# A global modeling study of biofuel-derived butanol emissions using the chemistry transport model, STOCHEM-CRI

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Research into $C_3$ and longer chain alcohols, such as butanol, as potential biofuels and/or fuel additives has become prevalent in recent years. There are many advantages over ethanol-derived biofuels. For example, butanols have energy densities and chemical structures which are much closer to the components found in gasoline, thus overcoming the miscibility issues associated with ethanol-based biofuels. They are also less hygroscopic, less volatile and less corrosive than ethanol, meaning that, as fuels, they can be shipped and distributed through existing infrastructure.

Producing and using butanol as a fuel will lead to its direct emission into the atmosphere, via incomplete combustion or leakage and evaporation, hence an understanding of the atmospheric processing and environmental impact is essential. Once emitted, butanol is predominantly removed from the atmosphere via reaction with the OH radical, which is a highly site-specific process. This means that each of the four butanol isomers lead to the formation of many different stable end product(s), thus meaning that the atmospheric impact of butanol will depend on the site at which the reaction takes place. A laboratory study by McGillen at al.[1] investigated the removal of the butanol isomers under atmospheric conditions, deducing the branching ratios and dominant reaction pathways associated with the OH radical initiated degradation.

This work applies the kinetic and product data from McGillen et al.[1] to the global chemistry transport model, STOCHEM-CRI, in order to simulate the atmospheric impacts associated with the global-scale use of butanol as a biofuel. This was initially achieved by running model simulations with original stable end-product branching ratios. Channel sensitivity simulations were then integrated, whereby the model assumed that the reaction of OH with butanol proceeds via one reaction pathway, in order to investigate the importance of the stable end product(s) in terms of atmospheric composition and oxidising capacity. It is found that for n-butanol in particular, the product branching ratios selected make a non-negligible difference to the local oxidising capacity.

[1]McGillen, M.R., Baasandorj, M. and J.B. Burkholder (2013), *Gas-Phase Rate Coefficients for the OH plus n-, i-, s-, and t-Butanol Reactions Measured Between 220 and 380 K: Non-Arrhenius Behavior and Site-Specific Reactivity*, J. Phys. Chem. A, 117(2), 4636-4656