

Detailed kinetic study of anisole pyrolysis and oxidation for understanding tar formation during biomass combustion and gasification

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Supplementary material

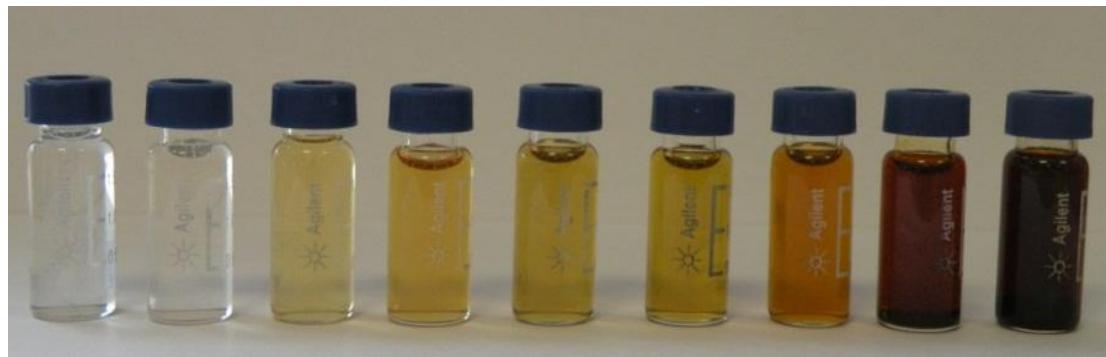


Figure S1. Solution recovered from condensers after the pyrolysis of anisole from 773 K to 1173 K (each 50 K) illustrating tar maturation. Samples collected by quenching of heavy products in liquid nitrogen and diluted after warming in acetone.

