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Doctoral thesis summary

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Title of the thesis	Characterization of atmospheric pollution dynamics in Spain by means of air quality modelling
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Atmospheric pollution causes large impacts on human health and societal economic interests and it is a threat for the ecosystems and the climate of the Earth. Improving the understanding of pollution dynamics is necessary to desing efficient air quality strategies that reduce the impacts of air pollution. This Ph.D. Thesis identifies the typical atmospheric conditions at synoptic scale that affect the Iberian Peninsula (IP) and uses them to explain the dynamics of the most relevant gaseous pollutants in Spain (nitrogen dioxide NO2, sulphur dioxide SO2, and ozone O3) by means of air quality modelling.

Circulation type classifications (CTC) summarise the continuum of atmospheric circulation into a discrete number of typical circulation types (CTs). For the 1983-2012 climatic period, a CTC is derived to be useful in the characterization of air quality dynamics over the IP. Sensitivity tests to classification techniques (principal components, correlation analysis, clustering) and other factors affecting the CTC (temporal and spatial resolution, domain size, etc.) are performed to objectivize the choice of the automatic set-up that maximizes its quality. The six identified CTs – described in terms of frequency, persistence, transitions, and location of pressure systems – are consistent with CTs found in the literature. The temporal stability of the CTC, evaluated following a cross-validation process that compares the results of the climatic and yearly CTs, leads to the identification of a representative year (2012). A representative day for each CT in 2012 is identified using an objective score that minimizes the differences of the daily and the average surface pressure CT grid.

The study of NO2, SO2, and O3 dynamics performed on the representative day of each CT focuses on the biggest Spanish urban areas (Madrid and Barcelona) and heavy industrial/electricity-generation areas such as Asturias (northern Spain) and the Algeciras bay (southern Spain). The state-of-the-art CALIOPE Air Quality Forecast System (CALIOPE-AQFS) that provides high-resolution data on emissions, meteorology, and pollutant concentration over Spain is the main tool used in the characterisation of pollution dynamics. The modelling system is also used to quantify the contribution of specific sources of pollutants – coal-fired power plants and on-road transport – by means of a brute-force approach and an emission-based source apportionment, respectively.

The CTs control the transport patterns of SO2/NO2/O3 in Spanish continental and Atlantic areas, whereas in Mediterranean coastal areas and over complex-terrains a combination of synoptic and mesoscale dynamics (sea-land and mountain-valley breezes) explains the pollutant concentration patterns. The power plants' contribution to surface concentration (up to 55 µgSO2 m-3 and 32 µgNO2 m-3) occurs mainly close to the source (< 20 km) related to vertical diffusion when the emission is injected within the planetary boundary layer. However, the SO2/NO2 plumes can reach distances higher than 250 km. The daily maximum O3 concentration attributed to the on-road transport emissions from Madrid and Barcelona contribute up to 24% and 8% to total O3 concentration, respectively, but it is particularly significant (up to 80-100 µg m-3 in an hour) to the O3 concentration peak during the central hours of the day in April-September. The long-range transport of O3 to the IP is controlled by the CTs and its concentration is very significant in the area of influence of Madrid and Barcelona, particularly under cold CTs (70-96%).

This Ph.D. Thesis has proven that CALIOPE-AQFS (1) is useful to characterise the 3-D dynamics of primary and secondary pollutants in Spain under typical CTs; (2) is able to attribute and quantify air pollution to its sources via brute force and source apportionment; and (3) has the potential to help in the design of specific, science-based abatement strategies that minimize air pollution impacts.

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Signature