DETERMINING BOUNDS FOR A PRESSURE HAZARD RATING TO AUGMENT THE NFPA 704 STANDARD

A Thesis

by

PHILLIP RAYMOND HODGE

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

December 2011

Major Subject: Chemical Engineering

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Approved by:

Chair of Committee,	Sam M. Mannan
Committee Members,	Debjyoti Banerjee
	Dan Shantz
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ABSTRACT

Determining Bounds for a Pressure Hazard Rating to Augment the NFPA 704 Standard.

(December 2011)

Phillip Raymond Hodge, B.S., Rice University

Chair of Advisory Committee: Dr. Sam M. Mannan

Hazard communication is an essential part of a comprehensive safety plan, especially for those facilities that contain reactive chemicals. There are a variety of means of communicating a chemical hazard, but one of the most prevalent in the United States is the Instability Rating found in the NFPA 704 standard. While the NFPA 704 identifies hazards associated with exothermically decomposing compounds, it neglects compounds that decompose endothermicly to form large quantities of gas. Such compounds have been known to cause accidents due to pressure buildup, such as in the BP Amoco Polymers explosion in 2001.

In this work, twenty-five compounds were examined via an APTAC to determine their pressure and temperature profiles. These profiles were then used to determine the amount of gas generated, the gas generation rate, the gas generation product, the onset temperature, and the instantaneous power density. These properties were analyzed to determine those that best represented the instability hazard of the chemical. Ultimately, the molar gas generation rate and onset temperature were chosen to rate the selected

chemicals, and new cut-offs were established to divide the chemicals into revised instability groupings.

Compounds that did not decompose in the temperature range examined were given the rating of zero. Compounds with low onset temperatures and high gas generation rates were assigned the rating of 4, while chemicals with high T_{onset} and low dn/dt_{maxn} were assigned a value of 1. Chemicals with high onset temperatures and high gas generation rates were grouped into rating 3. Group 2 included low onset temperature compounds with low gas generation rates. The cut-offs used to define these regions were 130°C for the onset temperature and 0.01 (1/min) for the gas generation rate. The ratings were found to be comparable to the current NFPA system, but improved upon it by providing a valid rating (group 1) for the chemicals that endothermically generated gas. Detailed plots of the data are provided as well as suggestions for future work.

DEDICATION

To Chemistry Lunch and the 8th Floor, because I wouldn't be here without them.

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I would like to express my sincerest thanks to Dr. Sam M. Mannan for the opportunities that he has given me to explore the many facets of process safety. His support and confidence have been much appreciated throughout this process.

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Finally, I would like to thank my wife who agreed to my hair-brained scheme to go back to school. She has vicariously experienced the ups and downs of my two years at A&M and now knows more than she ever wanted to know about adiabatic calorimetry. She agreed to the headache that is a Houston commute and continues to put up with me through it all. I don't know where I'd be without her.

NOMENCLATURE

APTAC	Automatic Pressure Tracking Adiabatic Calorimeter
ARC	Accelerated Rate Calorimeter
ASTM	American Society for Testing and Materials
avg	Average
CHETAH	Computer Program for Chemical Thermodynamic and Energy Release Evaluation
C_c	Heat capacity of the cell
C_s	Heat capacity of the sample
dn/dt	Molar gas generation rate
dn/dt_i	Molar gas generation rate for any given time
dn/dt_{max}	Maximum molar gas generation rate
dn/dt_{maxn}	Normalized maximum molar gas generation rate
dP/dt	Pressure rate
dP/dt_i	Pressure rate at any given time
dT/dt	Temperature rate
dT/dt_i	Temperature rate at any given time
DSC	Differential Screening Calorimeter
DTBP	Di-Tert-Butyl Peroxide
E_A	Activation energy
GGP	Gas Generation Product

HWS	Heat – Wait – Search
IPD	Instantaneous Power Density
k_i	Rate constant at any given time
lg	Large
m	Mass
m_c	Mass of the cell
m_s	Mass of the sample
md	Medium
min	Minute
mL	milliliter
MKOPSC	Mary K. O'Connor Process Safety Center
MW	Molar (or Molecular) weight
n	Number of moles
n_i	Number of moles of generated gas at any given time
n_{max}	Maximum number of moles of generated gas
n_{maxn}	Normalized maximum number of moles of generated gas
n_s	Number of moles of sample
NFPA	National Fire Protection Association
NO_x	Mono-Nitrogen oxides
NRIFD	National Research Institute of Fire and Disaster
P	Pressure
P_i	Pressure at any given time

P_0	Initial pressure
psi	Pounds per Square Inch
psia	Pounds per Square Inch Absolute
R	Ideal gas law constant
r_{decomp}	rate of decomposition reaction
s	Second
sm	Small
t	Time
T	Temperature
T_i	Temperature at any given time
T_{max}	Maximum temperature at the end of an exothermic reaction
T_{onset}	Onset temperature – temperature at which a reaction begins
T_0	Initial temperature
V	Volume
V_{cell}	Volume of the cell
$V_{v\text{-}s}$	Gas expansion volume
ΔH_{decomp}	Enthalpy of decomposition
Φ	phi factor
ρ_s	Density of the sample
°C	degrees Celcius

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1. INTRODUCTION

Reactive chemicals are those chemicals that are inherently unstable and susceptible to a rapid reaction mechanism, typically decomposition or polymerization. These chemicals may react alone or with other substances under specific conditions to liberate heat or gases in an uncontrolled manner. In 2002 the CSB released a study, Improving Reactive Hazard Management, which compiled twenty years of reactive chemical incidents (CSB, 2002a). The report estimated that eight serious reactive chemical incidents occur each year, causing an average of six fatalities per year. The CSB has affirmed that serious reactive chemical incidents continue to occur at an alarming rate (CSB, 2009).

While the hazards of reactive chemicals can be severe, they are balanced by a wide variety of useful chemistries that make them ideal reactants in the synthesis of pharmaceuticals, plastics, and other products. While some reactive chemicals may be replaced with inherently safer alternatives, it is still necessary and advantageous to use a wide range of reactive chemicals in some situations. As such, an emphasis needs to be placed on the correct management of the hazards from these chemicals.

In order to correctly utilize reactive chemicals, it is necessary to understand the conditions under which a chemical can undergo an uncontrolled reaction, as well as the likely results. This can be done in a variety of ways, ranging from expert opinion to quantitative structure property relationship (QSPR) or calorimetry. These methods range

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This thesis follows the style of the *Journal of Loss Prevention in the Process Industries*.

in their predictive ability and testing cost.

