

**Bases científico técnicas  
para la mejora de la  
calidad del aire en España**



**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación



## **Modelización de ozono troposférico para evaluar la eficacia de medidas sobre emisión de precursores**

**María Teresa Pay**, Oriol Jorba, Marc Guevara, Miriam Olid, Carles Tena, Dene Bowdalo, Hervé Petetin, Vanessa Nogueira Dos Santos and Carlos Pérez García-Pando

Earth Sciences Department – Atmospheric Composition Group

Colaboradores externos:

X. Querol (CSIC), S. Napelenok (U.S. EPA), G. Gangoiti (Uni. Vasc Country)

Valencia  
13 junio 2019



**GENERALITAT  
VALENCIANA**

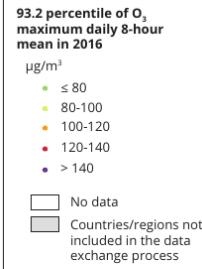
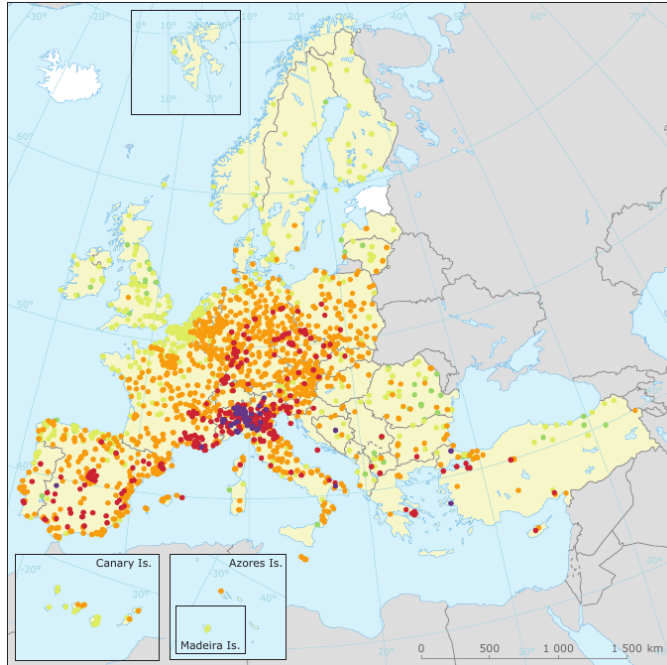


**GOBIERNO  
DE ESPAÑA**  
MINISTERIO  
PARA LA TRANSICIÓN ECOLÓGICA

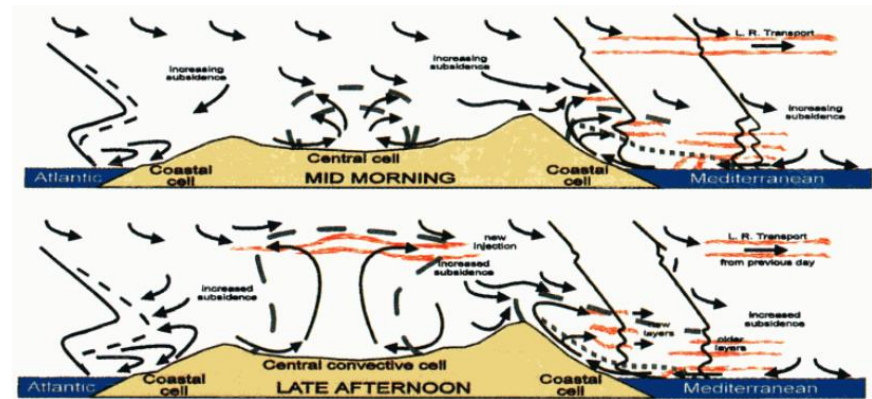
Fundación  
**Naturgy**

# Background and motivation

## O<sub>3</sub> concentration



## O<sub>3</sub> dynamic



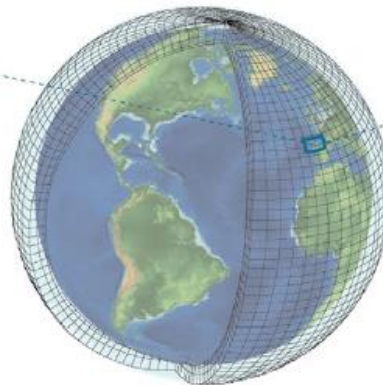
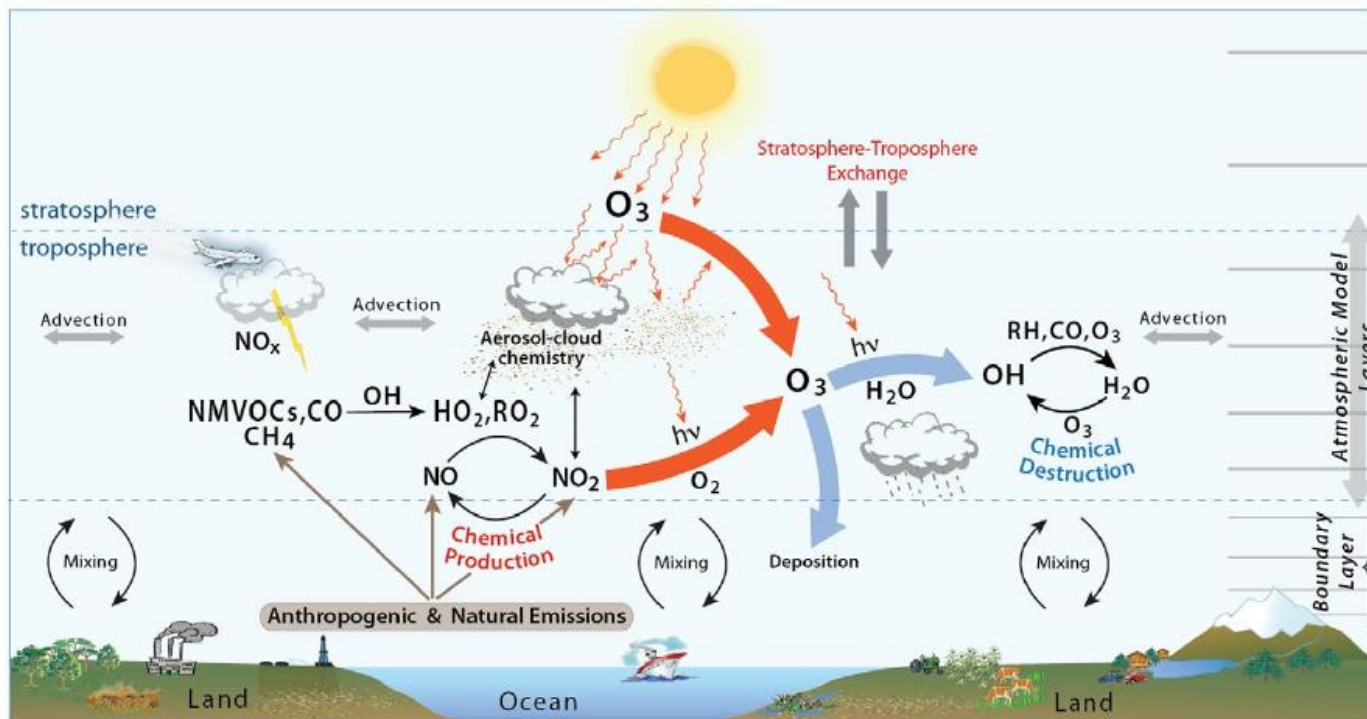
Sources: Millán et al., 1997, 2000, 2014; Gangoiti et al, 2001, 2002, 2006; Toll and Baldasano, 2000

Source: EEA (2018)

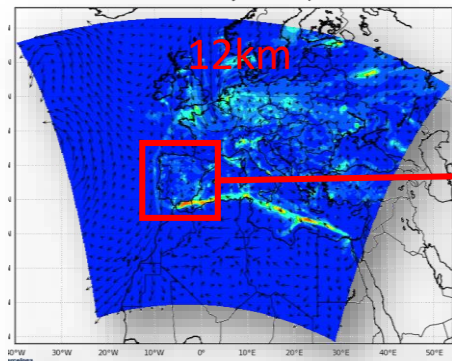
## Outline

1. How models forecast the O<sub>3</sub> episodes? → BSC research work on AQ modelling.
2. Who is responsible of the O<sub>3</sub> exceedances? → First results on source apportionment.

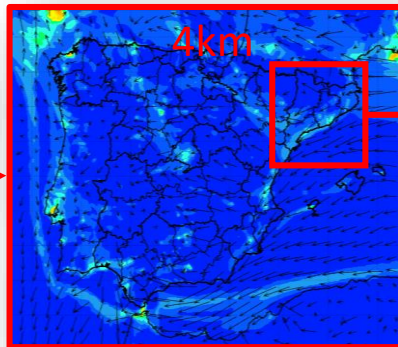
# 1. How models forecast the O<sub>3</sub> episodes?



