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A CHEMICAL KINETIC MECHANISM FOR THE COMBUSTION OF GASOLINE SURROGATE/ETHANOL/N-BUTANOL BLENDS

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Abstract. The use of gasoline/ethanol/n-butanol (GEB) blends in engines has been investigated intensively in the last decade. Ethanol has been used mainly in Brazil and the United States in fuel-flexible engines for several decades, as a blending agent to gasoline or used alone as a biofuel. In the near future, n-butanol could be also used in these blends given that its combustion properties are closer to those of gasoline than ethanol. The objective of the present work is to develop and validate a kinetic model for GEB blends by merging two kinetic models from the literature. The approach consists of carefully analyzing the common reaction packages in both kinetic models, so that the resulting merged model gives a good prediction of the ignition delay time and the laminar flame speed (LFS). The combined model is validated by performing numerical simulations of the combustion of gasoline/air, ethanol/air, n-butanol/air, and GEB/air in 0-D constant-volume auto-ignition and 1-D freely-propagating gaseous premixed flame configurations. Results are compared to those obtained using the original kinetic models as well as available experimental data from the literature. Finally, to evaluate the model performance, the LFS sensitivity analysis for the reaction rate constants is presented to identify important reaction pathways for the studied fuel blends.