Whichever means is used, it becomes necessary to disseminate this information in a clear and easily understood manner. Lack of awareness of the potential for reactive hazards is often cited as a cause of reactive chemical incidents (CSB 2009). As a means of mitigating this problem, several methods of communicating reactive hazards are in place. Material safety data sheets (MSDS) are often the primary means of hazard communication for a chemical, and may contain a variety of different measures of the reactivity of a chemical. Other commonly used methods are the Global Harmonized System for hazard classification and labeling of chemicals (GHS), the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), and the Hazardous Materials Information System (HMIS). While all these systems are in place, one of the most prevalent systems used in the United States is the NFPA 704.

The NFPA 704 standard classifies chemicals according to four separate categories: Health, Flammability, Instability, and Special Hazards. This results in the common safety diamond that appears on MSDSs, transports, and chemical labels. The Dow Fire and Explosion Index (FEI) incorporates the NFPA instability rating as well. Excluding special hazards, the categories are rated on a five-point scale (between 0 and 4). Though these classifications may be based on quantitative data, they are placed in categories based on relative boundaries established by the NFPA. The system was designed to allow workers and first responders an easy method of determining the relative threat when dealing with these chemicals. Though it is the instability rating of chief concern in this work, a brief explanation of the other ratings will be provided.

Health Hazard: The health hazard rating is based on the LC50 of the substance. LC50's are determined for inhaled, dermal, and oral routes of entry, and the most severe category is used to determine the health hazard rating. Only acute effects are considered for this number.

Flammability Hazard: The flammability rating is primarily based on flash points for liquids and particle size for dusts. There are special allowances made for chemicals which easily liberate flammable gasses or have self-contained oxygen.

Special Hazards: There are several special hazards that may be listed in a NFPA 704 diamond. The most common special hazards are water reactive and strong oxidizer. Radioactive materials and asphyxiants may also be labeled with a special hazard symbol.

Instability: The instability rating was originally called the reactivity rating. In its first incarnation, the instability rating was largely determined by qualitative assessment and expert opinion. The rating was augmented in 1997 by a method from Hofelich et al. (1997) which quantified the rating using a value called the Instantaneous Power Density (IPD). IPD was defined as the enthalpy of reaction multiplied by the initial reaction rate determined at 250°C expressed in Watts per milliliter per second. Although testing is the preferred method of obtaining parameters to determine instability, the NFPA 704 does allow for other methods such as the ASTM CHETAH program.

IPD methodology is effective in quantifying the relative hazards of exothermic reactions; however, it only considers reactive hazards associated with self-heating. While the potential to runaway is an important consideration, it is not the only parameter

that contributes to an unstable chemical. Another important parameter is the generation of gas.

Substantial gas generation often occurs during the exothermic decompositions associated with runaway but can occur during endothermic reactions as well (Barton & Rogers, 1997). Under IPD methodology these reactions would be classified as having an instability rating of 0. This failure can lead to unexpected events (Fenlon, 1987). For example, a lack of awareness of the instability of an endothermic process resulted in three fatalities in a BP Amoco Polymers nylon production facility (now Solvay Advanced Polymers, LLC) in March of 2001 (CSB, 2002b). Amodel (a polymer in the nylon family) was heated prior to being sequestered in a waste tank. As it cooled, the polymer blocked pressure valves and generated gas. Workers were killed while opening the tank to clean out the polymer. Although the reaction literature did mention the possibility of pressure generation at high temperatures, this information was not adequately communicated to operators. Other incidents involving gas generation can be found in Bretherick's Handbook (Urben, 2007).

As this incident shows, the current NFPA instability rating is not comprehensive enough to identify all reactive chemical hazards. In an effort to correct this, researchers at the Mary K. O'Connor Process Safety Center (MKOPSC) developed a methodology incorporating gas generation into the instability rating (Carreto-Vasquez et al., 2010). Carreto-Vasquez et al. sought to use an automatic pressure tracking adiabatic calorimeter (APTAC) to explore the gas evolution of several long chain polymers. They measured the maximum pressure as well as the maximum pressure rate and normalized these

values based upon the amount of material in the cell and the headspace in the cell. These processes will both be explored in further detail in the methodology section of this document.

Carreto-Vasquez et al. used these two measurements in an initial attempt to designate cut-offs for pressure generation hazards. To do this, they looked at a set of sample data obtained using an accelerating rate calorimeter (ARC). It was ultimately determined that the justification for the intervals was minimal and more detailed measurements were needed. This work seeks to expand upon the work of Carreto-Vasquez et al. by exploring how a broad range of common chemicals release gas when tested with an APTAC. The following sections will describe the methods of testing the chemicals and normalizing the data. The data will then be compiled and conclusions presented on the new proposed instability rating system.

2. METHODOLOGY

2.1 Chemical Selection and Preparation

Properly selecting a sample set is important when trying to draw inferences about the broad spectrum of available chemicals. The chemicals were principally drawn from three different lists. The following explains the rationale behind using each list.

There were several different considerations when selecting chemicals for this study. The first consideration was that chemicals from each of the five current NFPA classes be selected. As such, a minimum of three chemicals from each class was tested. A second criterion was that a preference would be given in the selection process to those chemicals that are produced and used in bulk across the chemical industry. Hofelich et al. used similar grounds for compiling their list of chemicals when proposing the IPD methodology. (Hofelich et al., 1997) Table 2.1 lists the chemicals tested by Hofelich et al.

The leading concern with the list from Hofelich et al. is a lack of chemicals in the 3 or 4 rating. To correct for this, chemicals that have known reactive hazards were added to this list. These chemicals were selected from the MKOPSC list of reactive chemicals that warrant further study, originally presented at the 3rd NRIFD Symposium in Mitaka, Tokyo, Japan (Rogers et al., 2004). Table 2.2 lists these chemicals. The chemicals were chosen based on a history of instability, the presence of reactive functional groups, or the ability to initiate free-radical reactions.

