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INTRODUCING A WORKFLOW FOR IMPROVING KINETIC MODELS: A CASE STUDY USING BUTANOL

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Side-by-side comparison of detailed kinetic models using a new tool to aid recognition of species structures reveals significant discrepancies in the published rates of many reactions and thermochemistry of many species. We demonstrate a new workflow that uses a combination of experimental data, data-science methods, and critical appraisal, to bring detailed kinetic models of combustion chemistry closer to the "truth". A recent kinetic model for the isomers of butanol was imported into a common database, along with parameters from over seventy other kinetic models from recent combustion literature. Individual reaction rate and thermodynamic parameters of species were varied using values encountered in the literature. We identify over 1600 conflicting parameters in other published kinetic models, rank them according to their impact on ignition delay times, then resolve the most important discrepancies by performing literature evaluations. The updated model is tested against a range of experimental data using the automated PyTeCK framework.