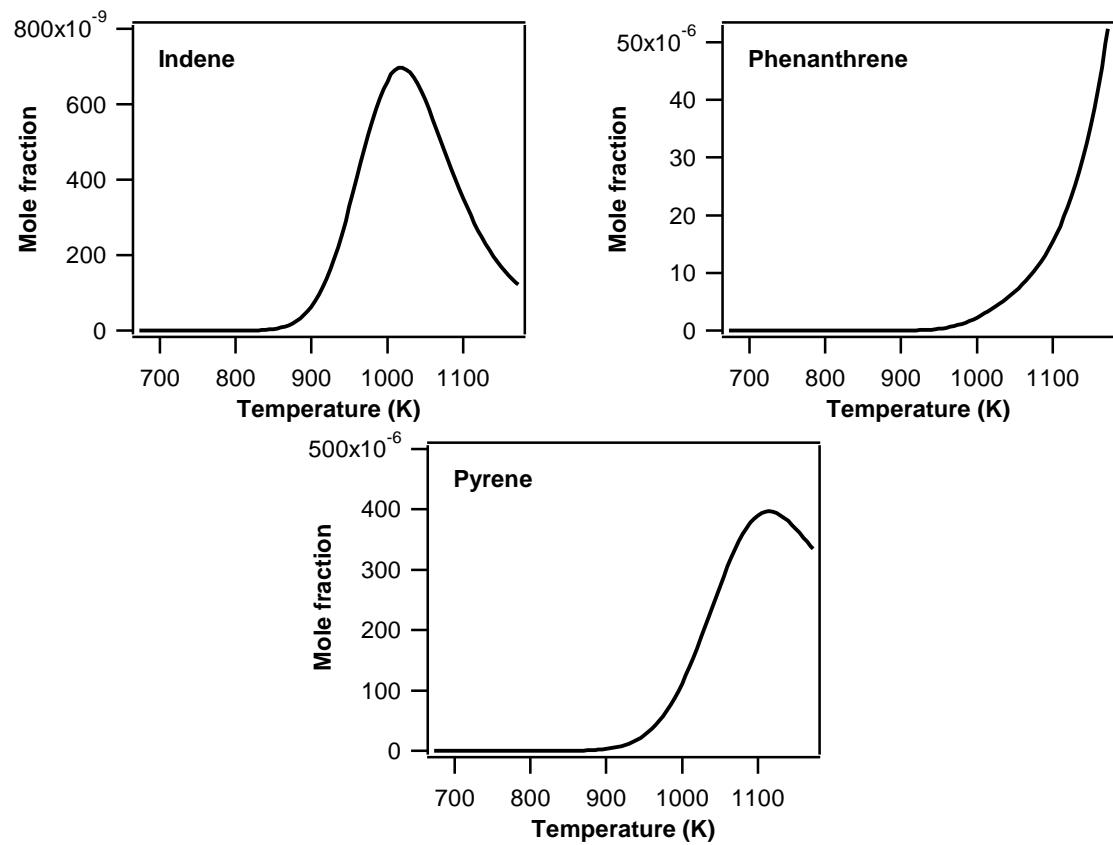


Figure S2 Anisole pyrolysis: simulated evolution of the mole fraction of some polycyclic at residence time 2sec and pressure 800 Torr.