Table 2.1
Chemical List from Hofelich et al. 1997

Chemical	NFPA ranking
Dioctyl Phthalate	0
Ethanolamine	0
Ethyl Alcohol	0
Isopropyl Alcohol	0
Methylene Chloride	0
Methyl Ethyl Ketone	0
Propylene Glycol	0
Acetone	0
Benzene	0
n-Butyl Alcohol	0
Ethyl Benzene	0
Ethylene Glycol	0
Phenol	0
Toluene	0
Bisphenol A	1
Maleic Anhydride	1
Acetic Acid	1
Cumene	1
DURSBAN**	1
Hydrogen Peroxide (40 – 60%)	1
Methyl Methacrylate	2
1,3-Butadiene	2
Acrylonitrile	2
Ethylene	2
Styrene	2
DOWICIL** 75	2
Hydroxylamine	3
Chloropicrin	3
Cumene Hydroperoxide	4
Di-tert-butyl Peroxide	4

* DURSBAN is a trademark of DowElanco
**DOWICIL is a trademark of the Dow Chemical Company

Table 2.2
MKOPSC List of Reactive Chemicals That Warrant Further Study

9,10-Dibenzocyclopentadiene	Di-tert-amyl peroxide	Methyl pentadiene
Acetal	Di-tert-butyl peroxide	Monomethyl ether
Acetic anhydride	Dicumyl peroxide	Nitric acid
Acetyl chloride	Dicyclopentadiene	Nitroanisole
Acetylene	Dinitroaniline	Nitrobenzene
Acrylic Acid	Dinitrobenzene	Nitrocellulose
Aluminum hydride	Dinitrocresol	Nitrocyclohexane
Amlene	Dinitrotoluene	Nitroethane
Amyl nitrate	Dintriophenol	Nitroglycerine
Barium Hydrides	Dioxane	Nitropropane
Benzoyl peroxide	Dipentene	Nitropyrene
Butadiene	Divinyl acetylene	Pentadiene
Butadiene	Ethyl nitrate	Pentene
Butene	Ethylene	Picric acid
Butyne	Ethylene glycol dimethyl ether	Propylene oxide
Chlorbutadiene	Ethylene oxide	Silane
Chlorosulfonic acid	Glyceryl trinitrate	Sulfuric acid
Chlorotrifluoroethylene	Hexene	t-Butyl alcohol
Cumene hydroperoxide	Hydrogen peroxide	Tert-butyl hydroperoxide
Cycloheptane	Hydroxylamine	Tetrahydronaphthalene
Cycloheptatriene	Isobutylene	Tetramethyl aluminum
Cyclohexane	Isohexene	Trinitrotoluene
Cyclohexene	Isoprene	Vinyl acetate
Cyclooctadiene	Isopropyl ether	Vinyl chloride
Di-borane	Methycyclopentane	Vinyl ethers
Di-isobutyl	Methyl i-butyl ketone	Vinyl pyridine

These lists provide an overabundance of chemicals to test, so the next goal became to limit the choices. The first means of limiting the chemicals was to have an authoritative value for the NFPA instability rating. NFPA 325M (NFPA 1994) was used for this purpose. Although all of the chemicals tested could not be found on this list, as it tends to favor the lower-rated chemicals, the majority of them are present. A final

limitation was a preference to test solids and liquids. One gas, ethylene oxide, was included, but due to testing constraints, solids and liquids were used for all other samples.

Since this research was conducted primarily to incorporate endothermic reactions which produce non-condensable gases, it would seem prudent to incorporate chemicals that exhibit this behavior. Four such chemicals were included. These chemicals were not found on any of the lists, but were chosen because of knowledge of their decomposition reactions. These chemicals do increase the number of 0 rated chemicals in the list, but will be considered a separate class in the analysis. Table 2.3 shows the final list of chemicals and the respective lists where they can be found. Four chemicals (picoline, water, ethylene oxide, and 2 – butanone peroxide) were included because they were previously tested by the MKOPSC and are indicated by the heading "tested".

Chemicals were tested as received to mimic typical storage conditions. The manufacturing company and purity of each chemical can be found in Table 2.4. While small amounts of contaminants are known to affect reactive chemicals (Dinh, 2008) it is unlikely that significant quantities of highly pure compound are stored long-term without some contamination. Regarding the presence of inhibitors or stabilizers in radical polymerizers, the choice to use the Heat-Wait-Search mode described below helps to alleviate these effects by allowing the chemical time to stabilize at a given temperature.

Table 2.3
Final Chemical List

Chemical Name	Instability	DOW List	MKOPSC List	NFPA 325M	Endothermic Potential	Tested
Isopropyl Alcohol	0	X		X		
Picoline	0					X
Polyacrylic Acid	0				X	
Polyarylamide	0				X	
Polyethylene Glycol	0				X	
Polyvinyl Acetate	0				X	
Water	0					X
Cumene	1	X	X	X		
Dicyclopentadiene	1		X	X		
Maleic Anhydride	1	X		X		
Manganese Carbonate	1				X	
Nitrobenzene	1		X	X		
Acrylonitrile	2	X	X	X		
Isoprene	2		X	X		
Methyl Methacrylate	2	X		X		
Styrene	2	X	X	X		
Vinyl Acetate	2		X	X		
2,4-Dinitroaniline	3		X	X		
Ethylene Oxide	3	X	X	X		X
Hydrogen Peroxide	3	X	X			
Hydroxylamine	3	X	X			
Nitroethane	3		X	X		
1,2-Dinitrobenzene	4		X	X		
2-Butanone Peroxide	4					X
Cumene Hydroperoxide	4	X	X	X		
Tertbutyl Peroxide	4	X	X			

Table 2.4
Chemical Origin and Purity

Chemical Name	Manufacturer	Avg. MW (g)	Purity (%)
Isopropyl Alcohol	OmniSolv	60.1	99.9
Picoline	OmniSolv	93.13	99.9
Polyacrylic Acid	Aldrich	450000	99.5
Polyarylamide	Aldrich	100000	99
Polyethylene Glycol	Aldrich	4600	99
Polyvinyl Acetate	Aldrich	100000	99
Cumene	Sigma Aldrich	120.19	99.9
Dicyclopentadiene	Sigma Aldrich	132.2	99
Maleic Anhydride	Sigma Aldrich	98.06	99
Manganese Carbonate	Sigma Aldrich	114.95	99.9
Nitrobenzene	Sigma Aldrich	123.11	99
Acrylonitrile	Aldrich	53.06	99
Isoprene	Sigma Aldrich	68.12	99
Methyl Methacrylate	Sigma Aldrich	100.12	99
Styrene	Aldrich	104.15	99
Vinyl Acetate	Sigma Aldrich	86.09	99
2,4-Dinitroaniline	Sigma Aldrich	183.12	98
Ethylene Oxide	Sigma Aldrich	44.05	99
Hydrogen Peroxide	Aldrich	34.01	12.5
Hydroxylamine	Aldrich	69.49	99.9
Nitroethane	Sigma Aldrich	75.07	98
1,2-Dinitrobenzene	Sigma Aldrich	168.11	97
2-Butanone Peroxide	Aldrich	210.22	35
Cumene hydroperoxide	Aldrich	152.19	88
Tertbutyl Peroxide	Sigma Aldrich	146.23	98

2.2 Automatic Pressure Tracking Adiabatic Calorimeter

The Automatic Pressure Tracking Adiabatic Calorimeter (APTAC) was used to examine each of the chemicals. The APTAC is a closed cell calorimeter that can run in several different modes that will be described later. The cell is placed inside a 500-mL pressurized vessel and is heated by four different heaters: top, bottom, side, and tube.

