

Non-Steady State Validation of Kinetic Models for Ethylene Epoxidation over Silver Catalysts

Lilliana Brandão¹ and Christian Reece^{1*}

1. Rowland Institute at Harvard, Harvard University, Cambridge, Massachusetts 02142, United States

*Corresponding author: christianreece@fas.harvard.edu

Supplementary Information

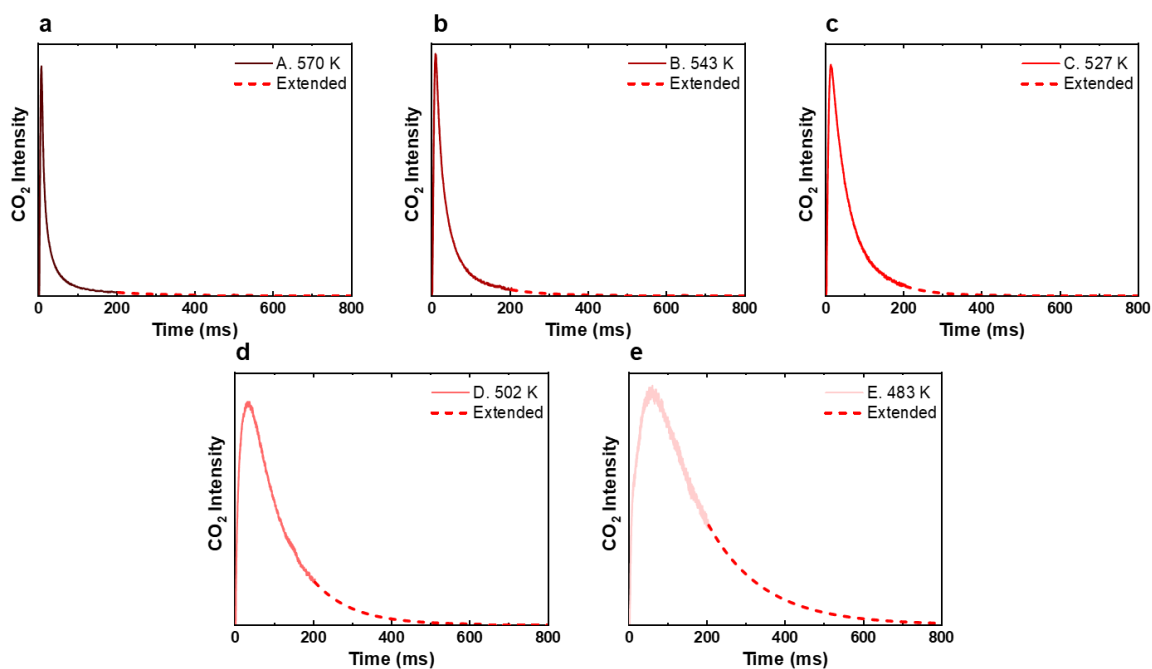


Figure S1. Extrapolated CO₂ response curves from the Gleaves-Madix experiment¹ where the tail of the curve is expanded to 1000 ms using a single exponential function fit to tail of the curve from 120 – 200 ms.² Experimental data was adapted from ref.¹

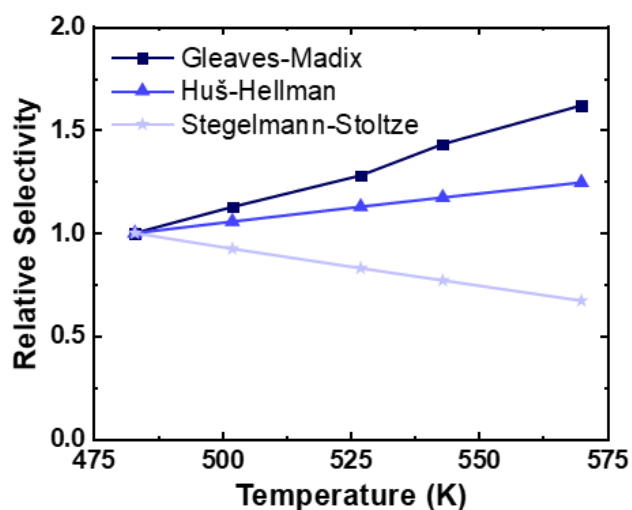


Figure S2. Experimental and simulated relative selectivity (normalised to 483 K) for the single-pulse experiments in which ethylene and O₂ were pulsed over the clean catalyst at varying temperatures from 483 – 570 K. Experimental data was adapted from ref.¹

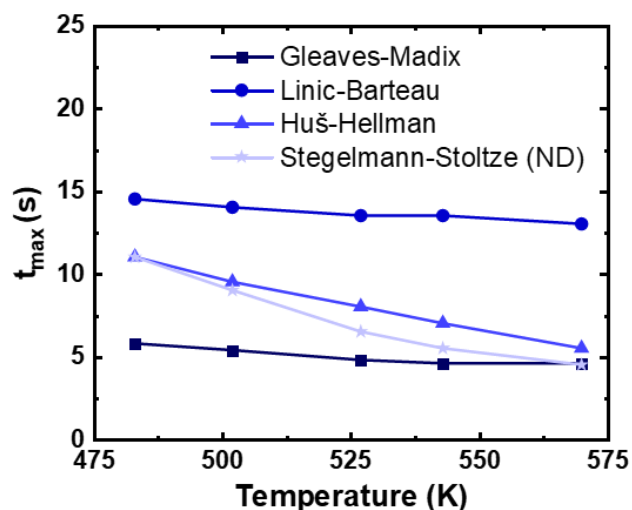


Figure S3. Experimental and simulated time of maximum ethylene oxide production (t_{\max}) as a function of temperature for the simulations with the Stegelmann-Stoltze model modified to turn off oxygen desorption (ND). Experimental data was adapted from ref.¹

References

- 1 J. T. Gleaves, A. G. Sault, R. J. Madix and J. R. Ebner, *Journal of Catalysis*, 1990, **121**, 202–218.

2K. Morgan, A. Goguet, C. Hardacre, E. V. Kondratenko, C. McManus and S. O. Shekhtman, *Catalysis Science and Technology*, 2014, **4**, 3665–3671.