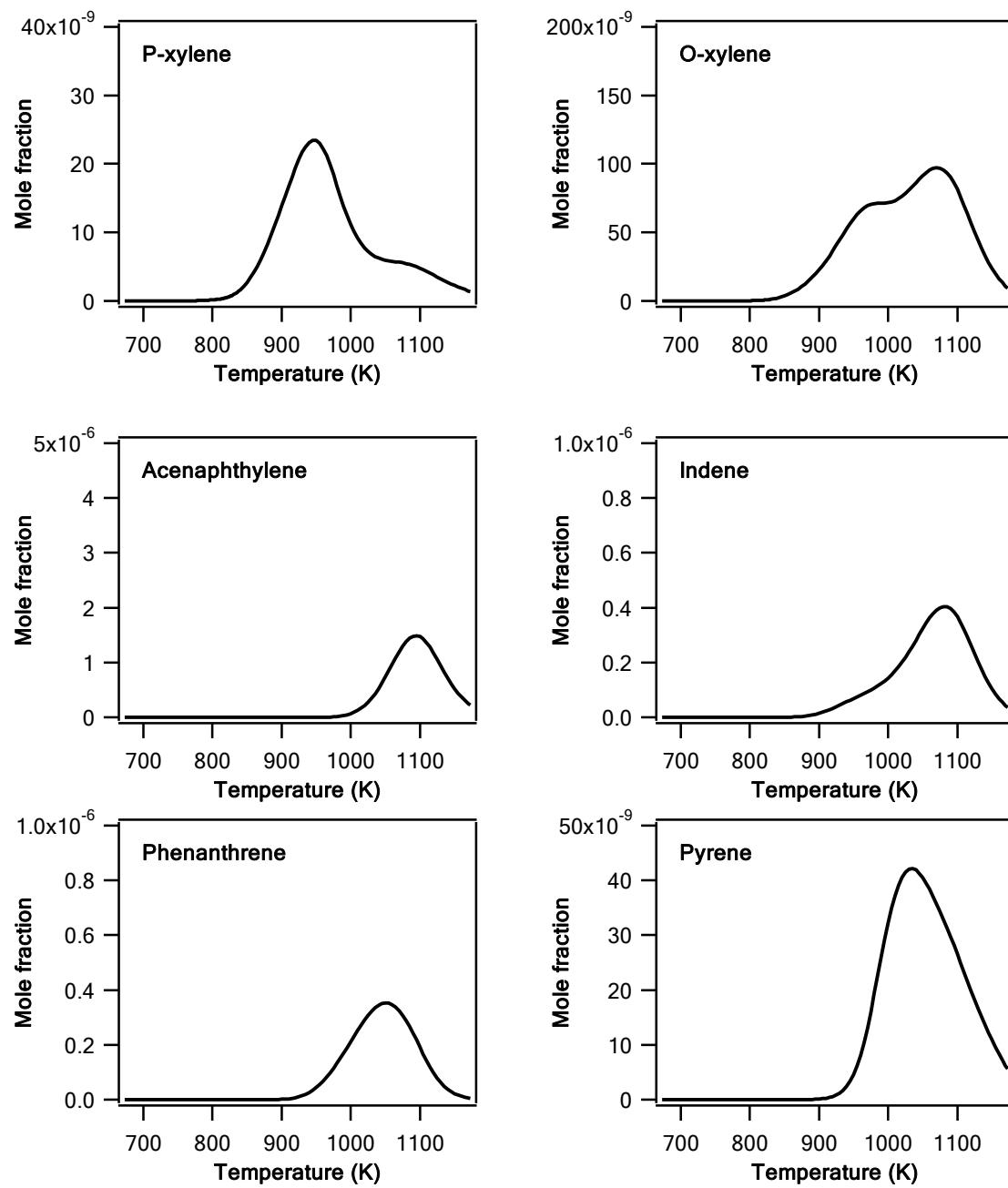


Figure S3 Anisole oxidation: evolution of the mole fraction of some aromatic and polycyclic species at residence time 2sec and pressure 800 Torr.