Measurements are taken by two pressure transducers and seven thermocouples. The pressure transducers measure pressure inside the cell as well as the pressure within the larger vessel. Four of the thermocouples are used to monitor the temperature of the heaters. The other three thermocouples measure the temperature of the gas inside the pressure vessel, the temperature of the sample cell's wall, and the temperature of the sample inside the cell. Pressures can be varied from 10 psia to 2000 psia, while the temperature range is from 0 to 500°C. The controlling software adjusts settings or will shut down the experiment if necessary to avoid exceeding these limits.

The APTAC can be operated in a variety of modes. Though only the Heat-Wait-Search (HWS) mode was used for this research, the other modes will be described briefly.

Heat-Soak-Search: In this mode the APTAC heats a sample to a desired temperature for a given time period. If an exotherm is detected during the soak period, the APTAC will switch to adiabatic mode and follow the exotherm. This mode is often used to test the efficacy of reaction inhibitors.

Heat Ramp: In this mode the APTAC heats the sample at a given rate until a given temperature is reached. No exotherm detection is provided in this mode and heating continues even during a reaction. This could cause heat loss from the sample to the environment if the self-heating rate exceeds the set heat rate of the experiment. This mode is often used as a screening tool prior to other, costlier tests being done.

Isothermal: In this mode the APTAC heats the sample to a given temperature and attempts to maintain that temperature inside the cell for a given time period.

Because the APTAC is not fitted with any cooling equipment, this mode is most effective at temperatures far above room temperature. This mode is often used to determine reaction kinetics.

HWS: This is the mode that will be used to test the samples for this research. In this mode the APTAC heats the sample to a given temperature and then attempts to maintain that temperature for a given time interval. During the wait period, the APTAC searches for exotherms. An exotherm is detected when the self-heating rate exceeds a user-selected value (normally 0.05°C/min). If an exotherm is not detected by the end of the interval the APTAC increases the temperature by a set amount (typically 10°C) and initiates the waiting period again. This cycle will repeat until a preset temperature cut-off is reached or an exotherm is detected. If an exotherm is detected by the APTAC it switches to adiabatic mode. While in the adiabatic mode, the calorimeter seeks to maintain zero heat flow across the cell boundary. It does this by adjusting the heaters to maintain the temperature outside the cell at the same level as that of the sample. Adiabatic mode continues until the self-heating rate falls below the user-defined rate or the defined temperature limit is reached. If the temperature limit is not reached, the APTAC switches back to the HWS mode and continues the experiment. Figure 2.1 shows a typical temperature profile from a HWS experiment.

As mentioned previously, the APTAC is a closed cell calorimeter. This means that there is no material flow in or out of the sample cell. This allows the machine to accurately measure the amount of gas produced during an experiment. Normally, to compensate for the high pressures generated in a closed cell test, thick walled cells are

needed to prevent failure of the cell. While many calorimeters make use of such cells (the accelerating rate calorimeter is a prime example), the thickness of the cells can cause strong deviations from adiabatic conditions. Deviations from adiabatic conditions create errors because process units approximate adiabatic conditions during runaway reactions (Wei et al., 2006). The APTAC, however, is able to use thin-walled vessels. It accomplishes this through pressure tracking. The pressure outside the cell is maintained at the same level as that inside the cell. If a set pressure difference between the two is exceeded, safety shut-offs stop the experiment to prevent cell rupture.

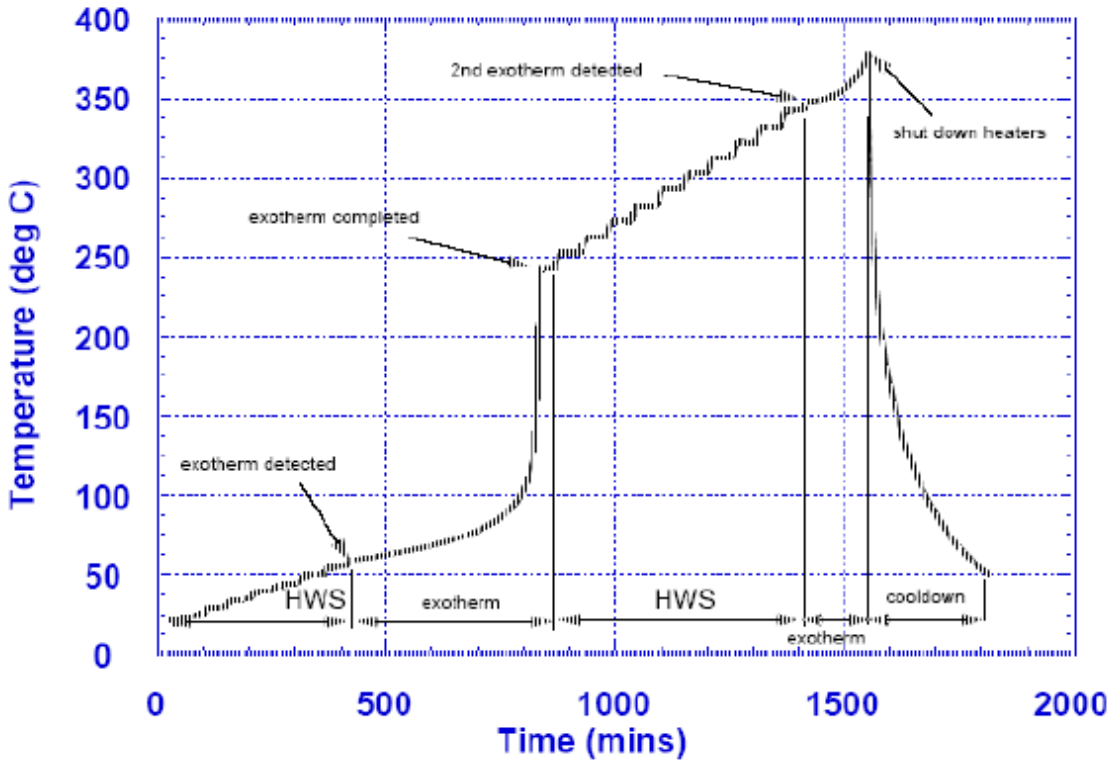

Fig. 2.1 Typical Temperature Profile from an APTAC HWS Experiment
(Extracted from the APTAC Manual)

The sample cell can be made from a variety of materials: glass, titanium, hastalloy, tantalum, and stainless steel. Because of the wide variety of chemicals studied, glass was chosen for the current set of experiments. Although this does make for thicker walled vessels, it also prevents accidental catalysis that could be caused by interactions with the various metallurgies. Table 2.5 details the normal parameters that were used to conduct the tests required for this thesis.