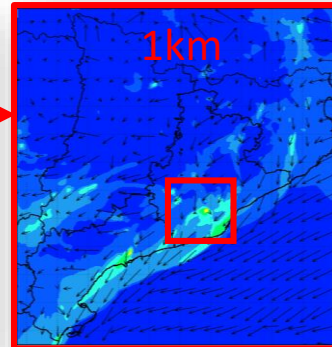
# CALidad del aire Operacional Para España (CALIOPE)



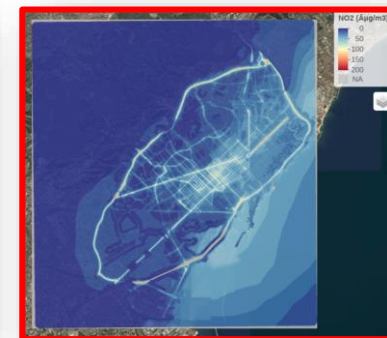
Pay et al. (2011; 2012 AE)



Baldasano et al. (2012 AE)



Pay et al. (2014 GMD)



Benavides et al. (2019 GMDD)



Citizen



Administrations

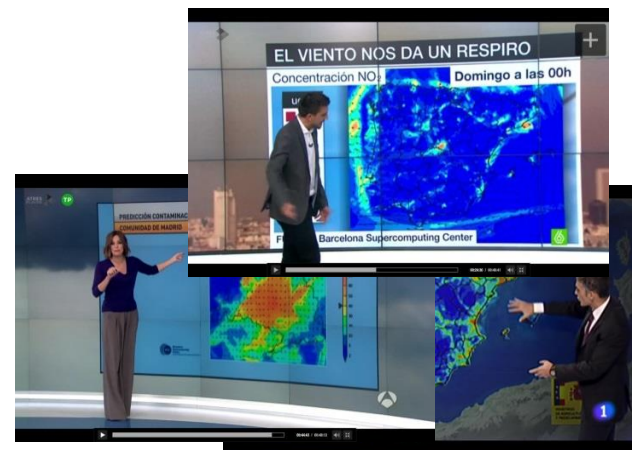
Medi ambient @mediambientat · 31 Jul 2018  
⚠️ AVIS PREVENTIU #ozóCAT. Es preveu superació del llindar d'informació (> 180 µg/m³ de mitjana horària) a la Plana de Vic i l'Alt Llobregat. A la resta, els nivells seran moderats a gairebé tot el territori. Més informació [bit.ly/2ry8PDd](https://bit.ly/2ry8PDd) #qualitaira

Mapa d'avisos:

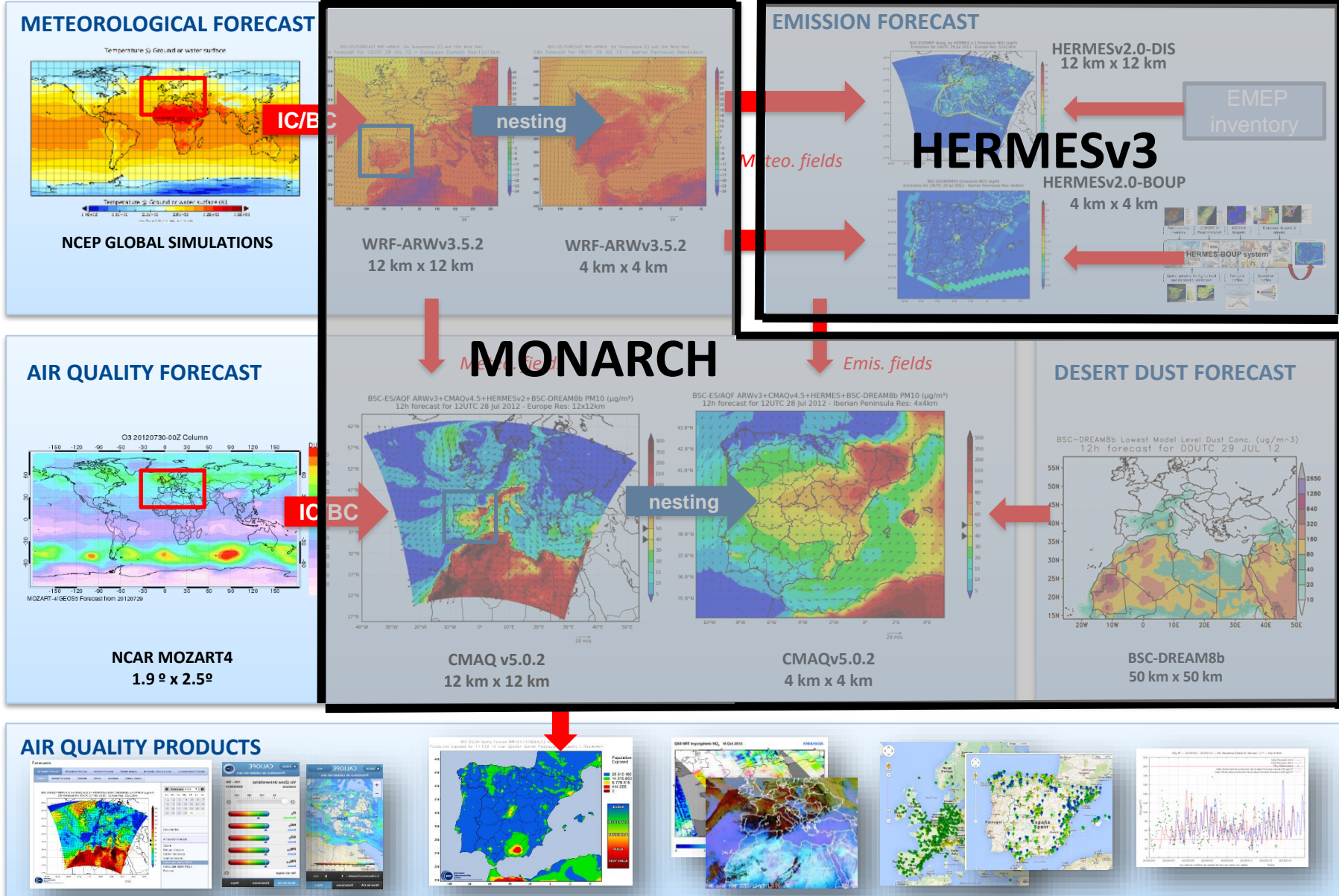
Sha realitzat un avis preventiu per possibilitat de superació del llindar d'informació.

- Sense avis
- Avis preventiu
- Superació del llindar

The media

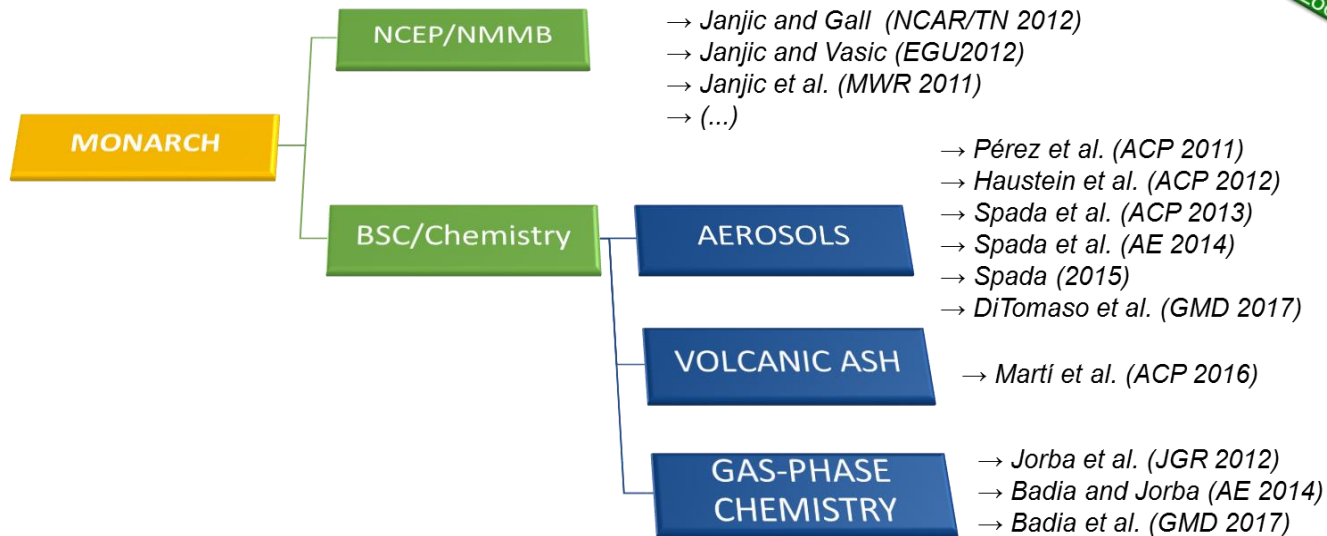
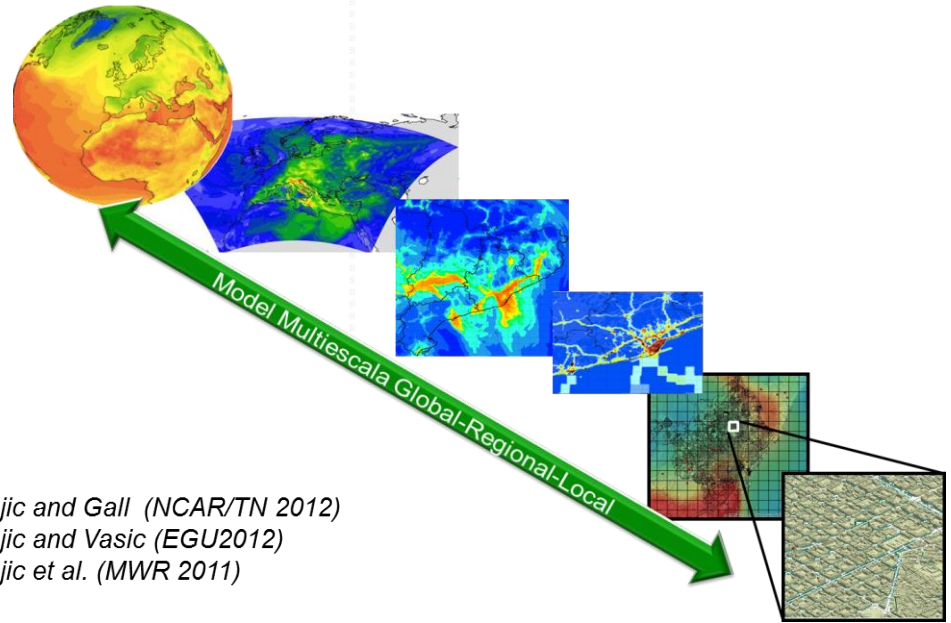


