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# Model calculations about effects of regenerative fuels on air quality

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Photochemical model calculations were performed to investigate the effects of the use of bio-ethanol and bio-diesel on air quality. The mesoscale meteorological model MM5 v3.7.4 was used to prepare the input data for the Eulerian photochemical dispersion model CAMx. Two simulations, each of 31 days, comprising January and July 2007, were performed, with additional days in advance to allow the model spin up. The simulations were conducted using five nested domains with horizontal grid resolutions from 64.8 to 0.8 km. The innermost domain spans 70.4 x 70.4 km in north-south and east-west direction and covers Vienna and its surroundings.
The Comprehensive Air quality Model with eXtensions (CAMx) v5.20 was used to calculate the photochemistry. The chemistry mechanism invoked was the SAPRC99 mechanism, which includes 217 reactions - 30 of which are photolytic - and 111 species (74 state gases, 21 state particulates and 16 radicals). The spatial resolution of the nested CAMx model grids was the same as in the MM5 calculations, with slightly smaller domain sizes, allowing "buffer cells" around the chemical grids. For both episodes, a reference run with present day emissions gave a reasonable agreement with available air quality measurements.
In a scenario calculation, assuming a substitution of fossil fuel for traffic with bio-ethanol, it was expected, that changes of the exhaust composition of vehicles with respect to the hydrocarbons have an impact on ozone in summer. However, since ozone production in northeast Austria is mainly nitrogen-oxide-controlled, only small changes in comparison to the reference calculation were observed. Nevertheless, changes in other compounds as an increase of the concentration of acetaldehyd might lead to a negative impact on health.
In the case of bio-diesel use, a reduction in the emission of particulate matter was assumed. In parallel, the scenario included the transition to modern exhaust treatment in diesel cars, which implies an increase of the NO2 partition in the nitrogen oxides emission. In particular in the vicinity of major traffic routes, an increase of the NO2 concentration was observed, due to the fine spatial resolution of the model. This increase might counteract the benefit of reduced aerosol concentrations on health in the scenario run. In some regions the enhanced formation of secondary nitrate aerosol also substitutes the reduction of primary aerosol.