Table 2.5
Normal Test Parameters

Setting	Value
Mode	HWS
Start Temp. °C	50.00
Final Temp. °C	350.00
Temp. Increment °C	10.00
Cool Down Temp. °C	50.00
Shutdown Temp. °C	390.00
Shutdown Temp. Rate °C/min	400.00
Exotherm Threshold °C/min	0.05
Exotherm Limit °C	390.00
Heating Rate, °C/min	2.00
Max Pressure psia	1050.00
Max Pressure Rate, psi/min	1000.00
Max Pressure Imbalance psi	50.00

2.3 Normalization and Data Manipulation

Pressure and pressure rate data are obtained from the APTAC. These pressures and pressure rates are then converted to a molar quantity of gas present in the sample and a molar rate of gas generation using the ideal gas equation of state. Equations 2.1 and 2.2 show the ideal gas equations for number of moles of gas generated and molar gas generation rate respectively (Iwata & Koseki, 2008).

Although gases deviate from the ideal gas law at high pressures, it is still a good approximation for the quantity of gas formed during decomposition. A more complex equation of state cannot be used without extensive knowledge about the composition of the gases formed in the headspace. Although these are assumed to be gases such as carbon monoxide, carbon dioxide, various NO_x compounds and water, without explicit knowledge of the relative composition of each of these, it is not feasible to use a more complicated equation of state. Furthermore, as the reaction proceeded the composition of the gas would change. This would necessitate a change in the constants used in more complicated equation of state.

In order to utilize the ideal gas equation of state, the volume of the cell must be known. The volume of the cell is determined by measuring the change in mass from an empty cell to one filled with water. This volume is then corrected using the initial volume of sample. Equation 2.3 demonstrates this. The volume of the sample is likely to change during the trial due to vaporization or thermal expansion of the sample. To limit the effect of vaporization, the APTAC is run at a minimum pressure of 100 psia. The change in volume likely contributes to some error in the molar conversions, but is thought to be small in relation to the overall volume of the cell.

Once the conversion to moles has been made, the values for n must be corrected for the initial amount of gas in the cell. Equation 2.4 demonstrates this. Variables with a subscript *i* in Equations 2.4 and 2.5 indicate that the variable is replaced with its value at a given time and then evaluated at all other times to create a complete data series and

0 indicates the initial value of that variable. Once this is done, the maximum values for the gas generated (n_{max}) and gas generation rate (dn/dt_{max}) are found.

Finally both parameters must be normalized based on the amount of material considered. The sample will be normalized on a per mol basis. This results in a pseudo-unitless value for the normalized maximum gas generated (n_{maxn}) and a pseudo-unitless rate for the normalized maximum gas generation rate (dn/dt_{maxn}). Equations 2.6 and 2.7 demonstrate this. These values will be multiplied to yield a gas generation product (GGP) as shown in Equation 2.8. Further data analysis is developed in the Results and Discussion section.

Equation 2.1

$$n = \frac{P \cdot V}{R \cdot T}$$

Equation 2.2

$$\frac{dn}{dt} = \frac{V}{R \cdot T} \cdot \left(\frac{dP}{dt} - \frac{P}{T} \cdot \frac{dT}{dt} \right)$$

Equation 2.3

$$V_{v-s} = V_{cell} - \frac{m_s}{\rho_s}$$

Equation 2.4

$$n_i = \frac{P_i \cdot V_{v-s}}{R \cdot T_i} - \frac{P_0 \cdot V_{v-s}}{R \cdot T_0}$$

Equation 2.5

$$\frac{dn}{dt}_i = \frac{V_{v-s}}{R \cdot T_i} \cdot \left(\frac{dP}{dt}_i - \frac{P_i}{T_i} \cdot \frac{dT}{dt}_i \right)$$

Equation 2.6

$$n_{maxn} = \frac{n_{max}}{n_s}$$

Equation 2.7

$$\frac{dn}{dt}_{maxn} = \frac{dn}{dt}_{max} \cdot \frac{1}{n_s}$$

Equation 2.8

$$GGP = n_{maxn} \cdot \frac{dn}{dt}_{maxn}$$

2.4 Thermal Properties Determination

The information gathered from the APTAC also allows for an examination of the thermal properties of the compounds. Both the onset temperature of the decomposition and the IPD of the material are measures of the instability of the compound. The onset temperature can easily be determined by examining the temperature output from the APTAC. The value for the IPD requires more analysis however.

IPD is calculated by finding the enthalpy of the decomposition and the initial reaction rate of the material calculated at 250°C. This is shown in Equation 2.9. The enthalpy of the decomposition is shown in Equation 2.10 and is a product of the specific heat capacity of the material, the phi factor of the experiment, and the difference in the onset temperature and maximum temperature reached by the compound under self-heating. All of these can be gathered from the APTAC output except for the phi factor which is a ratio of the heat capacity of the cell to the heat capacity of the sample material (Equation 2.11).

The kinetic component of the IPD calculation can be determined by Equation 2.12. The density of the compound is known, and IPD methodology defines the temperature to equal 250°C. To determine the value for the pre-exponential factor and the activation energy, the inverse temperature is graphed versus the natural log of the

rate constant, k. This creates a line with slope equal to the activation energy and y-intercept equal to the natural log of the pre-exponential factor as shown in Equation 2.13. Equation 2.14 can be used to determine the values for k.