# CALIOPE: main elements



# MONARCH: online weather-chemistry model

- Fully **on-line** coupling: weather-chemistry feedback processes
- In-house developed.
- **Multiscale**: global to regional (up to 1km) scales (nesting capabilities)
- **Data assimilation** system

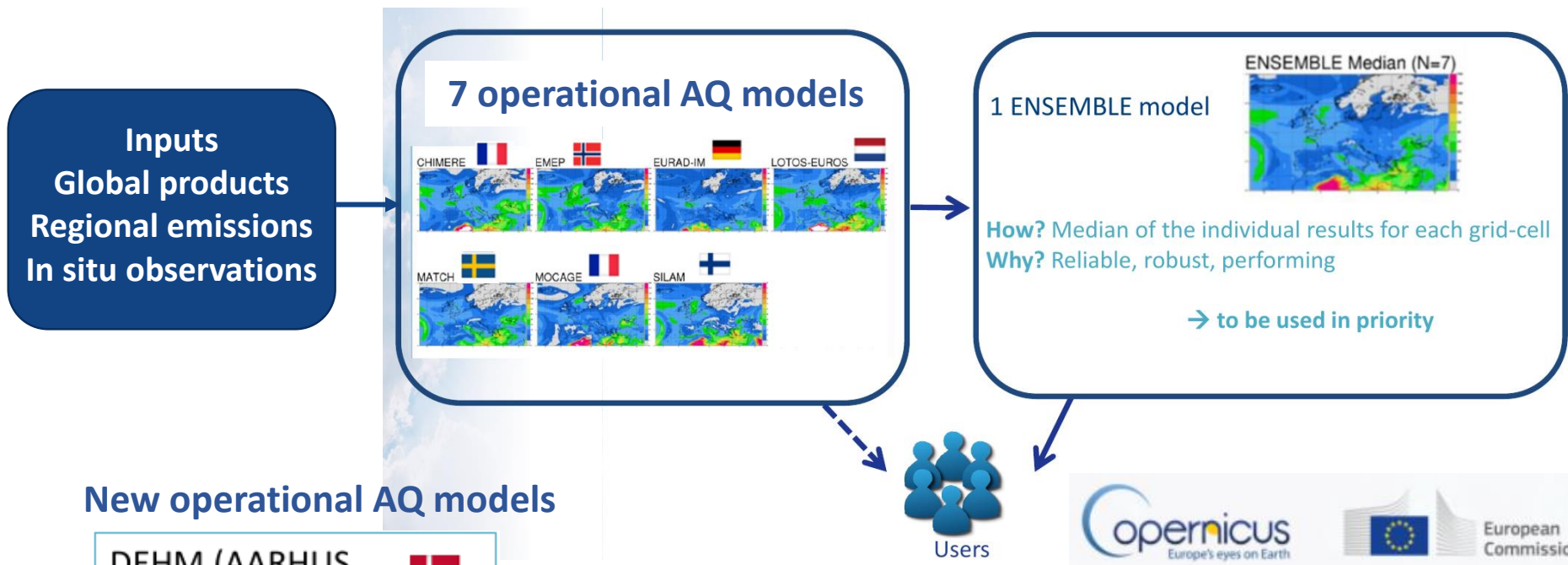


Funding:





# Copernicus Atmosphere Monitoring Service



## Regional air quality (CAMS\_50.II)



### New operational AQ models

DEHM (AARHUS University)   
GEM-AQ (IEP) 

### New candidates AQ models

MINNI (ENEA)   
MONARCH (BSC) 

### Products

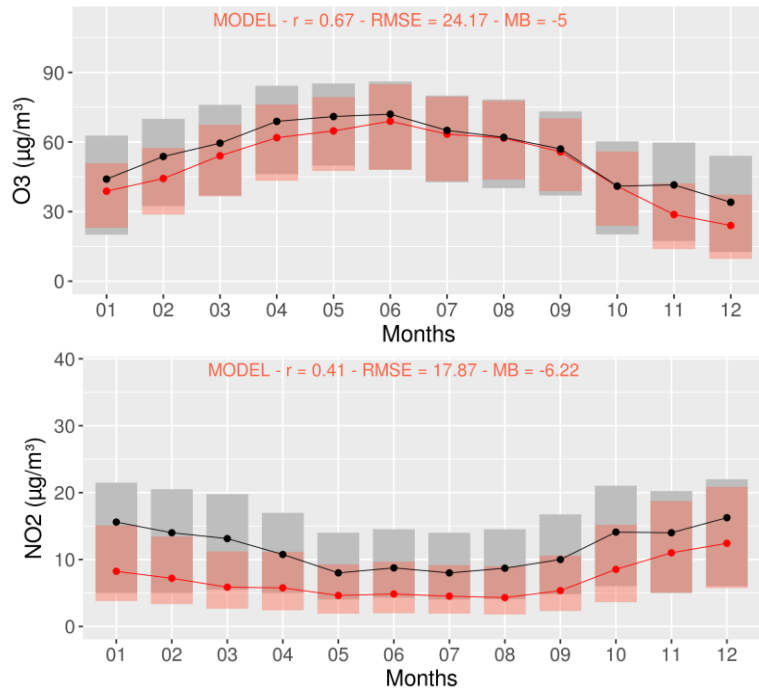
- NRT Individual & Ensemble 4-Day Forecasts
- NRT Individual & Ensemble Analyses (DD-1)
- NRT Validation & Statistics products
- Reanalyses (2014-2017)



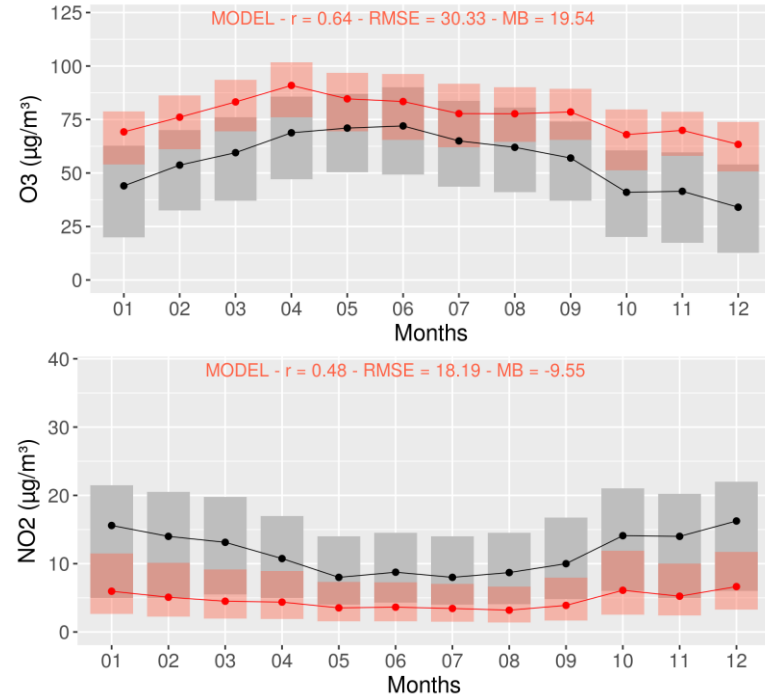
# MONARCH vs CALIOPE: annual cycle

Period: full year 2015

## MONARCH



## CALIOPE (WRF-CMAQ)

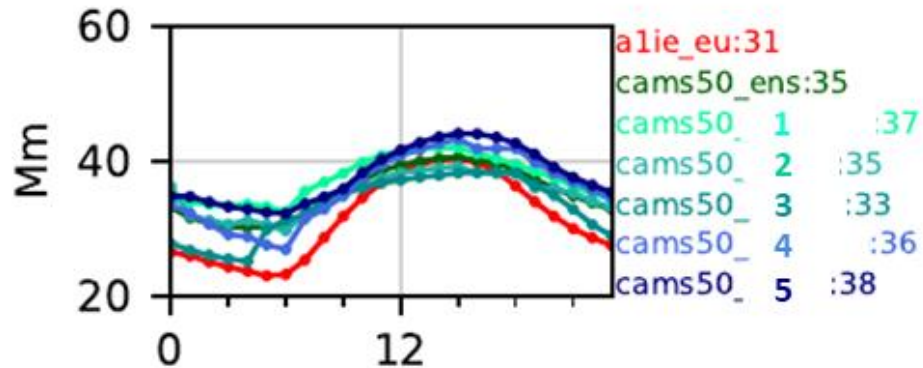
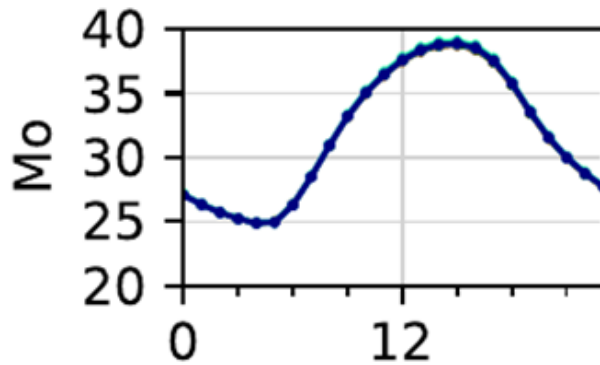


