations of CO appeared at the early points of trajectories.
- High distance values, indicate that the LRT of polluted air masses was responsible for high concentrations of CO.
- High concentration trajectories close to the surface, which originated in the Shandong Peninsula, passed over the Yellow Sea and landed in Seoul.
- The findings of this study regarding the trajectories and the origin of polluted air masses are similar to those of previous studies (Lee et al., 2019).

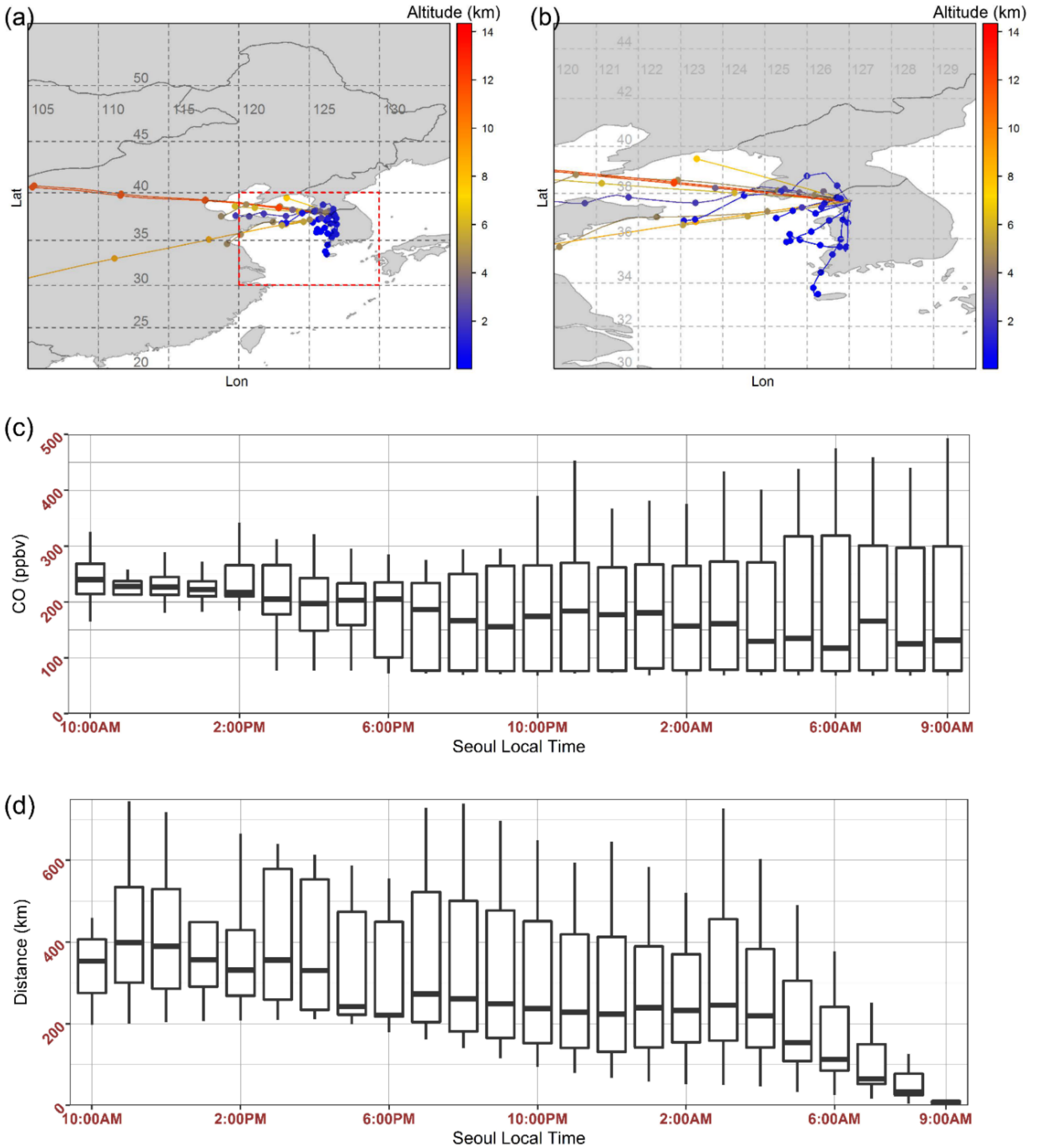

Figure 10: C-TRAIL output for the extreme pollution period (EPP) for Seoul as the receptor.