Equation 2.9

$$IPD = \Delta H_{decomp} \cdot r_{decomp}$$

Equation 2.10

$$\Delta H_{decomp} = C_s \cdot \phi \cdot (T_{max} - T_{onset})$$

Equation 2.11

$$\phi = 1 + \frac{m_c \cdot C_c}{m_s \cdot C_s}$$

Equation 2.12

$$r_{decomp} = \rho_s \cdot A \cdot e^{-E_A/R \cdot T}$$

Equation 2.13

$$\ln(k_i) = \ln(A) - \frac{E_A}{R \cdot T_i}$$

Equation 2.14

$$k_i = \frac{\frac{dT}{dt}_i}{T_{onset} - T_i} \cdot \frac{1min}{60s}$$

2.5 Precision and Normalization Studies

It is vital that the APTAC provides consistent results for the amount of gas generated. To ensure the precision of the APTAC data, multiple trials should be run. Due to the limited time frame and high number of samples selected for this study it is not feasible to run each of the compounds a statistically significant number of times. Instead one compound will be used to determine that the APTAC provides consistent results. The compound used will be tertbutyl peroxide. This compound was chosen because it is a well-studied compound with ample literature available for comparison. Moreover, the

compound has a low onset temperature that allows tests to be run more quickly. Finally, the reaction decomposes relatively cleanly, and only the normal cleaning regimen is required between each trial. Five trials will be conducted under as close to identical conditions as possible, and the resulting n_{maxn} and dn/dt_{maxn} values compared.

In addition to the precision study, a second study will be conducted to determine whether the volume of the reaction cell causes n_{maxn} and dn/dt_{maxn} to vary. Smaller reaction cells allow smaller sample sizes to be run. This can increase the coverage of the sample thermocouple. Not having sufficient coverage can lead to results deviating from adiabatic. Three different volumes of reaction cells will be used.

The final set of tests will be a normalization study. Three different initial amounts of tertbutyl peroxide will be tested to determine that normalizing the gas generated and the gas generation rate by the number of moles of sample results in a consistent value.

2.6 Measured Uncertainties, Calibration, and Cleaning Procedures.

The thermocouples measure the temperature to one thousandth of a degree Celsius. The pressure transducers measure to one hundredth of a psi. Masses were measured using a Metler Toledo balance accurate to the one hundredth of a gram.

The thermocouples were calibrated relative to each other to minimize temperature drift. This was done using the APTAC's calibration software using a clean glass cell. The calibration was performed every time the sample calorimeter was changed, the size of the cell was changed, or after every ten trials. Absolute calibration was handled by submersing the sample in deionized ice water.

Between trials the APTAC was cleaned using a variety of different physical and chemical methods to ensure that there was no cross contamination. The connectors exposed to chemicals during testing and the pressure lines of the APTAC were cleaned using water and acetone depending on the polarity of the chemical under consideration. This was done by physically scrubbing the lines and by flushing superheated solvent through the lines. In the cases of a more serious clog in the line, a small hand drill was used to remove the obstruction.

Prior to each trial, a leak test was performed. The location where leaks are of the most concern is in and out of the sample vessel. The cell was pressurized to above 100 psia and allowed to equilibrate for 30 minutes. At the end of this time the leak rate should be within the range of +/- 0.01 psi/min. If the pressure rate was outside this region then the vessel was inspected, modifications were made to fittings, and the leak test conducted again until the pressure rate fell within the expected range.

The APTAC was tested using a standard sample of 20% tertbutyl peroxide in toluene prior to any tests being conducted and compared to open literature values to check for accuracy. Figure 2.2 shows the results of this test and Figure 2.3 shows the standard results from the ATPAC manual. The tests show good agreement. Figures 2.2 and 2.3 were run in titanium cells. Figure 2.4 shows the same test run in a glass cell. The maximum heat rate is lower for this test due to the increased phi factor which is to be expected with glass, but otherwise the tests show good agreement.

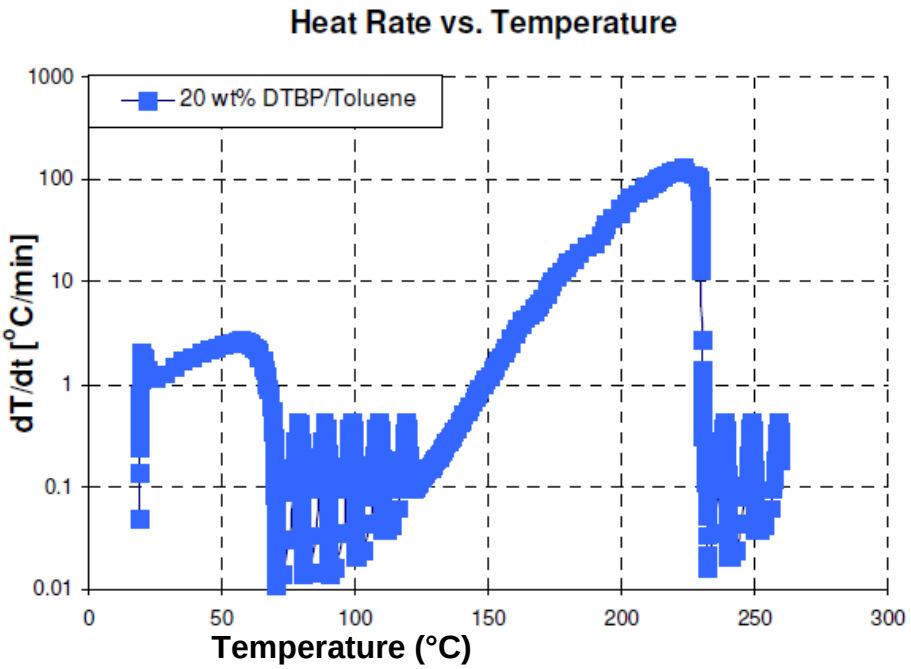

Fig. 2.2 APTAC Accuracy Check 20% Tertbutyl Peroxide in Toluene (Dinh 2008)

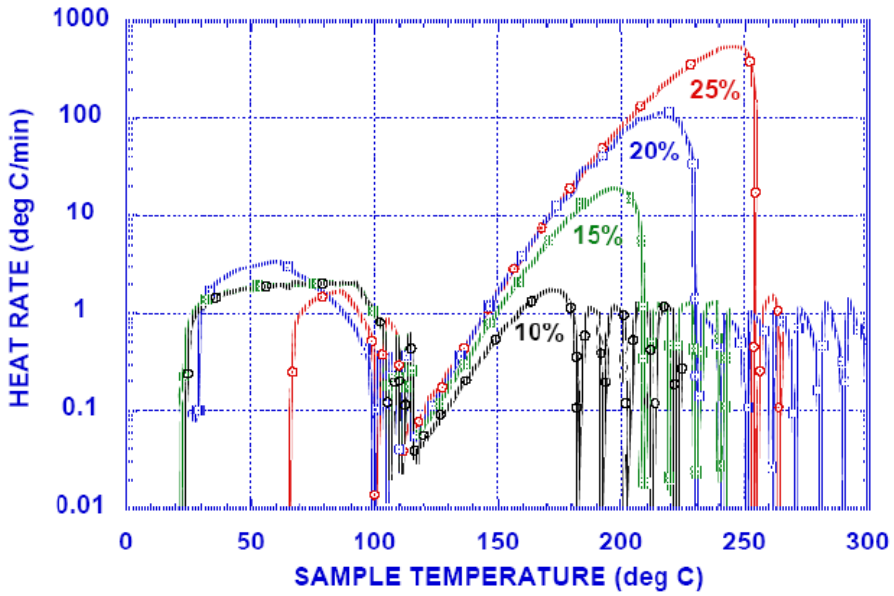

Fig. 2.3 APTAC Standard Curves (Extracted from the ATPAC Manual)