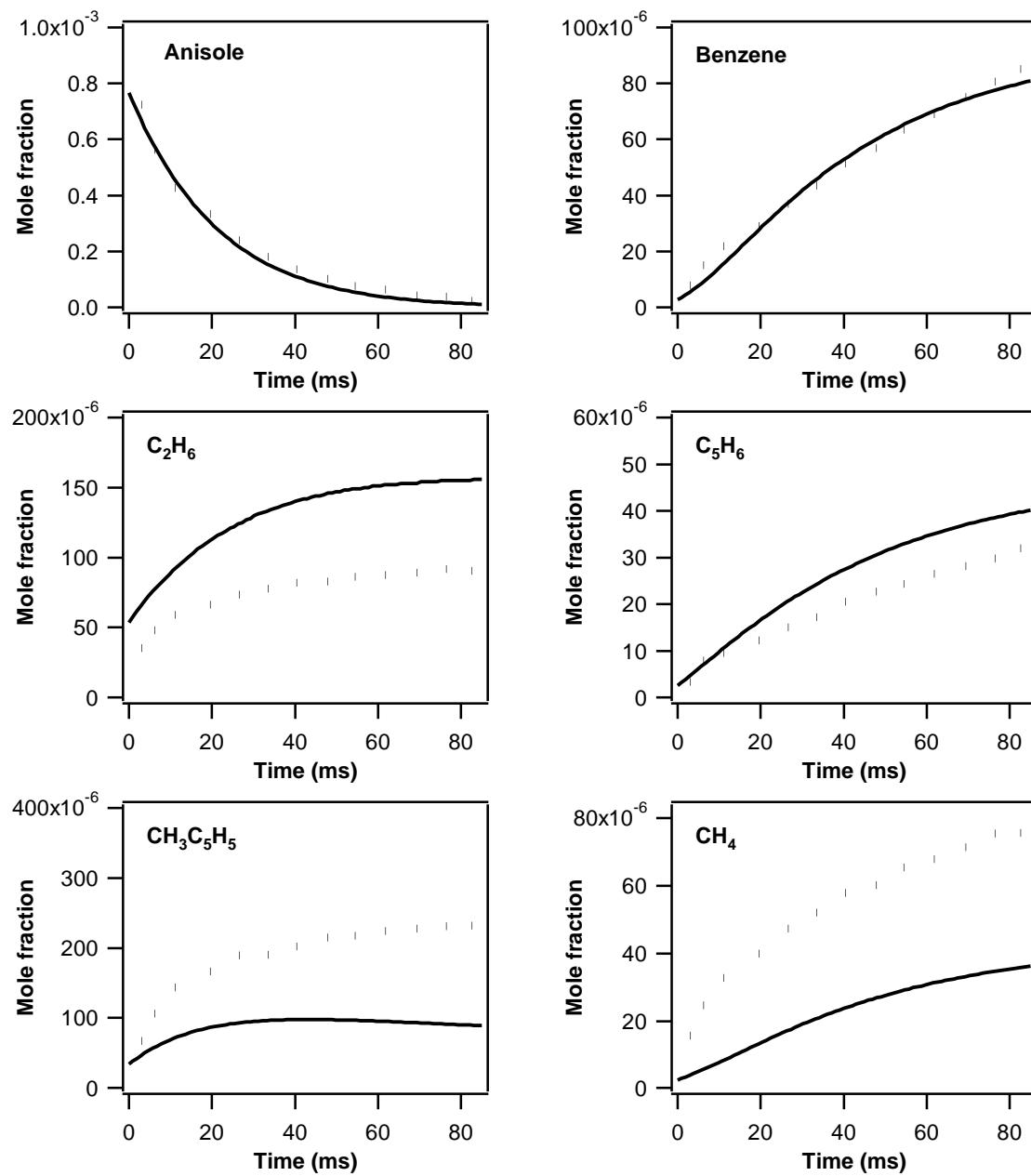


Figure S4 Anisole pyrolysis : measured pyrolysis products from the Pecullan et al. [18] study with comparison to predictions of proposed kinetic model. $X_{\text{anisole}} = 1077 \text{ ppm}$, $T = 1003 \text{ K}$, $P = 1 \text{ atm}$.