EIONET 2015 validated (rural, suburban, urban)

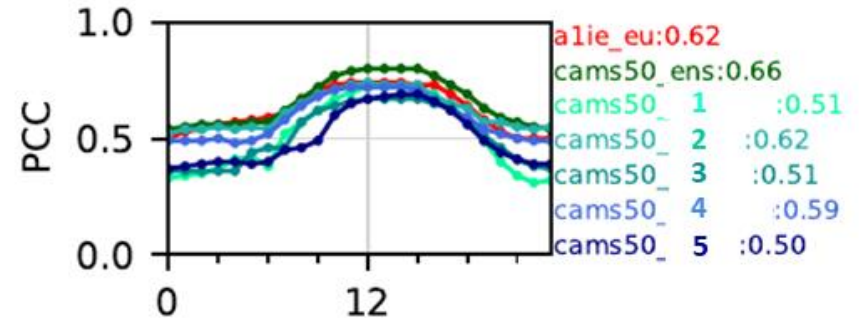
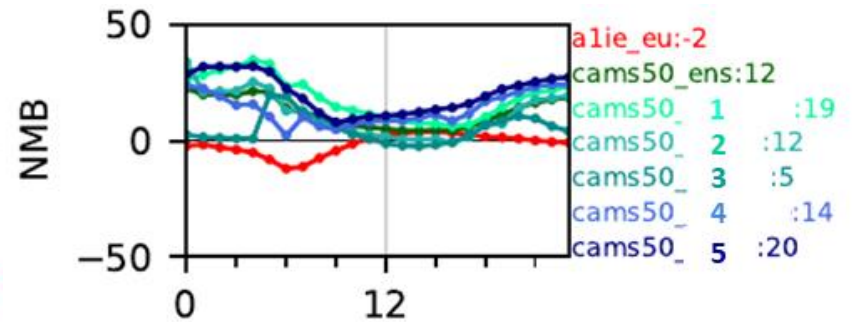
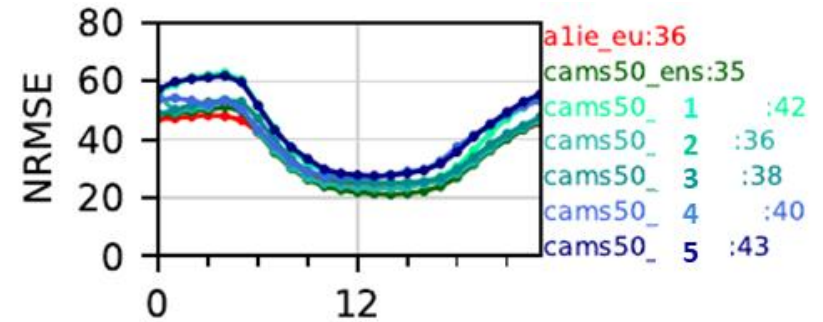
- 958 stations (O<sub>3</sub>)
- 774 stations (NO<sub>2</sub>)

# MONARCH vs CAMS: O<sub>3</sub>

Period: 20160801-20160901

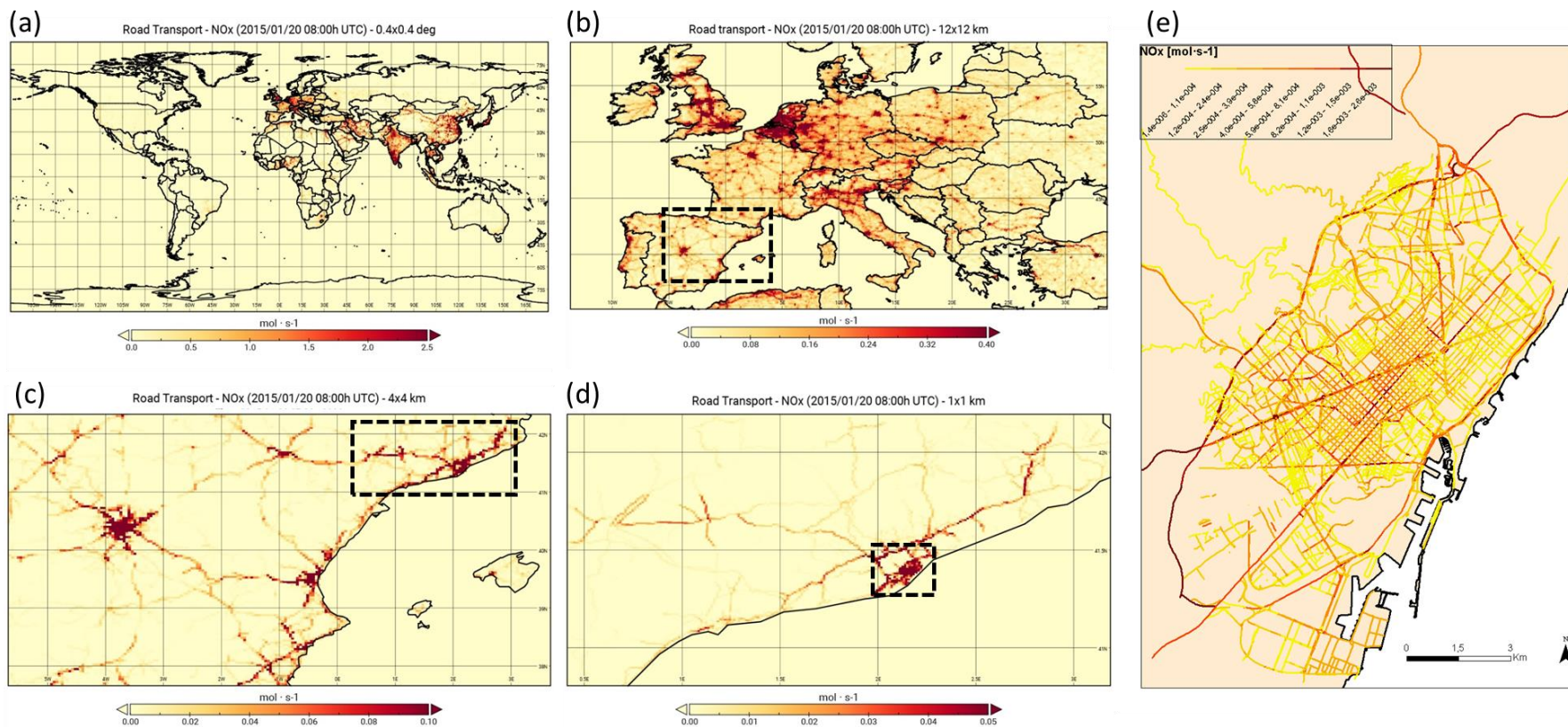


113 EBAS stations



# HERMESv3

A python-based, open source, parallel and multiscale emission modelling framework that processes and estimates gas and aerosol emissions for use in atmospheric chemistry models.

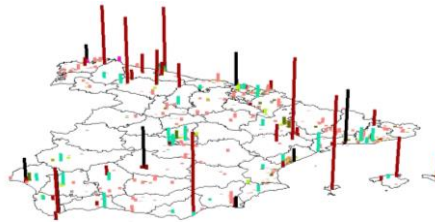


# HERMESv3\_BU: Bottom-up module

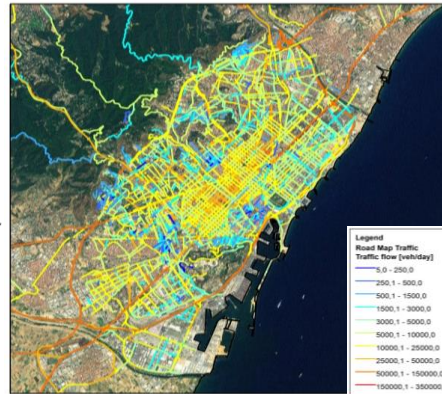
An **emission model** to estimate emissions at the source level (e.g. road link) combining state-of-the-art **bottom-up methods** with **local activity and emission factors**



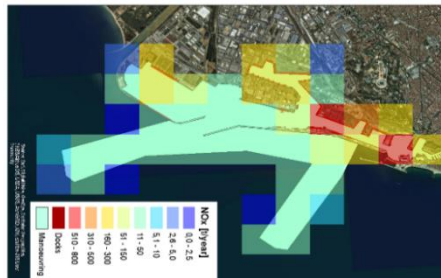
**Point Source**  
 $P$   
 $(x, y)$



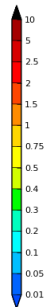
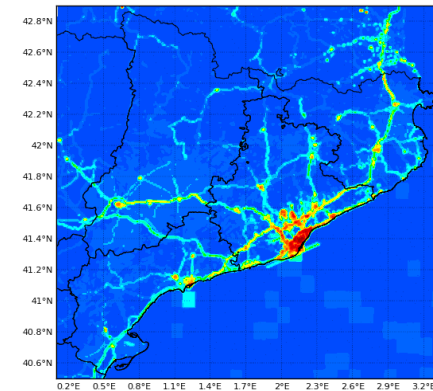
**Line Source**  
 $S$   
 $a$   
 $\{P_1, \dots, P_n\}$