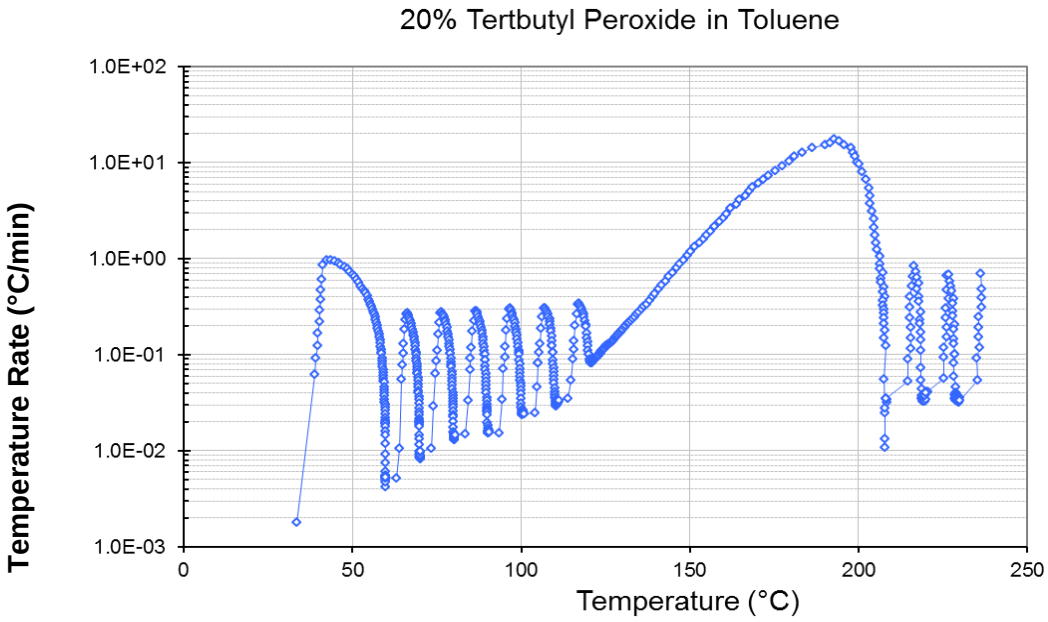

Fig. 2.4 APTAC Accuracy Check 20% Tertbutyl Peroxide in Toluene – Glass Cell

3. RESULTS AND DISCUSSION

3.1 Normalization Study

The five identical tests for DTBP are summarized in Table 3.1. The results and graphs of individual tests can be found in Appendix A. The tests showed a strong repeatability. The value for n_{maxn} shows an average value of 2.20 +/- 0.120. The value for the dn/dt_{maxn} is 0.0217 +/- 0.00602 1/min. All errors in this thesis are calculated at a 95% confidence interval using a standard normal Gaussian distribution. The gas generation rate has a higher relative variability, but this can be attributed to the fact that the molar rate is two orders of magnitude smaller than the maximum amount of gas generated. Overall these results show that the APTAC provides consistent measurements and a low variance.

Table 3.1
Repeatability Study

Name	n_{max} (mol)	dn/dt_{max} (mol/min)	n_{maxn}	dn/dt_{maxn} (1/min)	GGP (1/min)
DTBP 1.3g-1	1.98E-02	9.43E-05	2.18E+00	1.04E-02	2.25E-02
DTBP 1.3g-2	2.15E-02	2.06E-04	2.32E+00	2.21E-02	5.13E-02
DTBP 1.3g-3	2.11E-02	2.43E-04	2.30E+00	2.65E-02	6.11E-02
DTBP 1.3g-4	1.84E-02	2.00E-04	1.98E+00	2.15E-02	4.25E-02
DTBP 1.3g-5	2.10E-02	2.62E-04	2.23E+00	2.78E-02	6.18E-02
averages	2.04E-02	2.01E-04	2.20E+00	2.17E-02	4.79E-02
+/- error	1.13E-03	5.70E-05	1.20E-01	6.02E-03	1.42E-02

The second set of normalization tests was designed to look at the role that the volume of the sample played on the values obtained for the test. The results are displayed in Table 3.2 and individual tests are listed in Appendix A. The value for n_{maxn}

shows an average value of 1.76 +/- 0.343. The value for the dn/dt_{maxn} is 0.0148 +/- 0.00165 1/min. Once again the relative errors for these tests are small. Surprisingly the value for dn/dt_{maxn} had a lower error than the previous trial. One would expect the larger phi factors of the larger containers to play a role in the rate of gas generation, but perhaps the increased volume for expansion helped to counter this effect. The value for n_{maxn} does have a higher variance than the previous set of trials, by a factor of three. This indicates that changes in the cell size may cause increased error in this quantity. As such, it would appear that the methodology adequately accounts for the difference in volume, and any size cell could be used. To decrease the number of variables, however, the large-sized sample cell will be used for all cases.

Table 3.2
The Effect of Volume on the Test Procedures

Name	n_{max} (mol)	dn/dt_{max} (mol/min)	n_{maxn}	dn/dt_{maxn} (1/min)	GGP (1/min)
DTBP 0.5g-lg	5.32E-03	5.97E-05	1.47E+00	1.65E-02	2.42E-02
DTBP 0.5g-md	7.09E-03	4.77E-05	2.07E+00	1.40E-02	2.90E-02
DTBP 0.5g-sm	6.20E-03	4.96E-05	1.74E+00	1.39E-02	2.43E-02
averages	6.21E-03	5.24E-05	1.76E+00	1.48E-02	2.58E-02
+/- error	1.00E-03	7.32E-06	3.43E-01	1.65E-03	3.06E-03

The final set of preliminary tests was run to determine if the APTAC could provide consistent results when using different sample sizes. This is primarily a concern for designing a standardized test across chemical species. The results appear to show good agreement when a per-mole normalization is used, with one caveat. Multiple tests with DTBP resulted in an explosion incident which led to ruptured cells. These explosion incidents resulted in larger than expected pressure and pressure rate values.