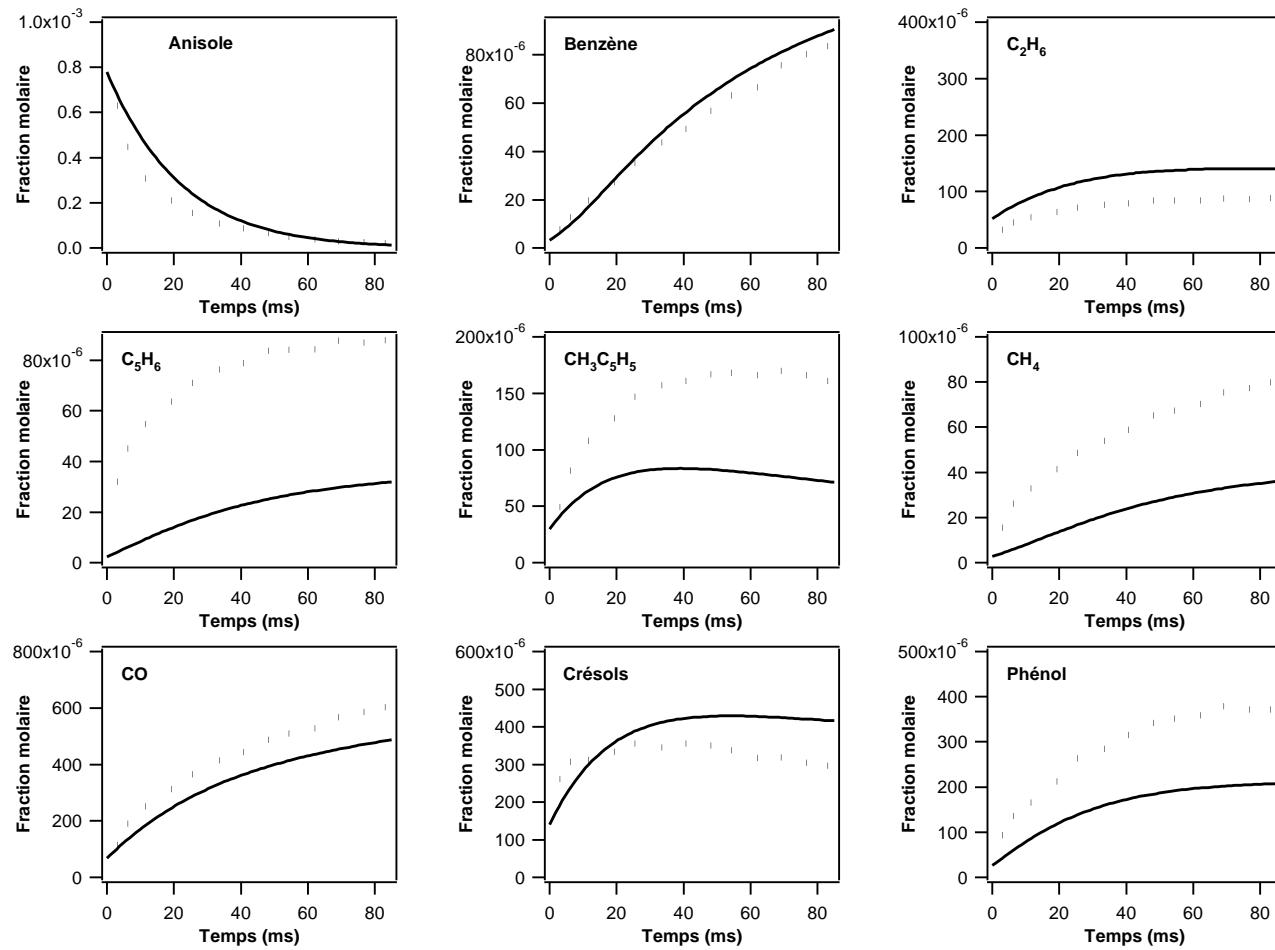


Figure S5 Anisole oxidation : measured products from the Pecullan et al. [18] study with comparison to predictions of proposed kinetic model. $X_{\text{anisole}} = 1079 \text{ ppm}$, $T = 1001 \text{ K}$, $P = 1 \text{ atm}$, $\phi = 1.05$.

