Supporting Information

Process Safety Considerations for the Use of 1 M Borane Tetrahydrofuran Complex Under General Purpose Plant Conditions

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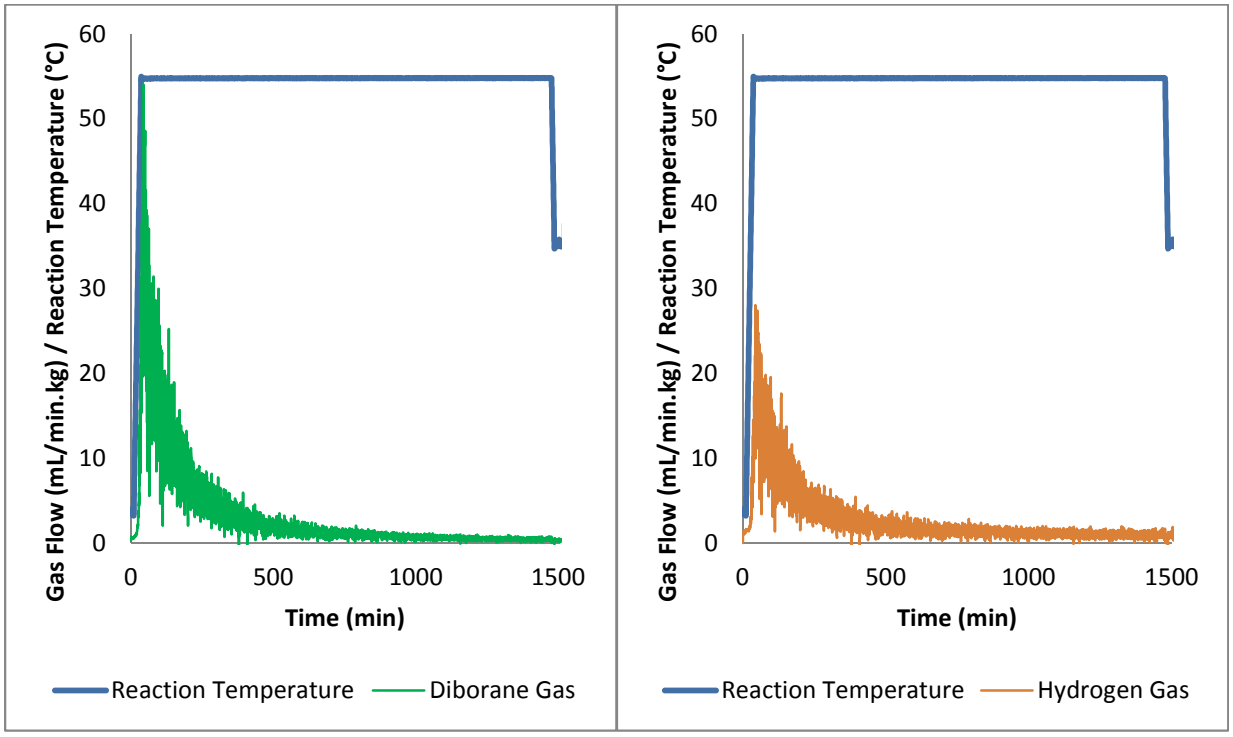
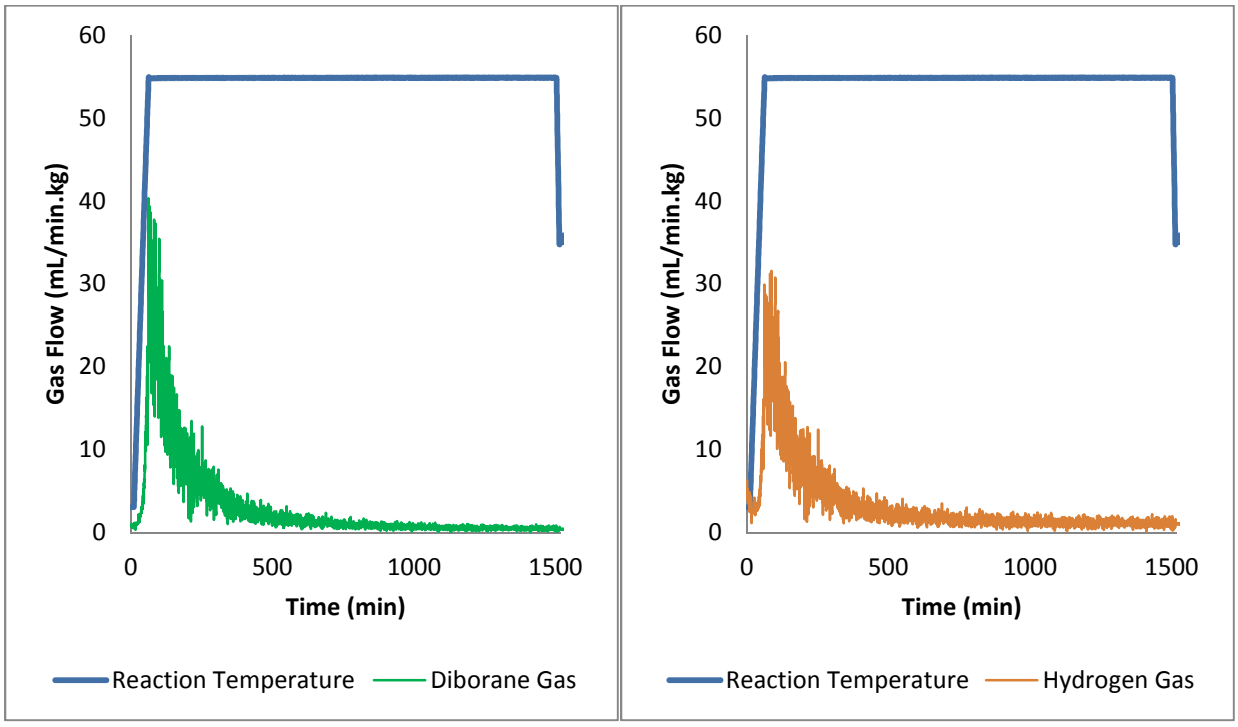
Headspace mass spectroscopy traces for BTHF aging studies

