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Representing isoprene epoxydiols derived secondary organic aerosol (IEPOX-SOA) in chemistry climate models: comparing explicit, simplified and empirical approaches

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Isoprene is the most abundant non-methane volatile organic compound in the atmosphere that substantially contributes to secondary organic aerosol (SOA) concentrations globally. Here we compare modeling approaches of various complexity that are used to represent the isoprene epoxydiols derived SOA (IEPOX-SOA) which is observed to be the dominate fraction of total isoprene SOA. Empirical SOA schemes such as two-product and volatility basis set (VBS) approaches, are the most commonly used approaches, although they do not account for the IEPOX-SOA dependency on aerosol acidity and its water content, which are critical factors for its formation rate. A fully explicit modelling of isoprene SOA chemistry has been applied in some studies but remains computationally expensive owing to the many species and reactions included, which makes it difficult to use for long-term chemistry climate simulations. We have developed an additional simplified parameterization for IEPOX-SOA, based on an approximate analytical solution of the relevant portion of the isoprene chemical mechanism. The new parameterization can retain the key physico-chemical dependencies of the full mechanism, by directly calculating the IEPOX-SOA yield and formation timescale using the current model fields of oxidant concentrations, NO, aerosol acidity and other key properties. We use the GEOS-Chem v11-02-rc global model to intercompare the new simplified parameterization, the two empirical treatments for isoprene SOA (the VBS approach and a fixed 3% yield parameterization), and the detailed full chemistry. The simplified parameterization captures the global tropospheric burden of IEPOX-SOA and its spatio-temporal distribution vs. those simulated by the full chemistry, while the constant 3% yield and VBS deviate strongly. Evaluation results for various schemes against global AMS measurements and implications on the future isoprene SOA predictions are also discussed.