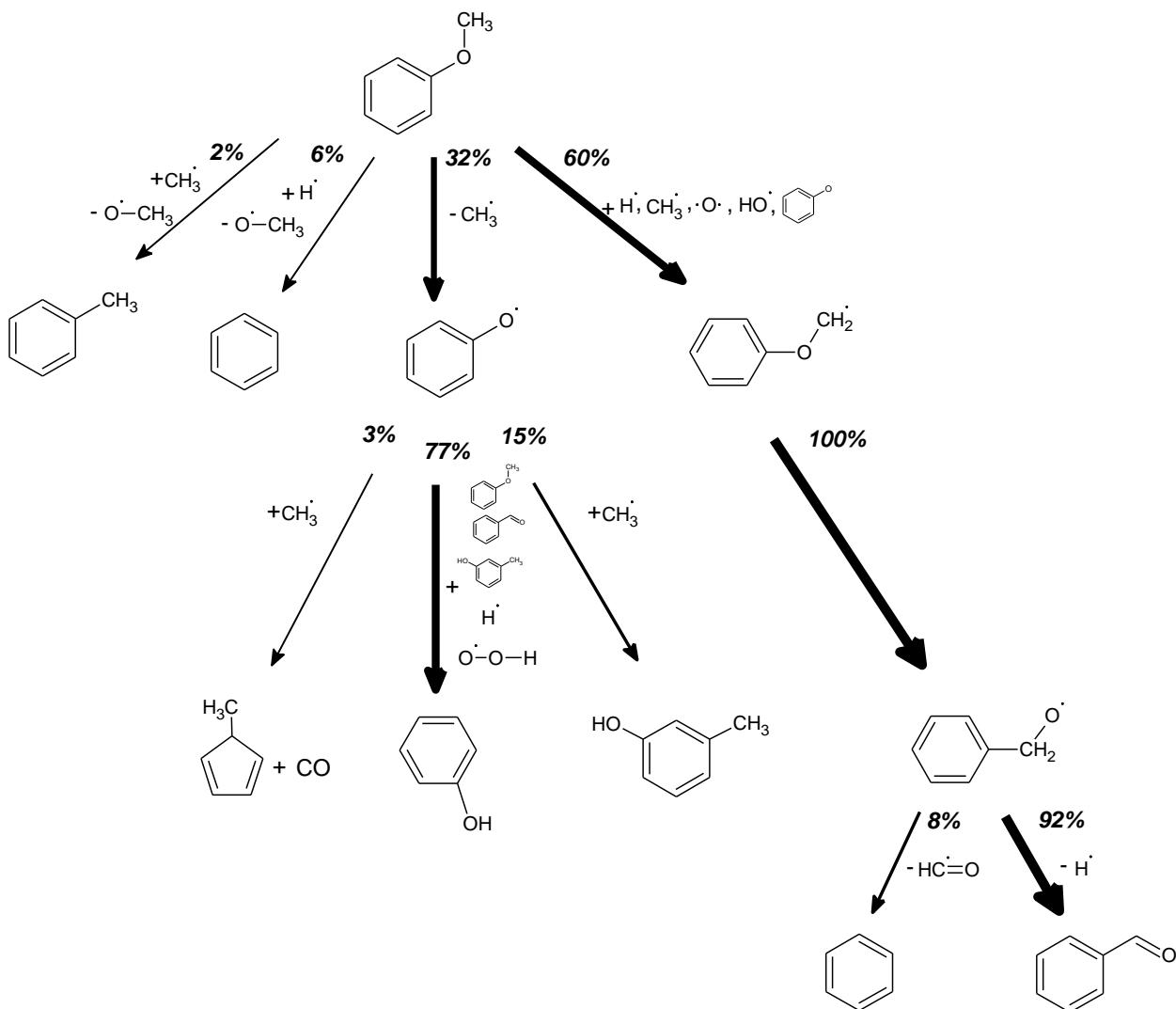


Figure S6 Reaction flux analysis for anisole oxidation. Conditions: 800 K, 800 Torr, residence time of 2 s corresponding to 16.8% anisole conversion. Given reaction fluxes (numbers associated with arrows) are relative to the consumption of a given species.