Note: Gas flow data normalized to the amount of fresh BTHF charged.

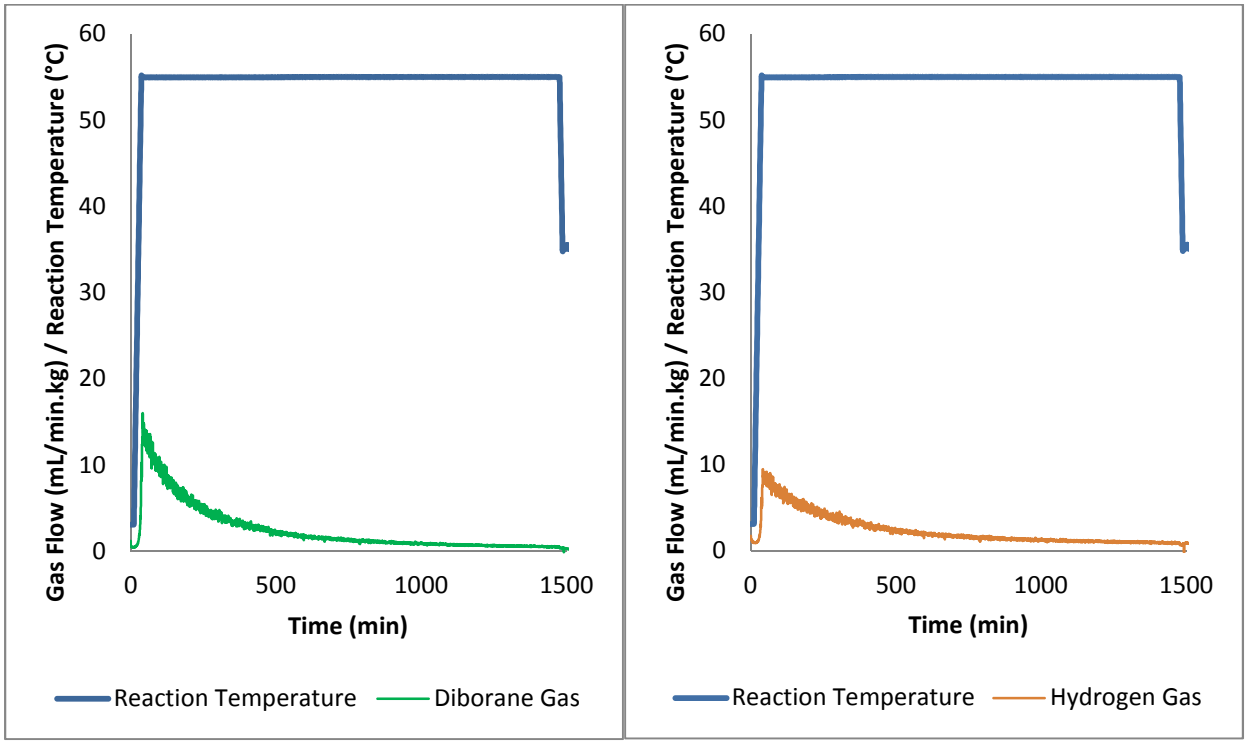
Run 1:



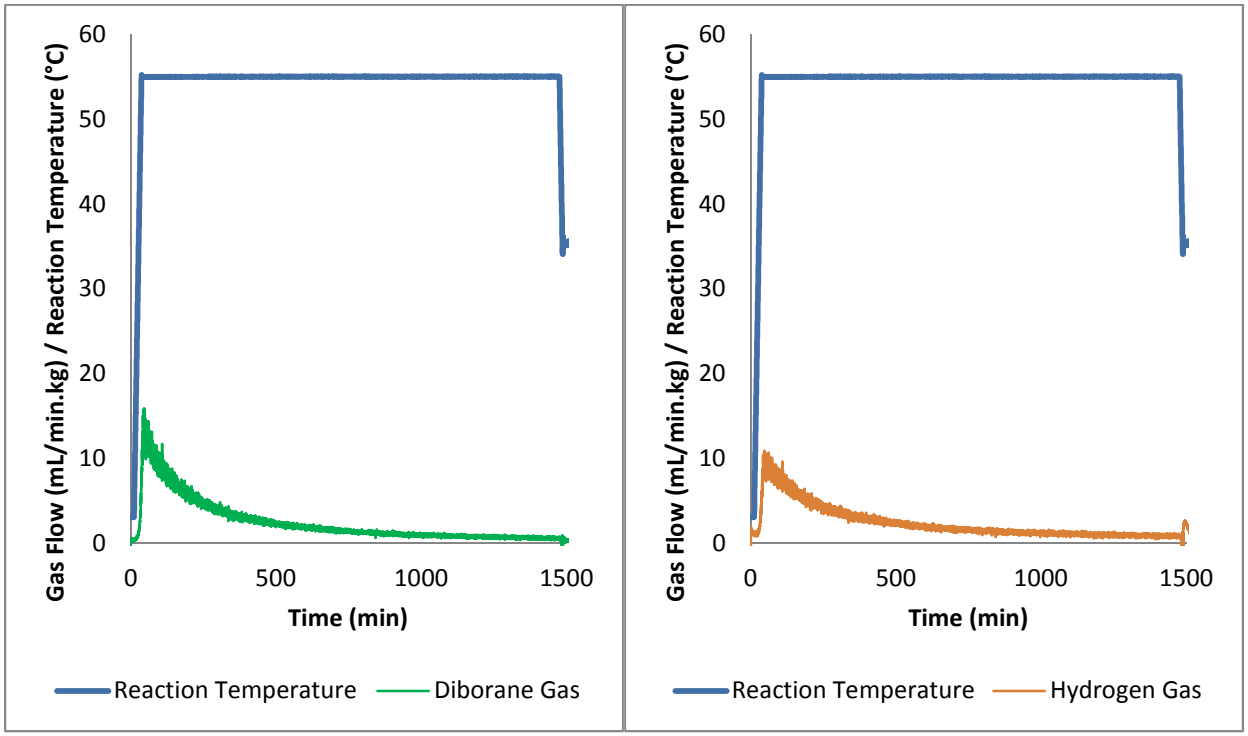
Run 2:



