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A FAST, ULTRACONDENSED CARBON BOND IV PHOTOCHEMICAL MECHANISM FOR APPLICATION IN REGIONAL AIR QUALITY MANAGEMENT MODELS

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This paper reports the development of an ultra-condensed photochemical mechanism that may be used to model rapidly the consumption of mixtures of volatile organic precursor (VOC) compounds and the formation of photochemical oxidants such as ozone. The mechanism is based on the Carbon-Bond IV mechanism and comprises 22 lumped species and 34 reactions. The mechanism produces very similar results to the Carbon-Bond IV mechanism but requires less than one-thirtieth of the computation time. This computational speed is similar to that of the GRS1 mechanism, but the new mechanism has significant advantages in that it appears to be more representative than GRS1 and also models VOC consumption. A representative mixture of VOC precursors was modelled using the ultra-condensed mechanism, the CBIV-99 mechanism and the GRS1 mechanism. Diurnal profiles of temperature and radiation at the summer solstice for Brisbane, Australia, were used to calculate photolysis rate coefficients. The new mechanism provides very similar results to the CBIV mechanism for ozone and other species, while the GRS1 mechanism predicts ozone concentrations that increase too rapidly and rise too far. The rapid speed and the accuracy of the mechanism make it suitable for combination with transport models such as TAPM for use in the development of regional air quality management strategies. The ability to model the consumption of VOC allows for the estimation of secondary organic aerosol (SOA) formation using standard methodologies.