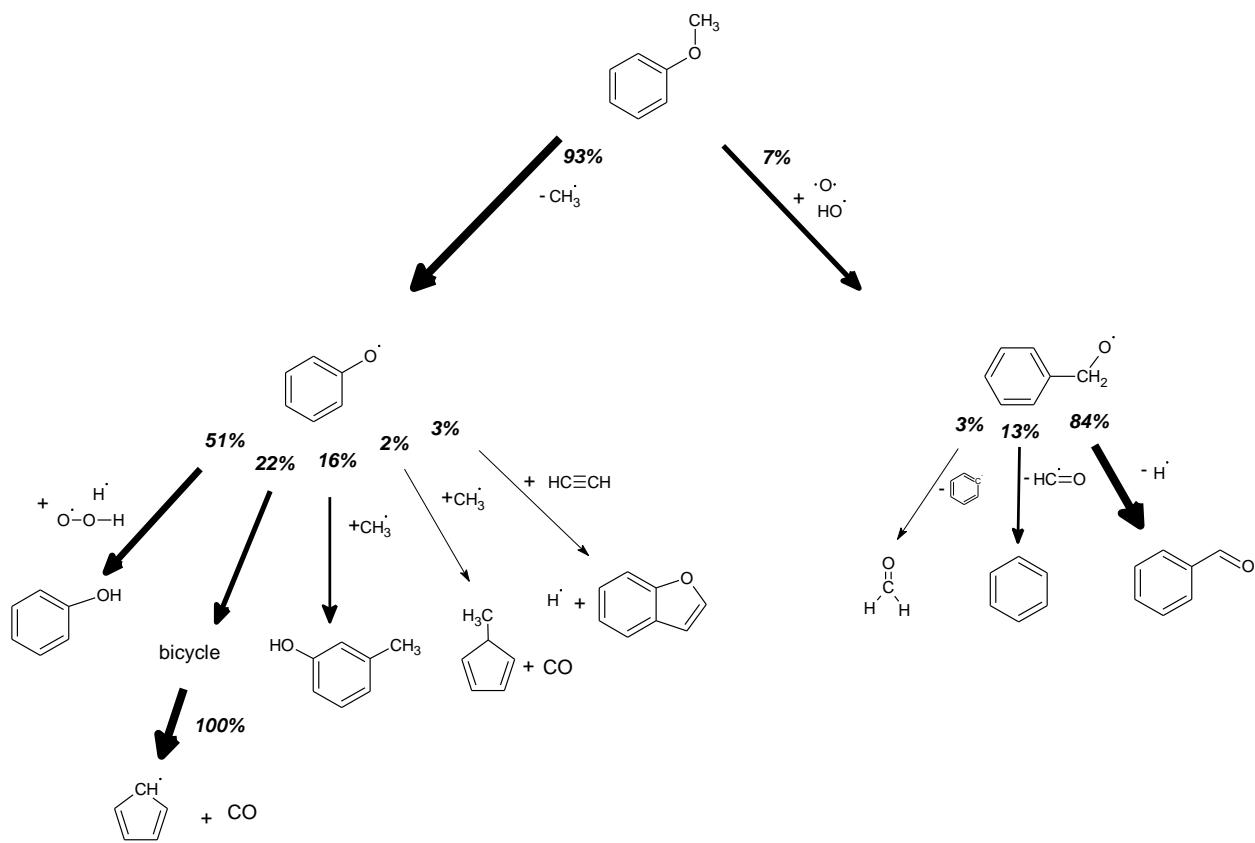


Figure S7 Reaction flux analysis for anisole oxidation. Conditions: 1000 K, 800 Torr, residence time of 2 s corresponding to 99.9% anisole conversion. Given reaction fluxes (numbers associated with arrows) are relative to the consumption of a given species.

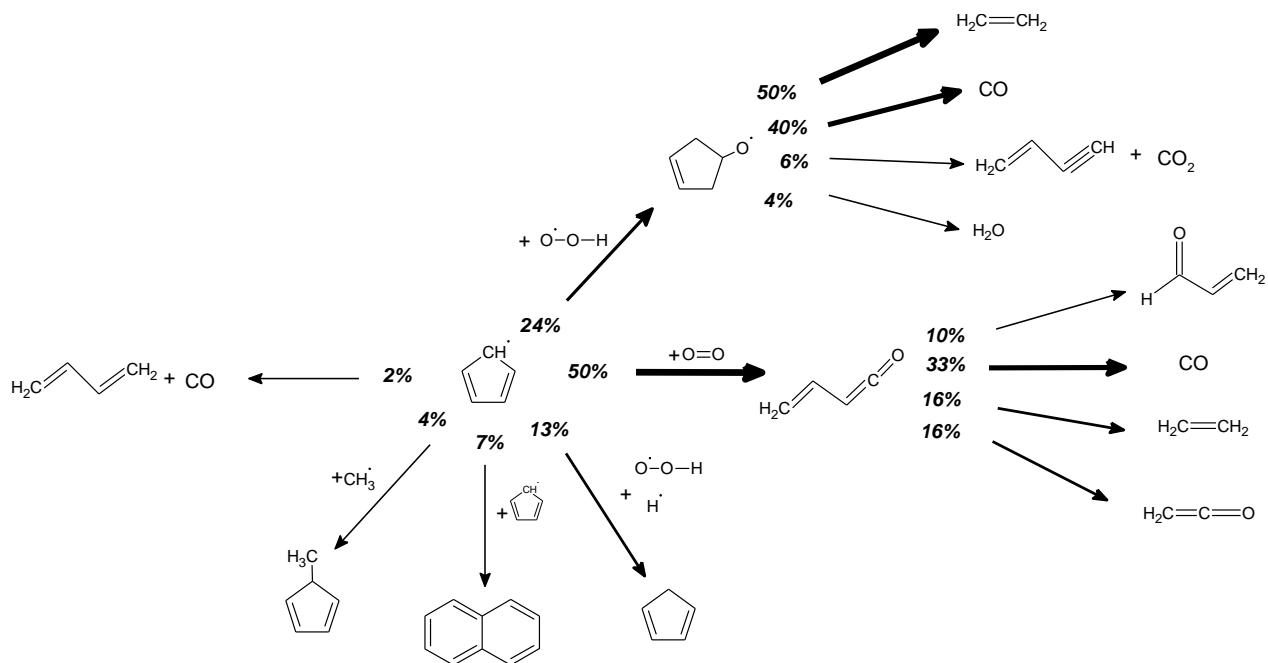


Figure S8 Reaction flux analysis for cyclopentadienyl oxidation (continuation of figure S7) Conditions: 1000 K, 800 Torr, residence time of 2 s corresponding to 99.9 % anisole conversion. Given reaction fluxes (numbers associated with arrows) are relative to the consumption of a given species.