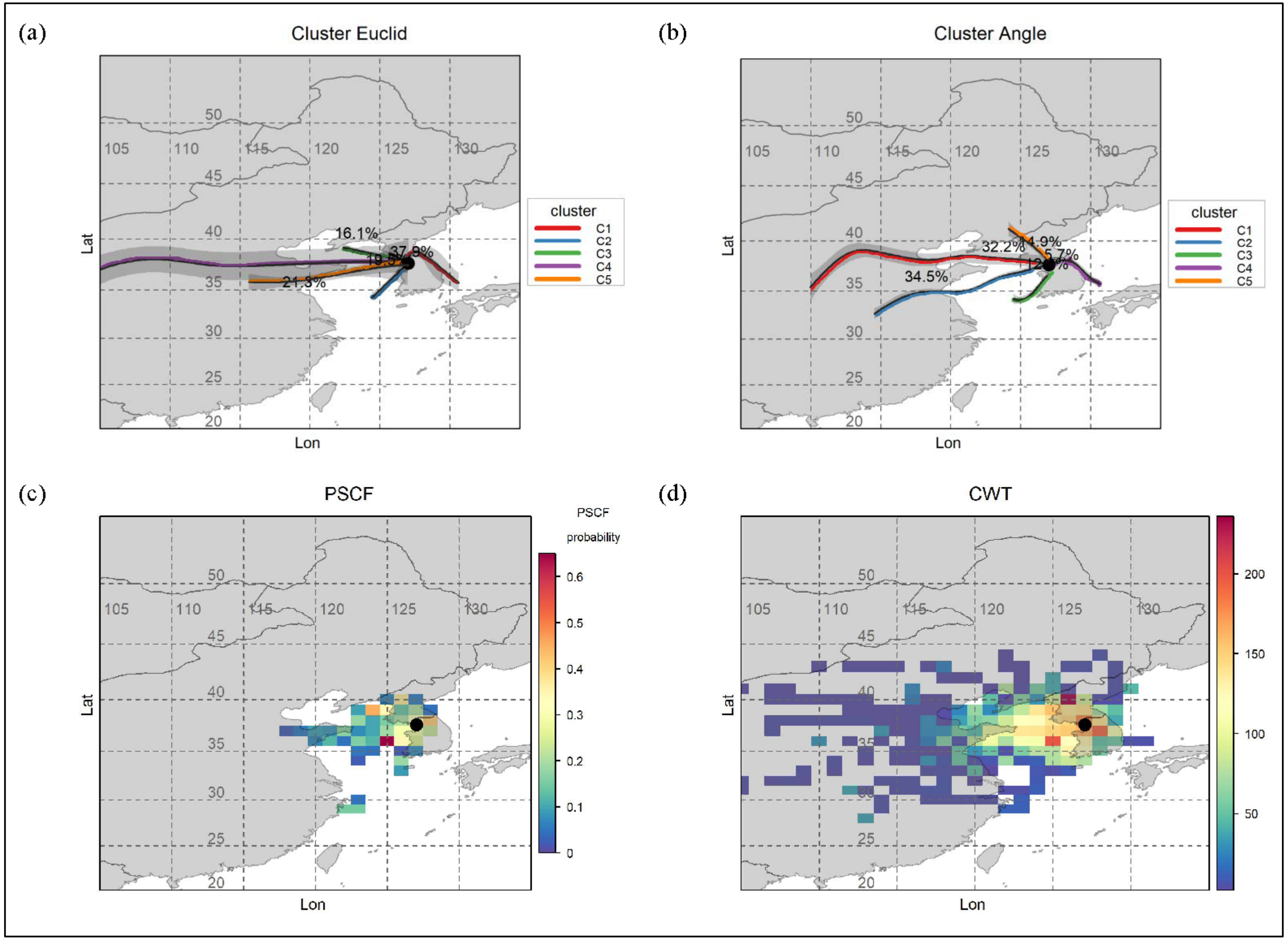

Figure 12: (a) Trajectories clustered by the Euclidian distance function, (b) trajectories clustered by the angle distance function, (c) the potential source contribution factor plot, and (d) the concentration-weighted trajectory plot

Conclusion

- Introduced C-TRAIL Lagrangian output, extracted from the Eulerian CMAQ model.
- C-TRAIL directly linked the trajectories of pollution from the source to the receptor.
- Investigated the pollution status of originated air masses for May 2016 over East Asia.
- C-TRAIL represents a practical tool for ascertaining the impact of long-range transport on species concentrations over a receptor by simultaneously providing concentrations and trajectories.
- C-TRAIL can be applied to LRT-impacted regions such as East Asia, North America, and India.
- An effective tool for establishing a link between real sources of pollution to a receptor

Code availability:

- Detailed description of the model:

https://doi.org/10.5194/gmd-13-3489-2020

- C-TRAIL v1.0 model source code:

https://doi.org/10.5281/zenodo.3885782

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