Influence of Water on the Regional Modelling of Organic Aerosol Using a Volatility Basis Set Approach

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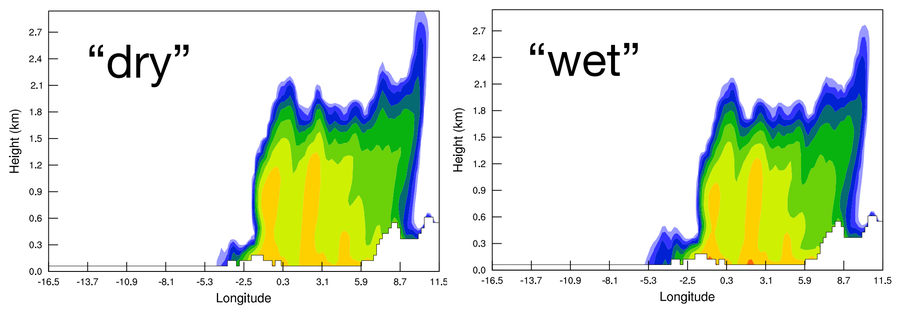
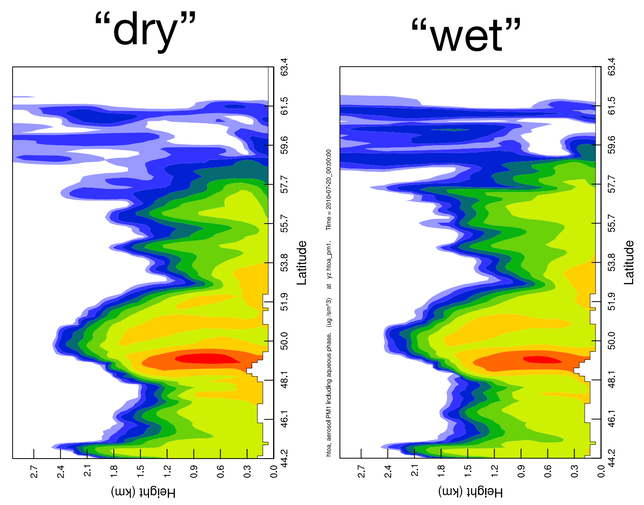
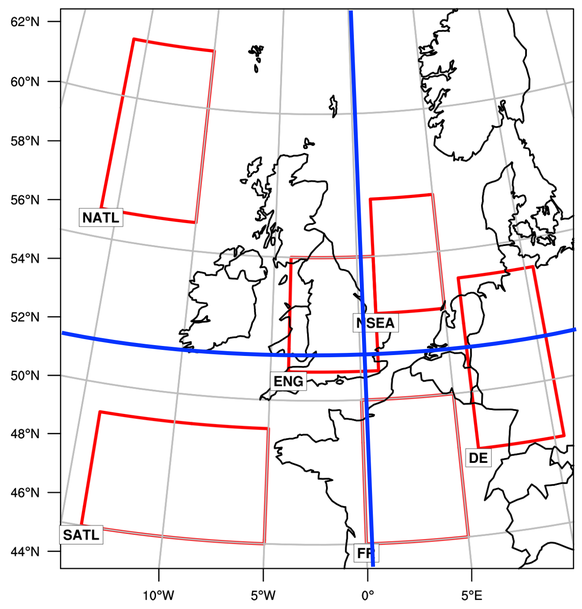
The Volatility Basis Set (VBS) approach has been used for several years to represent the formation of organic aerosol from volatile and semi-volatile organic compounds emitted by burning carbon-based fuels. The evolution of organic aerosol can be controlled by a range of factors: from reaction rates for oxidation, through to branching ratios of products from these reactions, which have been widely investigated. It can also be influenced by the simultaneous co-condensation of water along with the organic compounds, increasing the absorptive mass and so further increasing the uptake of organic compounds. This process is not currently taken into account in most VBS schemes, but in this study we investigate it's importance to organic aerosol growth.

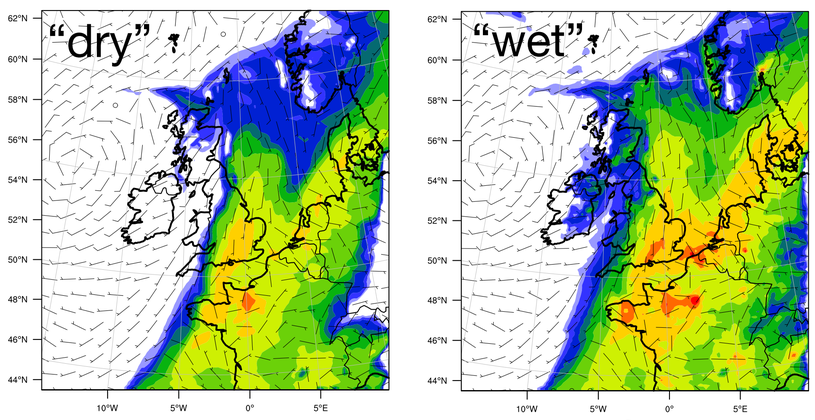
Vertical Profiles of OM PM1 mass loadings







Ground-level OM mass loadings and O:C ratio



Legend

"Fresh" Condensed

"Aged" Condensed

"Fresh" Gas-phase

"Aged" Gas-phase

Model Setup:

WRF-Chem v3.4.1, with CBM-Z chemistry and (8 section) MOSAIC aerosol.

