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Title:	Case study of the diurnal variability of chemically active species with respect to boundary layer dynamics during DOMINO
Authors:	Sinha, V. (/jspui/browse?type=author&value=Sinha%2C+V.)
Keywords:	Atmospheric Chemistry Boundary Layer Chemical Reaction
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Citation:	Atmospheric Chemistry and Physics, 12 (12), pp. 5329-5341
Abstract:	We study the interactions between atmospheric boundary layer (ABL) dynamics and atmospheric chemistry using a mixed-layer model coupled to chemical reaction schemes. Guided by both atmospheric and chemical measurements obtained during the DOMINO (Diel Oxidant Mechanisms in relation to Nitrogen Oxides) campaign (2008), numerical experiments are performed to study the role of ABL dynamics and the accuracy of chemical schemes with different complexity: the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4) and a reduced mechanism of this chemical system. Both schemes produce satisfactory results, indicating that the reduced scheme is capable of reproducing the O ₃ -NO _x -VOC-HO _x diurnal cycle during conditions characterized by a low NO _x regime and small O ₃ tendencies (less than 1 ppb per hour). By focusing on the budget equations of chemical species in the mixed-layer model, we show that for species like O ₃ , NO and NO ₂ , the influence of entrainment and boundary layer growth is of the same order as chemical production/loss. This indicates that an accurate representation of ABL processes is crucial in understanding the diel cycle of chemical species. By comparing the time scales of chemical reactive species with the mixing time scale of turbulence, we propose a classification based on the Damköhler number to further determine the importance of dynamics on chemistry during field campaigns. Our findings advocate an integrated approach, simultaneously solving the ABL dynamics and chemical reactions, in order to obtain a better understanding of chemical pathways and processes and the interpretation of the results obtained during measurement campaigns.
Description:	Only IISER authors are available in the record.
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