Run 3:

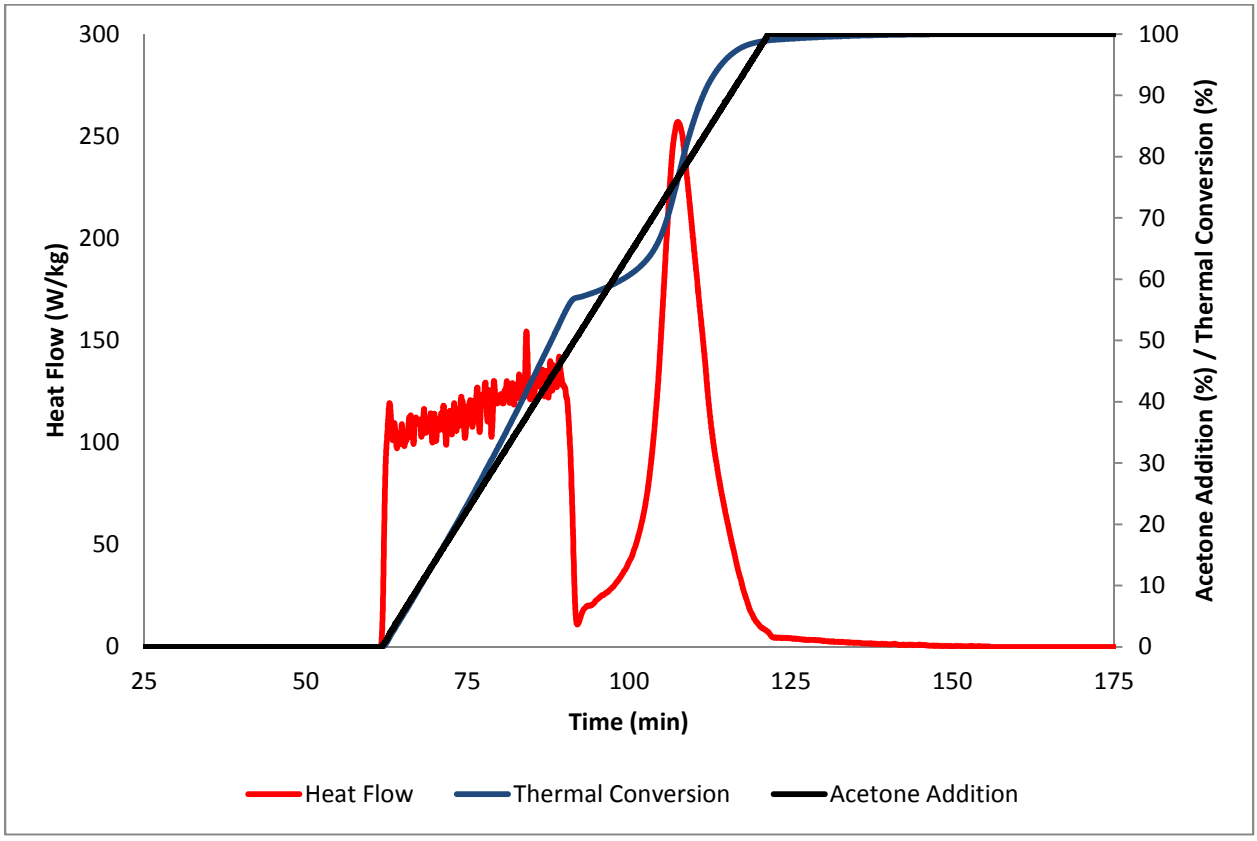

Gas Flow (mL/min.kg) / Reaction Temperature (°C)
60
50
40
30
20
10
0
0
500
1000
1500
Time (min)
Reaction Temperature
Diborane Gas
Gas Flow (mL/min.kg) / Reaction Temperature (°C)
60
50
40
30
20
10
0
0
500
1000
1500
Time (min)
Reaction Temperature
Hydrogen Gas

