Autoigniton of *n*-Butanol at Elevated Pressure and Low to Intermediate Temperature

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Introduction and Objectives:

- *n*-Butanol is a second generation biofuel that shows promise to replace other biofuels such as ethanol
- *n*-Butanol can be produced sustainably from waste products, can be distributed in currently existing infrastructure, and has a higher energy content than ethanol
- Although work is rapidly accumulating on *n*-butanol combustion, little has been done at high pressure and low to intermediate temperature
- Goal is to provide validation data using a heated rapid compression machine at high pressure and low to intermediate temperature

Rapid Compression Machine:

- Single, retractable, piston
- Piston is pneumatically driven and hydraulically stopped
- Piston is machined with crevices to control the roll-up vortex effect
- Pressure and temperature from TDC reported as compressed conditions
- The RCM has the ability to vary compressed temperature and compressed pressure independently

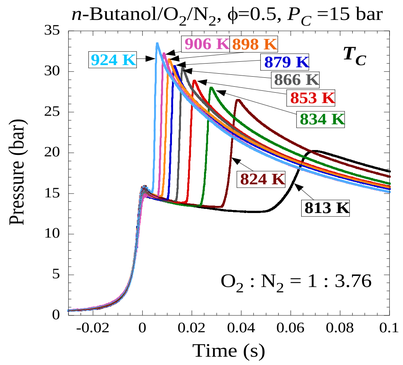
Experimental Conditions:

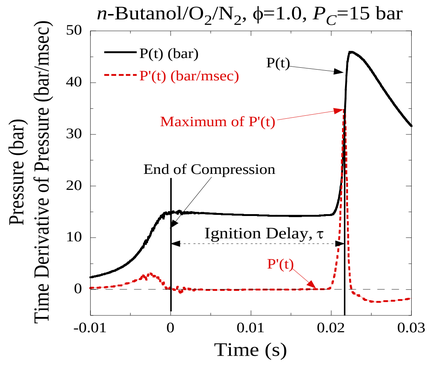
- Compressed Temperature Range: 675-925 K
- Fuel loading conditions are chosen to cover ranges not explored previously
- Fuel and oxygen concentrations are varied independently to reveal the effect of each on ignition delay

Mole Percentage (%)				
n-Butanol	**O_2**	**N_2**	**ϕ**	**P_C (bar)**
3.38	20.30	76.32	1.0	15
3.38	20.30	76.32	1.0	30
1.72	20.65	77.63	0.5	15
6.54	19.63	73.82	2.0	15
3.38	40.60	56.02	0.5	15
3.38	10.15	86.46	2.0	15
1.69	20.30	78.01	0.5	15
6.76	20.30	72.94	2.0	15

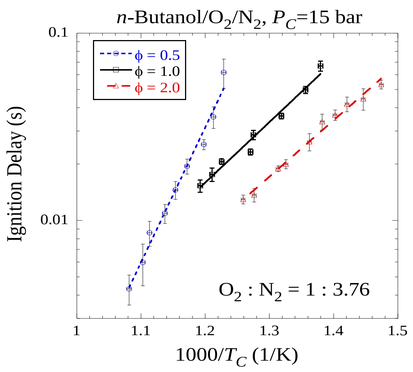
Experimental Results:

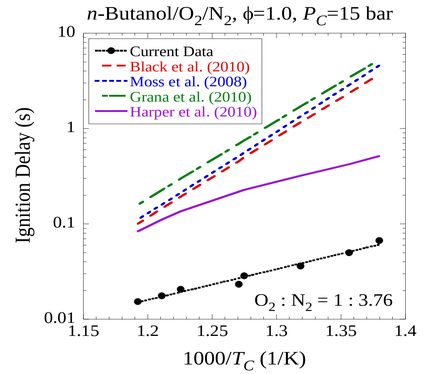
- Ignition is defined by the local maximum of the derivative
- No negative temperature coefficient region or two stage ignition observed for any of the conditions studied here





- Ignition delay is dependent on equivalence ratio
- Lower equivalence ratios are less reactive in the temperature range studied here
- Data appear to intersect around 850-900 K – this indicates that dependence on equivalence ratio may change in different temperature ranges
- Simulations using mechanisms available in the literature severely over-predict the ignition delay





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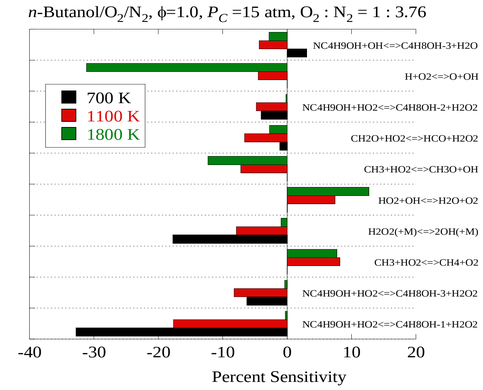
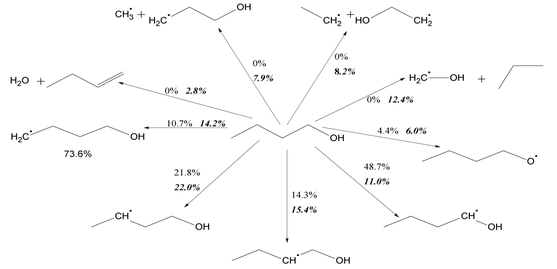
Modeling Results:

- Brute force sensitivity analysis of ignition delay to reaction rates is conducted on the mechanism from Black et al. (2010)
- The most sensitive reaction at low temperature is H-abstraction from *n*-butanol by HO_2 to form α-hydroxybutyl

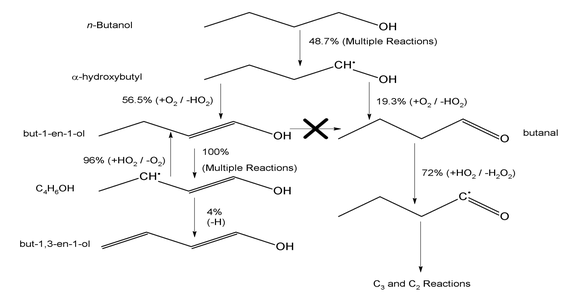


- Reaction path analysis of the mechanism from Black et al. (2010) reveals several important fuel decomposition pathways
- The most important pathway at low temperature is the formation of α -hydroxybutyl, in agreement with the sensitivity analysis



Reaction path analysis of the mechanism by Black et al. using constant volume, adiabatic simulations at initial conditions 15 atm, ϕ=1.0 and 800 K (plain text) and 1600 K (bold, italic text)

- Several fuel decomposition pathways have been reported in the literature (Zhang and Boehman (2010)), but are missing from the mechanism by Black et al. (2010)
- These missing pathways, or other pathways which are using incorrect estimates for reaction rates, may be causing the discrepancy between experimental results and simulations



Extension of the previous reaction path analysis at 800 K, 15 atm, and ϕ=1.0. The X indicates that pathway is not present

References:
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