**Area Source**  
 $F$   
 $A$   
 $\{S_1, \dots, S_n\}$



BSC-ES/HERMESv2 Emissions NO<sub>2</sub> (kg/h)  
 Emissions for 08UTC 25 Feb 2016 - Catalonia Domain Res: 1x1km



## 2. Who is responsible of the O<sub>3</sub> exceedances?

- Which are the economic activities responsible for high O<sub>3</sub>? (**sectors**)
- Where do the precursors responsible for O<sub>3</sub> exceedances come from? (**regions**)

**Unraveling the origin of the high surface O<sub>3</sub> concentrations** in Spain is a previous step to design mitigation strategies:

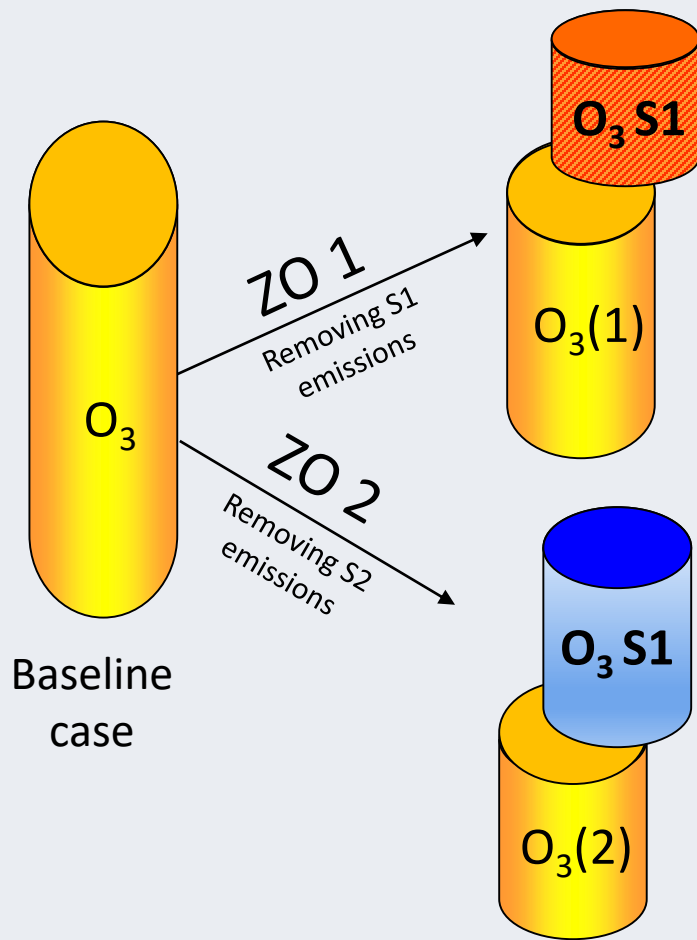
- Quantifying the O<sub>3</sub> contribution from:
  - the **NO<sub>x</sub>/VOC emission sectors within Spain.**
  - the **external contribution** (O<sub>3</sub> produced outside Spain).
- Using the **Integrated Source Apportionment Method** together with a **high detailed emission model.**



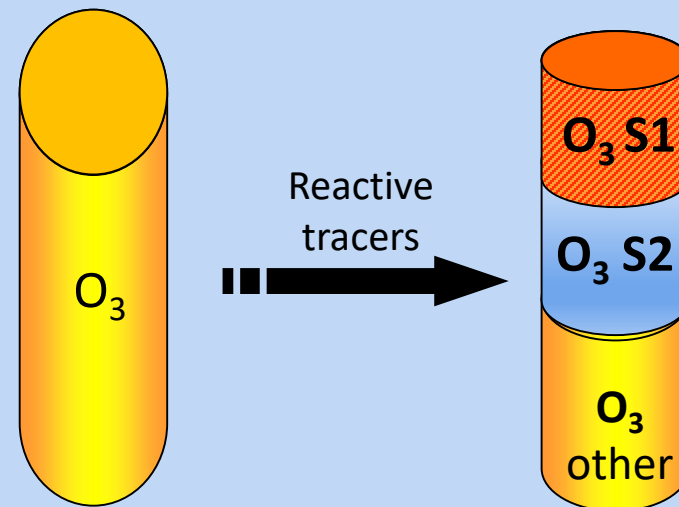
# Source apportionment modelling

Emissions  
are critical

## Zero-Out (ZO)



## Tagging



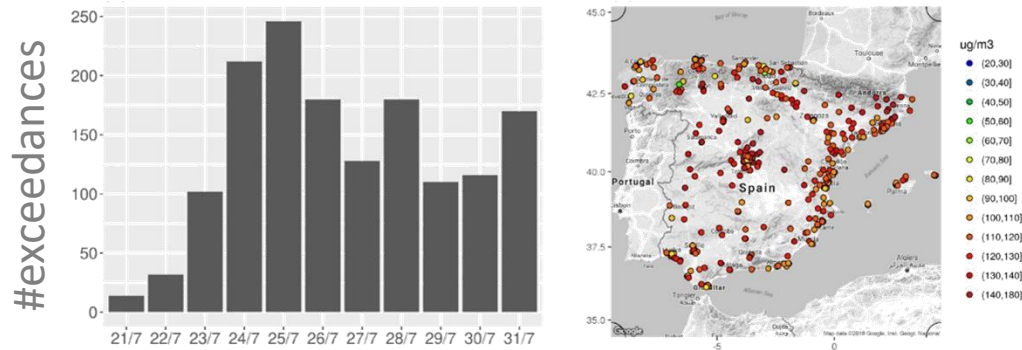
## Advantages

- Time saving (one simulation)
- Mass consistency
- Real atmospheric conditions
- Fully traceable

# O<sub>3</sub> source apportionment in the Iberian Peninsula

Pay et al., 2019. Atmos. Chem. Phys. 19, 5467–5494

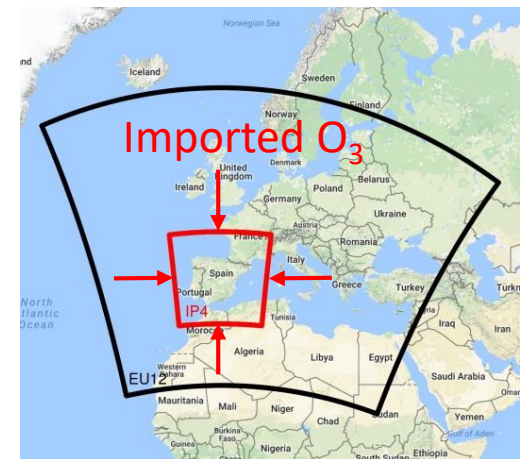
## O<sub>3</sub> episode: 21-31 July 2012



