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Evaluation of the pathways of tropospheric nitrophenol formation from benzene and phenol using a multiphase model

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Abstract. Phenols are a major class of volatile organic compounds (VOC) whose reaction within, and partitioning between, the gas and liquid phases affects their lifetime within the atmosphere, the local oxidising capacity, and the extent of production of nitrophenols, which are toxic chemicals. In this work, a zero-dimension box model was constructed to quantify the relative importance of different nitration pathways, and partitioning into the liquid phase, of mono-aromatic compounds in order to help elucidate the formation pathways of 2- and 4-nitrophenol in the troposphere. The liquid phase contributed significantly to the production of nitrophenols for liquid water content (L_c) values exceeding $3x10^{-9}$, and for a range of assumed liquid droplet diameter, even though the resultant equilibrium partitioning to the liquid phase was much lower. For example, in a "typical" model scenario, with $L_c=3x10^{-7}$, 58% of nitrophenol production occurred in the liquid phase but only 2% of nitrophenol remained there, i.e. a significant proportion of nitrophenol observed in the gas phase may actually be produced via the liquid phase. The importance of the liquid phase was enhanced at lower temperatures, by a factor ~1.5-2 at 278K c.f. 298K. The model showed that nitrophenol production was particularly sensitive to the values of the rate coefficients for the liquid phase reactions between phenol and OH or NO_3 reactions, but insensitive to the rate coefficient for the reaction between benzene and OH, thus identifying where further experimental data are required.

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