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The Master Chemical Mechanism (MCM) – Updates and Improvements

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The Master Chemical Mechanism (MCM) is a near-explicit chemical mechanism describing the detailed gas phase tropospheric degradation of a series of primary emitted volatile organic compounds (VOCs). The mechanism is constructed according to a set of rules as defined in the latest mechanism development protocols (Saunders et al., *Atmos. Chem. Phys*., **3**, 161-180, 2003 and Jenkin et al., *Atmos. Chem. Phys.*, **3**, 181-193, 2003). Rate constants and product channel branching ratios are taken from the latest experimental data or are estimated from structure activity relationships (SARs). Some strategic simplifications are applied in order to limit the number of reactions but retain the essential elements of the chemistry. The latest version of the MCM, MCMv3.1 is available on the new MCM website: **http://mcm.leeds.ac.uk/MCM/**. MCMv3.1 contains 135 primary emitted VOCs which lead to a mechanism containing *ca.* 5900 species and 13500 reactions.

The primary objective of the new MCM website is to make navigation around the MCM clearer and easier for the user. The website has three main self-explanatory functions; **Browse**, **Search** and **Extract**. A permanently displayed **Mark List** effectively acts as a "shopping basket" for collecting species of interest as you browse the MCM for mechanism extraction. The **Browse** facility enables the user to look through the MCM by category where the species names now have structures associated with them. The **Search** function allows the user to search the MCM either by SMILES string notation or by the unique MCM species name. The new **Extract** utility can ex-

tract subset mechanisms from the MCM for the species listed in the **Mark List** in various formats including FACSIMILE, KPP, FORTRAN, and XML, therefore making the MCM more accessible to an increasingly wide range of modellers.

Current and future developments/improvements of the MCM focus on some of the more fundamental aspects of the mechanism. The MCM is being extended for free tropospheric conditions. The protocols are to be revised in line with recent experimental data and new SARs developed. Certain reactions ($e.g.$ oxy radical reactions) are not adequately parameterised for the upper troposphere and will be re-examined.