## Contributions: anthropogenic emissions + imported O<sub>3</sub>

Sectors accounting  
92% of the total NO<sub>x</sub>

- Others
- Power Plants
- Industry
- On-road transport
- Non-road transport

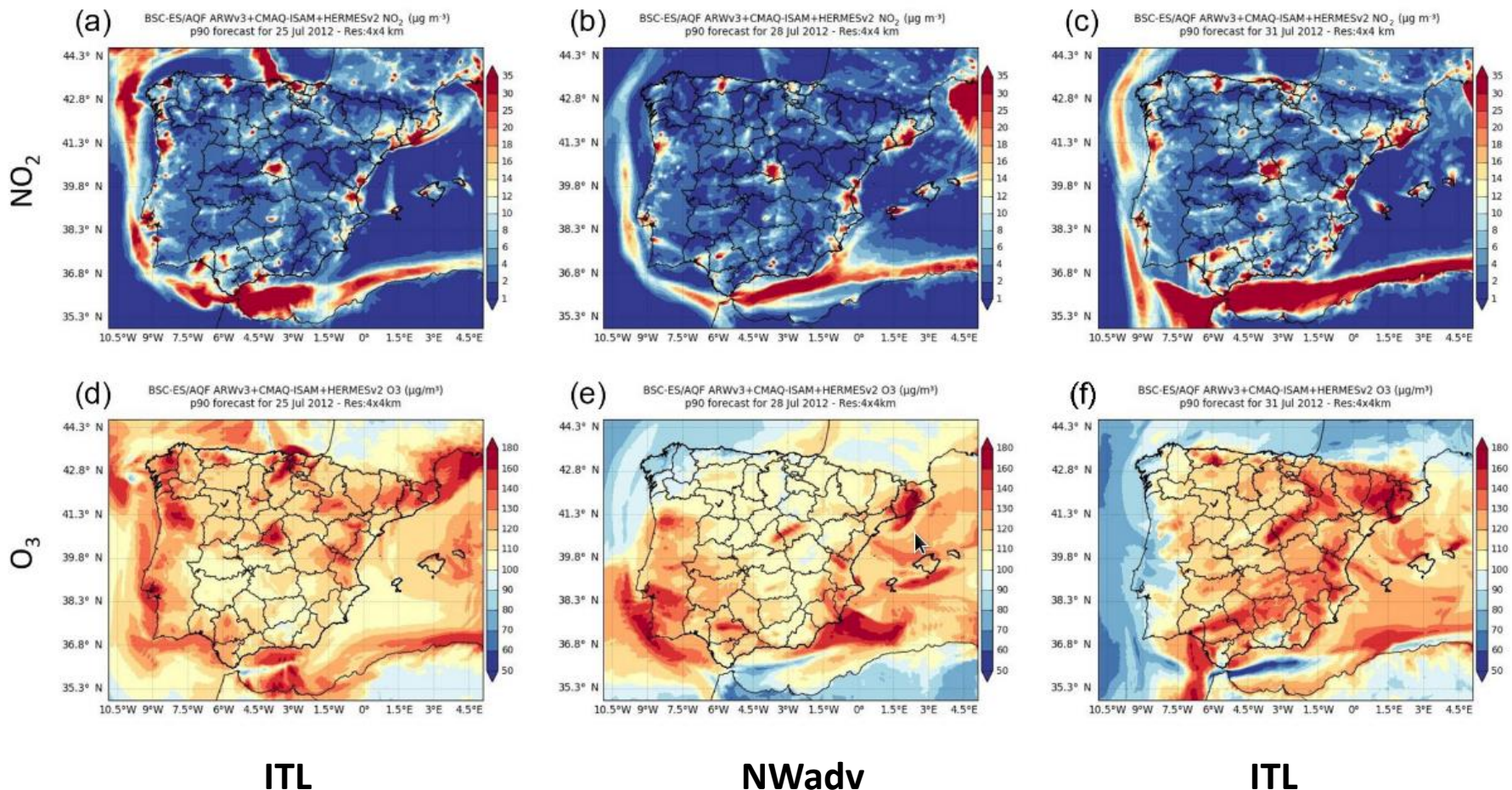


# NO<sub>2</sub> and O<sub>3</sub> concentrations

25 July

28 July

31 July



Iberian Thermal Low (ITL) and NW advection (NWadv) represent 44% of the days in the IP both taking place in summer (*Valverde et al., 2015*)



# O<sub>3</sub> contributions (p90 concentrations)

Power Plants

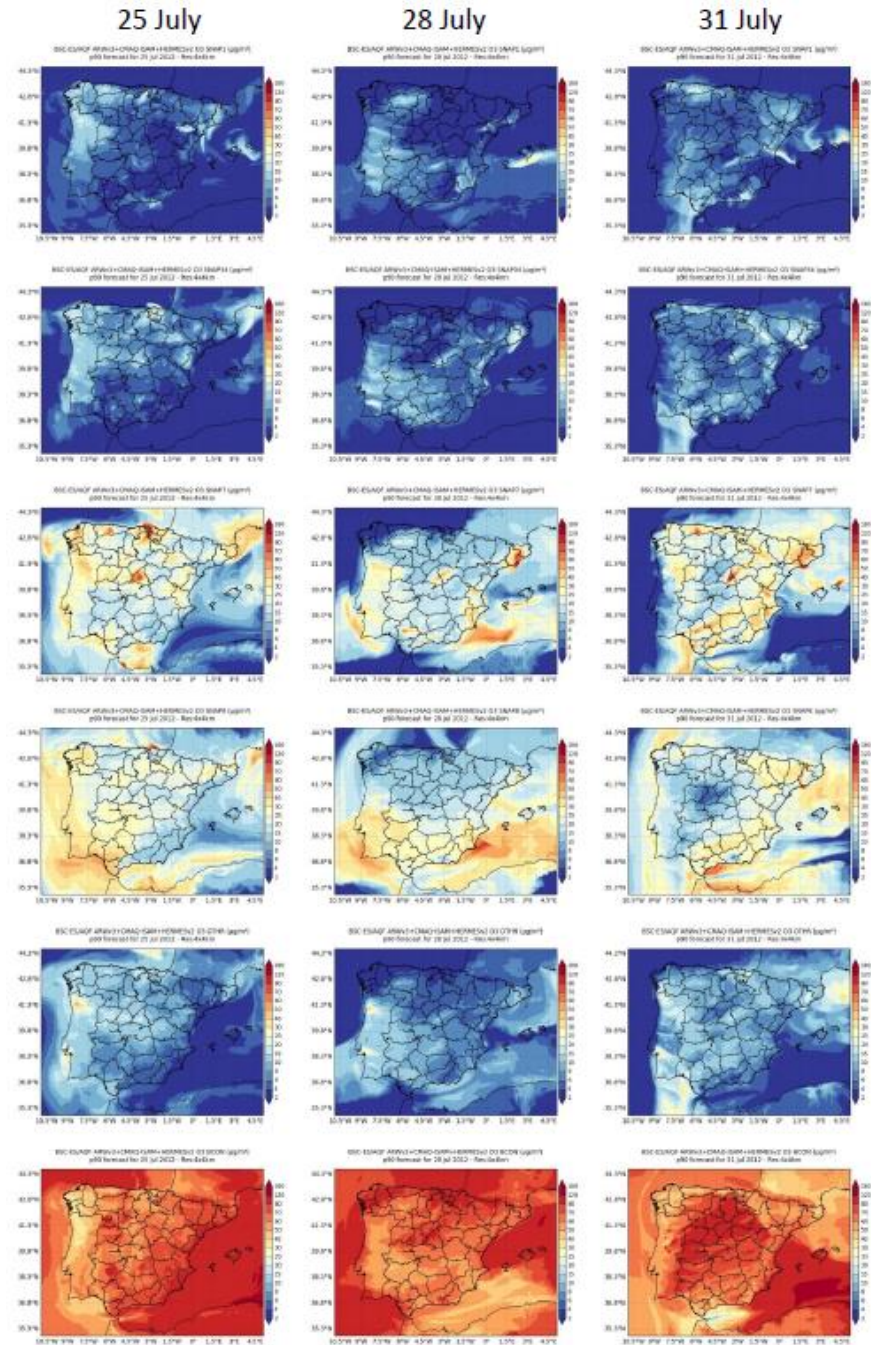
Industry

On-road

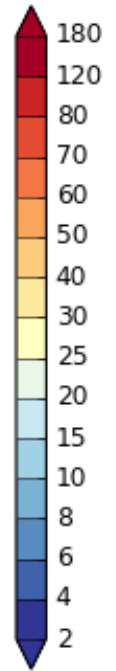
Non-road

Others

Imported



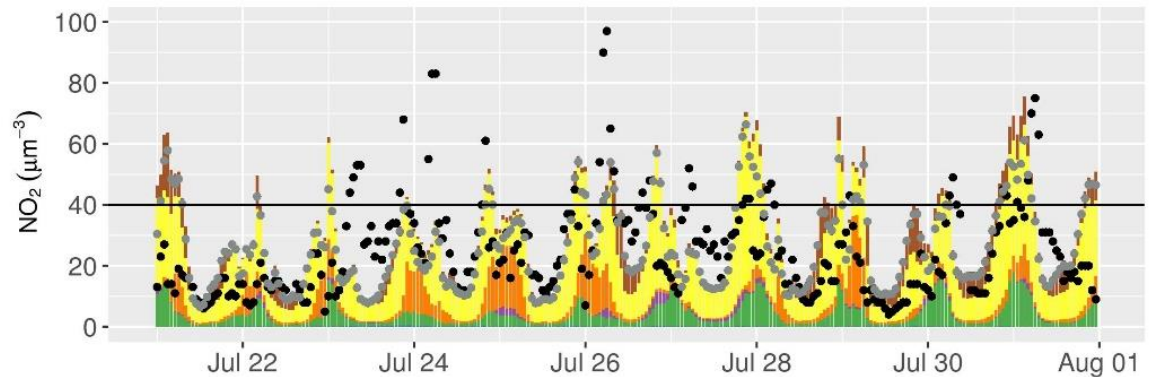
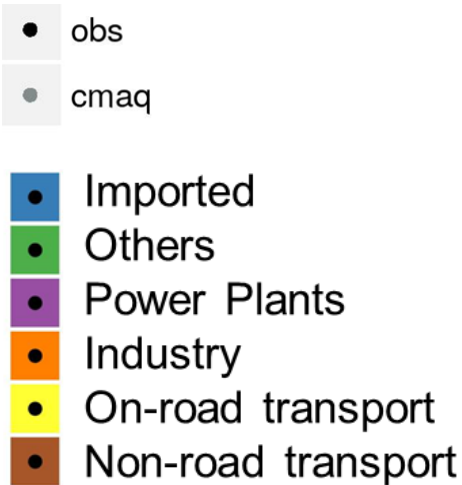
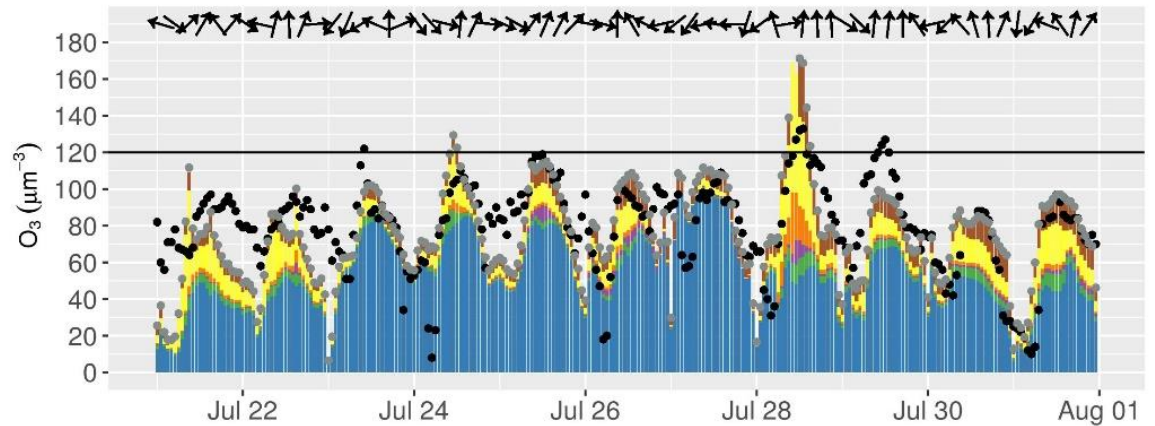
O<sub>3</sub>  
[µg/m<sup>3</sup>]



