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# A mechanistic model for simulating position-specific carbon isotopic compositions of thermogenic propane and precursors

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Position specific isotope analysis (PSIA) of thermogenic propane provides a valuable tool to investigate propane's origin, fate, and mechanisms of formation[1]. However, understanding the link between the observed carbon PSIA signals of propane and the associated underlying mechanisms still requires a more sophisticated model. Our study developed a mathematical framework to simulate position specific carbon isotopologues of propane and its precursors based on their bond-cleavage reaction pathways[2]. The model allows integrating multiple signals, including temperature, and isotopic signatures of mother compounds, and is validated by precisely reproducing the experimental PSIA data obtained during cracking of different kerogens. Also, the initial carbon isotopic signatures as well as the initial fraction of two possible mother compounds in kerogen are determined. Thus, our model serves as a novel tool for quantitive and mechanistic analysis of PSIA signals of thermogenic propane to investigate fate of propane in subsurface.

[1] Zhang, Li, Jiang & Xiong (2022). **166**: 104379.

[2] Jin & Peng (2024), The Innovation Geoscience **2**(1): 100054.