Run 4:


Gas Flow (mL/min.kg) / Reaction Temperature (°C)
60
50
40
30
20
10
0
0
500
1000
1500
Time (min)
Reaction Temperature
Diborane Gas
Gas Flow (mL/min.kg) / Reaction Temperature (°C)
60
50
40
30
20
10
0
0
500
1000
1500
Time (min)
Reaction Temperature
Hydrogen Gas

Heat flow trace for the addition of acetone to fresh BTHF

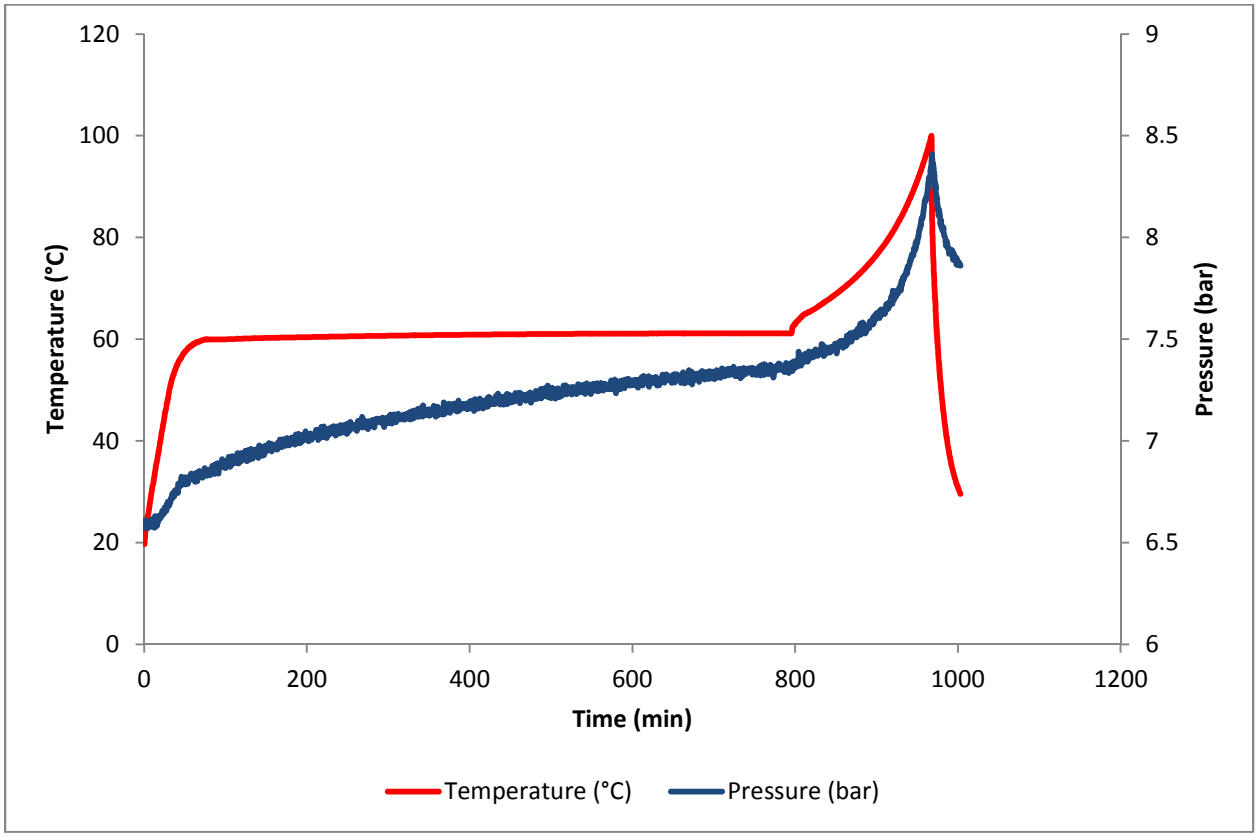
Note: Heat flow data is normalized to the amount of BTHF charged



The destruction of fresh BTHF is performed at 35 °C and uses an excess of acetone. Two distinct exothermic events are observed in the overall heat flow profile during the addition of acetone, with heat flow quickly returning to baseline after the addition is complete. The reaction mixture is then aged, followed by the addition of isopropyl alcohol. No additional heat output or significant gas evolution is observed during the age period or IPA addition, confirming the complete destruction of BTHF. Water is added, driving the reaction to the final boric acid species.