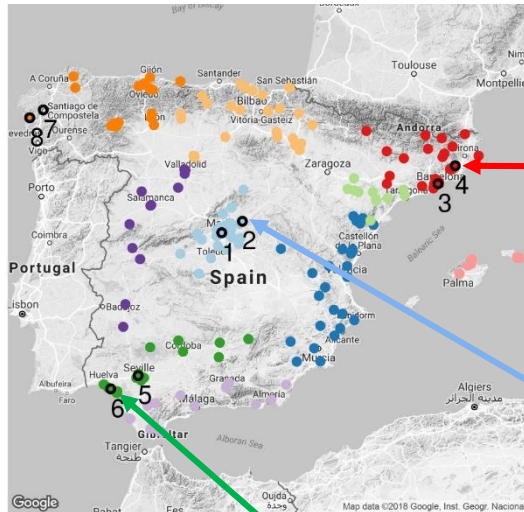
# O<sub>3</sub> contribution in urban areas



## (3) Urban station – Palau Reial (Barcelona)



# O<sub>3</sub> contribution in background areas



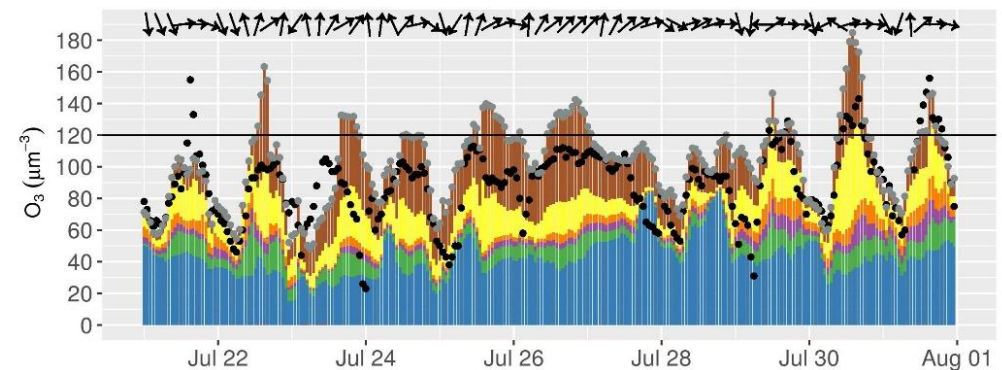
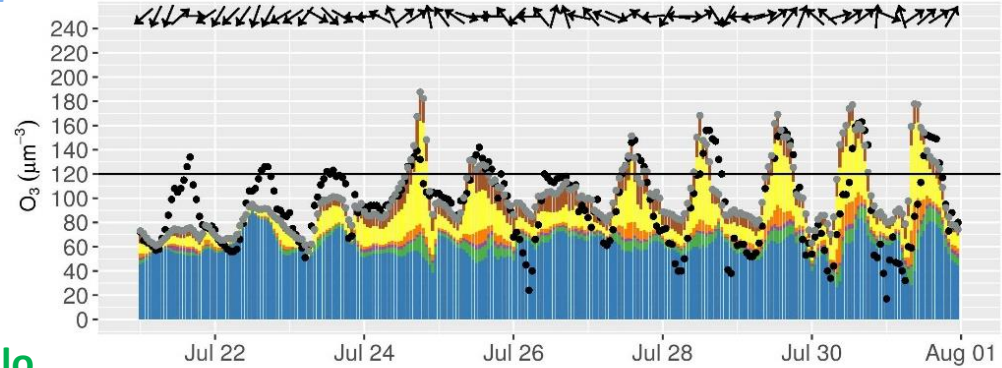
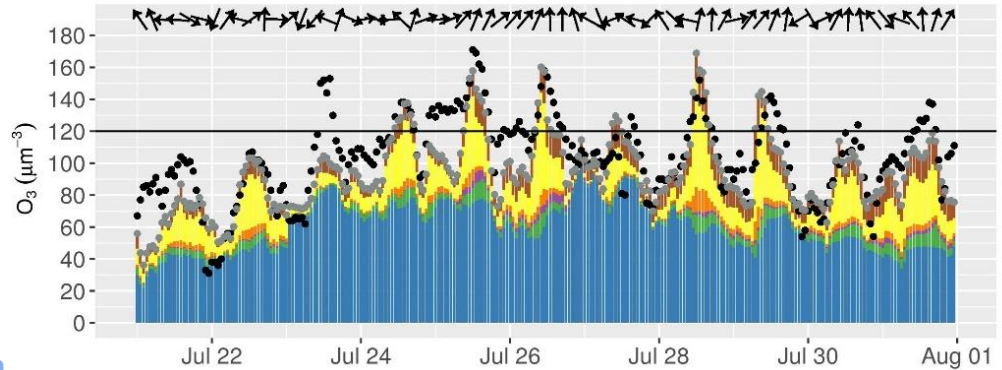
(4) Montseny

(2) Gadálajara

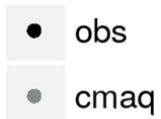
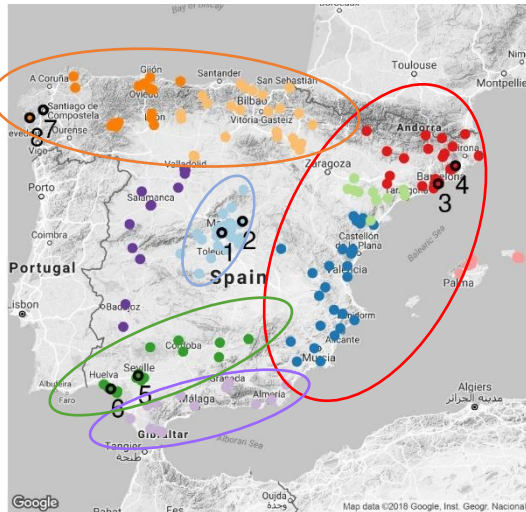
(6) El Arenosillo

- obs
- cmaq

- Imported
- Others
- Power Plants
- Industry
- On-road transport
- Non-road transport



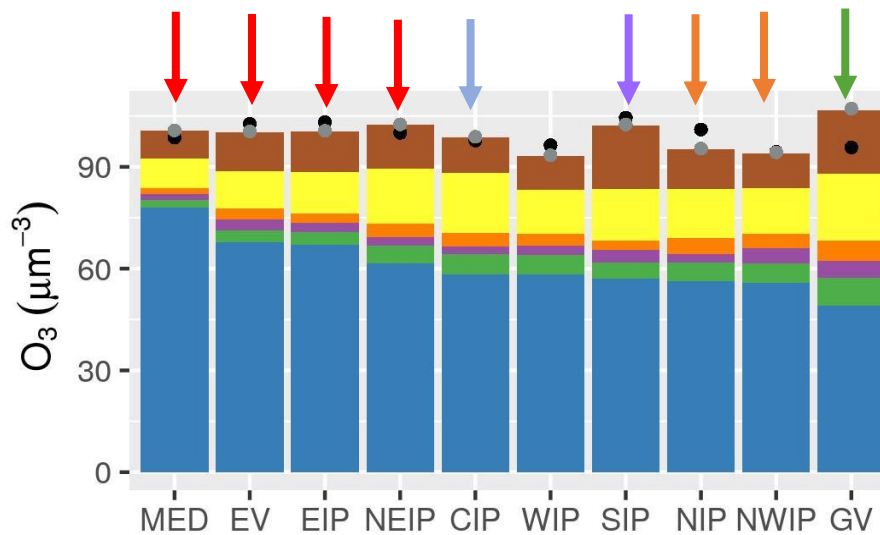
# Regionalization of source-sector contribution



- Imported
- Others
- Power Plants
- Industry
- On-road transport
- Non-road transport