This includes a 9-bin VBS, modified to account for the effect of associated water in the calculation of the equilibration of semi-volatile organic compounds.

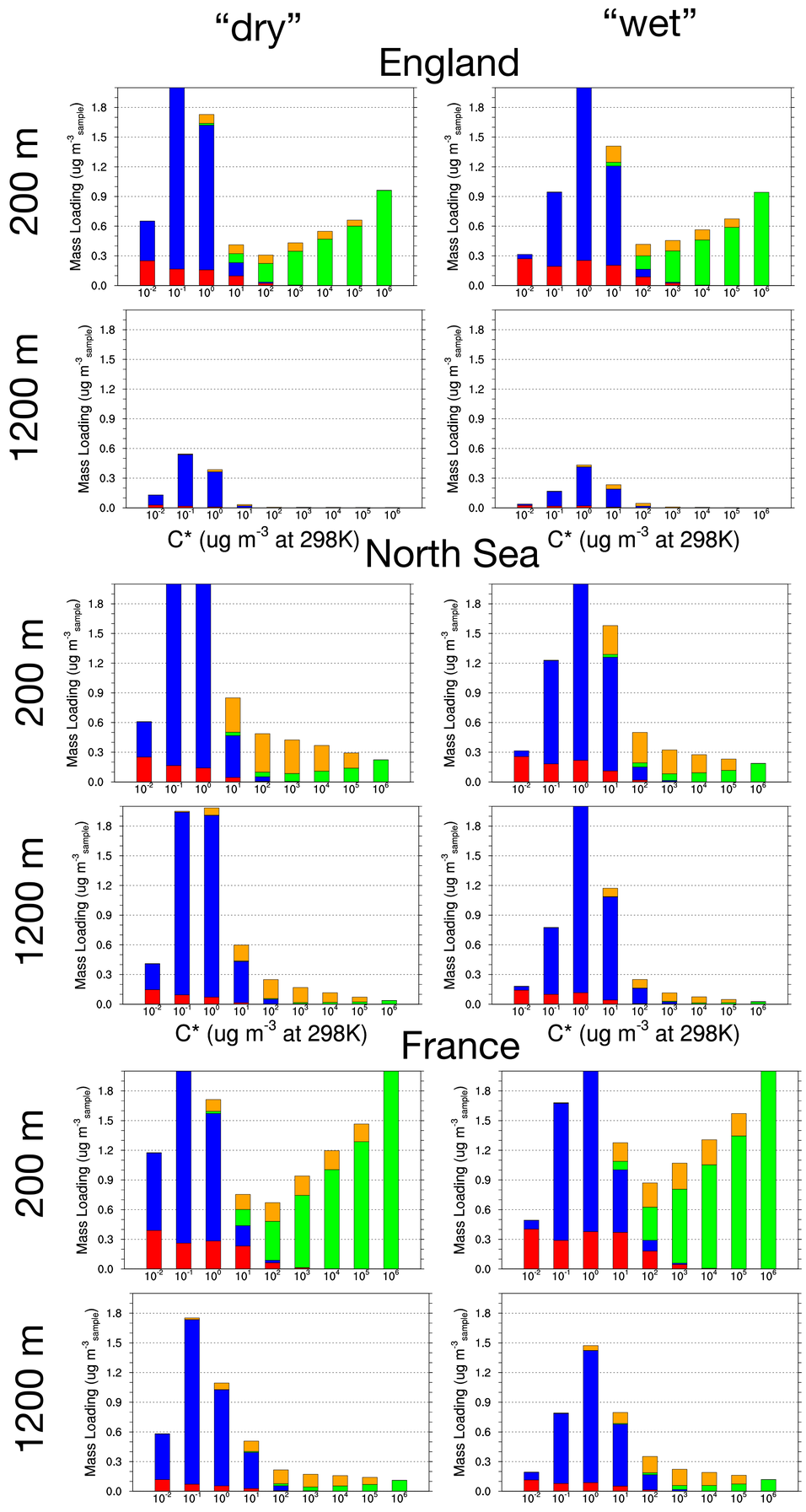
Model Configuration:

15 km grid spacing, 40 vertical model levels.
Meteorological inputs from ECMWF ERA-40 reanalysis.
Chemical boundaries from MOZART-4 and MACC models (no OM or VBS at boundaries for these simulations).
Emissions from combined NAEI and TNO databases.
Simulation period is 10th-21st July 2010 (plots for 0000z on 20th July 2010).

Scenarios:

"Dry" - standard VBS setup
"Wet" - water associated with organics used for VBS partitioning

Volatility Distributions



Conclusion

Including water association increases the absorptive mass of the organic aerosol - increasing the partitioning of VBS compounds into the condensed phase. This increases the condensed mass - principally close to source, as more high C* compounds are drawn into the condensed phase, but also in more remote regions of the model domain. It also stalls the gas-phase driven ageing of the VBS compounds, reducing the increase in O:C ratio due to this process.