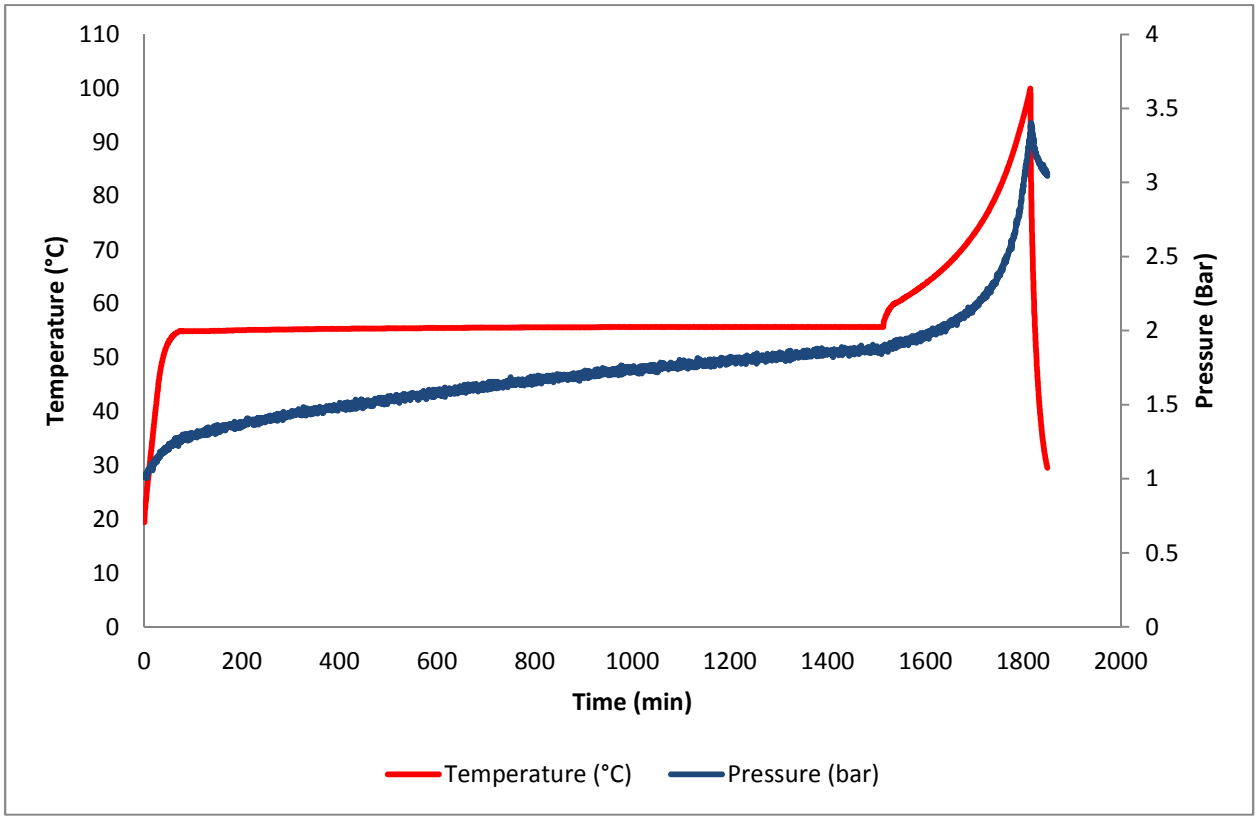
ARC traces for fresh BTHF

Fresh BTHF at 60 °C for 12 hours



On completing the isothermal aging period of 12 hours at 60 °C, the sample went into exothermic tracking immediately upon achieving the next heating step.

Fresh BTHF at 55 °C for 24 hours



On completing the isothermal aging period of 24 hours at 55 °C, the sample went into exothermic tracking immediately upon achieving the next heating step.