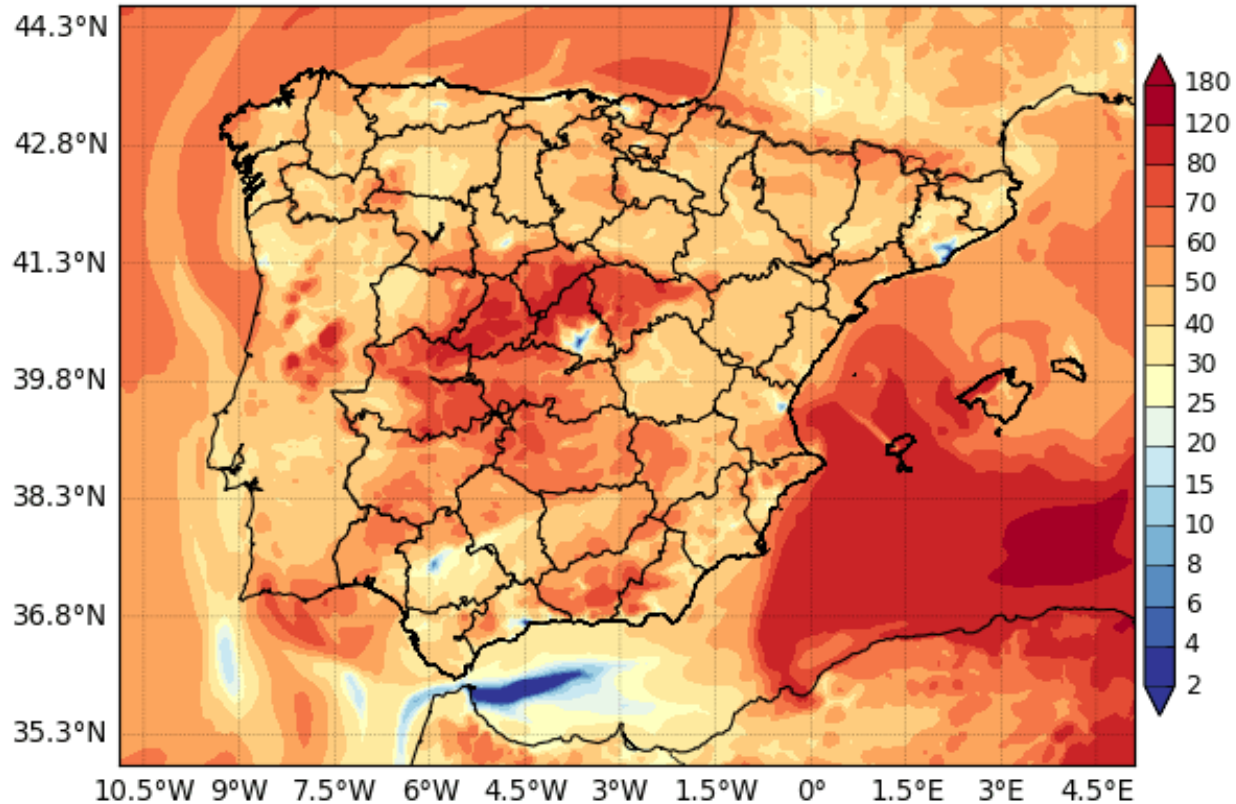
Daily mean contribution during  
DMA8 > 120  $\mu\text{m}^3$



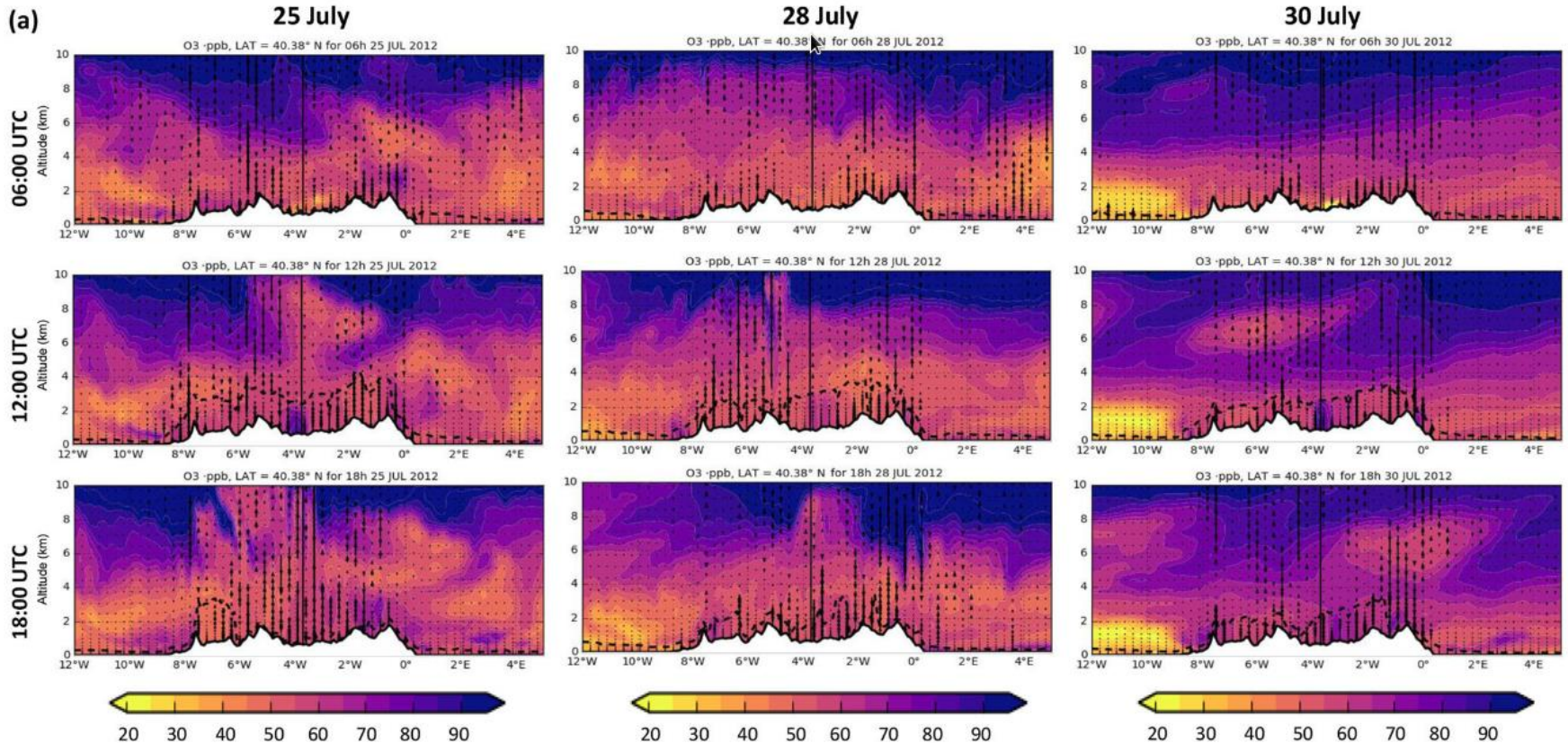
$r = 0.79$  (without GV)

# Imported O<sub>3</sub> concentration

BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> BCON ( $\mu\text{g}/\text{m}^3$ )  
00h forecast for 00UTC 31 Jul 2012 - Res:4x4km



# O<sub>3</sub> vertical distribution



# Conclusions

## 1. The improvement of models is necessary to improve the diagnosis of O<sub>3</sub>

- emission + meteorology + chemistry + boundary conditions

## 2. The O<sub>3</sub> problem in Spain is local, regional and hemispheric.

- **Imported O<sub>3</sub>** to the IP is a main contributor to ground-level O<sub>3</sub> concentration overall: 70-80% NW advections and 30-40% during stagnant conditions.
- **Regional/local source** contributions dominate O<sub>3</sub> during peaks:
  - Central and NE IP: the highest **road transport** contribution to O<sub>3</sub> (up to 40% in daily peak during events).
  - Industrial regions: **energy generation and industrial processes** contribute to O<sub>3</sub> up to 11%.
  - All sub-regions: the **non-road transport** is a contributor as significant as the road transport (10-19%).

## 3. Integrated source apportionment useful tool:

- Identification of potential errors in emission estimates
- Design more cost-efficient mitigation plans (together with source sensitivity).

# Ongoing research work

## 1. Source apportionment for O<sub>3</sub>

- Expand the quantification of the source contribution to O<sub>3</sub> in Spain including:
  - (1) different O<sub>3</sub> episodes
  - (2) multiyear O<sub>3</sub> seasons.
- Focus on main Spanish O<sub>3</sub> basin:
  - (1) Quantify the contribution of key emission sectors.
  - (2) Quantify the relative importance of imported vs regional/local O<sub>3</sub>.

## 2. Source apportionment for PM2.5

- At the Spanish urban level:
  - (1) Region (urban/national/transboundary) and sector contribution.
- At the European level focus on agriculture:
  - (1) Health and economic cost of agricultural production and consumption.



# Thank you!



**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación



Atmosphere  
Monitoring Service



GOBIERNO  
DE ESPAÑA

MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD



## Acknowledgments

- Spanish Ministry of Economy and Competitiveness (PAISA , CGL2016-75725-R).
- “Red Española de Supercomputación” (AECT-2017-1-0008).
- PRACE for awarding access to MareNostrum 4 through the eFRAGMENT project.
- The Copernicus Atmosphere Monitoring Service (CAM50, CAMS81) on behalf of the European Commission.
- AXA Research Fund.

## References:

- Pay, M.T., Gangoiti, G., Guevara, M., Napelenok, S., Querol, X., Jorba, O., Pérez García-Pando, C. *A source apportionment assessment of ozone concentrations in peak summer events over the Iberian Peninsula*. Atmos. Chem. Phys., 19, 5467 -5494, 2019
- Guevara, M., Tena, C., Porquet, M., Jorba, O., and Pérez García-Pando, C.: *HERMESv3, a stand-alone multiscale atmospheric emission modelling framework – Part 1: global and regional module*, Geosci. Model Dev., 12, 1885-1907, 2019