# A comprehensive two-scale model for predicting the oxidability of fatty ester mixtures

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The intricate mechanisms of oil thermo-oxidation and their accurate prediction have long been hampered by the combinatory nature of propagation and termination reactions involving randomly generated radicals. To unravel this complexity, we suggest a two-scale mechanistic description that connects the chemical functions (scale 1) with the molecular carriers of these functions (scale 2). Our method underscores the importance of accounting for cross-reactions between radicals in order to fully comprehend the reactivities in blends. We rigorously tested and validated the proposed two-scale scheme on binary and ternary mixtures of fatty acid methyl esters (FAMEs), yielding three key insights: (1) The abstraction of labile protons hinges on the carrier, defying the conventional focus on hydroperoxyl radical types. (2) Termination reactions between radicals adhere to the geometric mean law, exhibiting symmetric collision ratios. (3) The decomposition of hydroperoxides emerges as a monomolecular process above 80°C, challenging the established combinatorial paradigm. Applicable across a wide temperature range (80°C to 200°C), our findings unlock the production of blends with controlled thermo-oxidation stability, optimizing the use of edible oils across applications: food science, biofuels, and lubricants.