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Building tailored chemistry sets for plasma modelling using a statistical approach embedded in an online engine. JONATHAN TENNYSON, MALA VIRDEE, MARTIN HANICNEC, University College London, SEBASTIAN MOHR, Quantemol Ltd — The Quantemol Plasma Chemistry Generator (QPCG) helps explore the vast number of potential chemical species and reactions present in plasma systems. Critical to the understanding and development of complex plasmas is the identification of important chemical species and reactions present, often a resource and time intensive endeavour. QPCG suggests chemical species, important reactions and cross-section data for a given mixture of feed gases, helping researchers to curate self-consistent sets of chemical reactions that are specific to the system of interest. First, constituent plasma species are obtained from the Quantemol Database (QDB, Tennyson et al, Plasma Sources Sci. Technol. (2017) 055014) based on the composition of the feed gases. Potential reactants and products for a hypothetical reaction are combined iteratively from these species to form sets of allowed chemical reactions. Classification of these reactions into different process types, using models of reactions already available in QDB, facilitates selection of important reactions based upon process parameters. Finally, rate coefficients and/or cross sections are obtained from QDB, where available, or by analogy with similar reactions. By reducing the time needed to assemble a chemistry set, QPCG provides quick fundamental insights into plasma chemistries, accelerating the development and optimisation of new plasma systems and their applications. Examples of generated chemistry sets will be presented.

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