While the threat of explosion is an important consideration when determining a chemical's instability, this is already handled by other aspects of the NFPA standard. Table 3.3 shows the averaged results of all tests run. When the explosion events are removed the normalization appears to be much more consistent with the previous findings. Table 3.4 displays these results. The value for n_{maxn} shows an average value of 1.75 +/- 0.447. The value for the dn/dt_{maxn} is 0.0168 +/- 0.00541.

It is important to note that many effects such as autocatalysis and phi factor are dependent on the amount of material in the cell. While neither of these effects is likely to contribute to variance in the amount of gas generated, it can play a role in the molar rate of generation. To mitigate these errors, compounds will be run on an equimolar basis whenever possible.

Table 3.3
Normalization Study – All Tests

Name	n_{max} (mol)	dn/dt_{max} (mol/min)	n_{maxn}	dn/dt_{maxn} (1/min)	GGP (1/min)
DTBP 1.3g-avg	2.04E-02	2.01E-04	2.20E+00	2.17E-02	4.79E-02
DTBP 3g-lg	1.70E-02	1.00E-04	7.85E-01	4.63E-03	3.64E-03
DTBP 0.5g-lg	5.32E-03	5.97E-05	1.47E+00	1.65E-02	2.42E-02
DTBP 6g-lg	2.23E-02	2.78E-02	5.25E-01	6.55E-01	3.44E-01
DTBP 18g-lg	5.84E-02	8.85E-02	4.75E-01	7.20E-01	3.42E-01
DTBP 0.9g-lg	1.00E-02	7.71E-05	1.57E+00	1.21E-02	1.91E-02
averages	2.22E-02	1.95E-02	1.17E+00	2.38E-01	1.30E-01
+/- error	1.51E-02	2.85E-02	5.50E-01	2.79E-01	1.32E-01

Table 3.4
Normalization Study – Explosion Incidents Removed

Name	n_{max} (mol)	dn/dt_{max} (mol/min)	n_{maxn}	dn/dt_{maxn} (1/min)	GGP (1/min)
DTBP 0.5g-lg	2.04E-02	2.01E-04	2.20E+00	2.17E-02	4.79E-02
DTBP 0.5g-md	5.32E-03	5.97E-05	1.47E+00	1.65E-02	2.42E-02
DTBP 0.5g-sm	1.00E-02	7.71E-05	1.57E+00	1.21E-02	1.91E-02
averages	1.19E-02	1.13E-04	1.75E+00	1.68E-02	3.04E-02
+/- error	8.71E-03	8.72E-05	4.47E-01	5.41E-03	1.74E-02

3.2 Test Results

The results of the various chemical trials are displayed in Table 3.5. As noted above, explosion events can give higher values than normal for maximum pressure rate. In addition, a few chemicals reached the maximum temperature for the APTAC while in exotherm mode. This prohibits a true measure of the maximum temperature and may impact the maximum amount of gas generated. Trials with either of these concerns are included in Appendix B along with the summary tables and graphs used to obtain these data points.

It should be noted that dicyclopentadiene was removed from the study. This chemical caused blockages in the APTAC's pressure lines and created substantial problems with the pressure transducers, yielding poor-quality pressure data. The blockage was believed to have been caused by dicyclopentadiene vapors that condensed in the small pressure tubing leading to the pressure transducer. Extensive cleaning and refurbishing was needed to remove the blockages, and subsequent trials were deemed too likely to result in damage to the equipment.

Table 3.5
Gas Generation Hazard Summary

Appendix	Name	n_{maxn}	dn/dt_{maxn} (1/min)	GGP (1/min)	T_{onset} (°C)	IPD (W/mL)
6.1	1, 2 - Dinitrobenzene	1.40E+00	1.21E-01	1.70E-01	190	3.56E-01
6.2	2 - Butanone Peroxide	4.56E-01	1.37E+00	6.25E-01	80	2.22E+06
6.3	2, 4 - Dinitroaniline	4.89E+00	9.40E+00	4.60E+01	180	7.57E-01
6.4	Acrylonitrile	5.21E-01	9.84E-03	5.13E-03	100	8.73E-01
6.5	Cumene	0.00E+00	3.16E-04	0.00E+00	130	1.18E+00
6.6	Cumene Hydroperoxide	1.16E+00	3.56E-01	4.14E-01	120	3.41E+02
6.7	Ethylene Oxide	1.31E+00	1.40E+00	1.84E+00	180	2.36E-03
6.8	Hydrogen Peroxide - 12.5%	2.26E+00	8.14E-01	1.84E+00	140	7.47E+02
6.9	Hydroxylamine Chloride	8.27E-01	5.76E-02	4.76E-02	150	3.63E+04
6.10	Isoprene	3.99E-01	1.18E-03	4.72E-04	90	4.42E-01
6.11	Isopropyl Alcohol	8.14E-01	6.19E-03	5.04E-03	N/A	0.00E+00
6.12	Maleic Anhydride	7.93E-01	2.14E-01	1.70E-01	220	5.32E-02
6.13	Manganese Carbonate	1.27E-01	2.89E-04	3.66E-05	140	7.93E-02
6.14	Methyl Methacrylate	6.24E-01	1.35E-02	8.43E-03	100	2.43E+02
6.15	Nitrobenzene	6.54E-01	1.94E-03	1.27E-03	190	8.84E-01
6.16	Nitroethane	2.38E-01	1.30E-02	3.08E-03	160	1.56E+00
6.17	Picoline	7.04E-01	4.72E-03	3.32E-03	N/A	0.00E+00
6.18	Polyacrylic Acid	1.04E+00	4.08E-03	4.23E-03	260	0.00E+00
6.19	Polyarylamide	5.87E-01	5.66E-03	3.32E-03	300	0.00E+00
6.20	Polyethylene Glycol	3.18E-03	1.19E-03	3.80E-06	290	0.00E+00
6.21	Polyvinyl Acetate	7.65E-01	3.83E-03	2.93E-03	240	0.00E+00
6.22	Styrene	1.24E-01	9.67E-03	1.20E-03	120	3.85E+01
6.23	Tertbutyl Peroxide 1.3g-avg	2.20E+00	2.17E-02	4.79E-02	100	8.88E+01
6.24	Vinyl Acetate	5.52E-01	7.85E-03	4.33E-03	160	4.05E+02
6.25	Water	1.12E-01	3.44E-03	3.84E-04	N/A	0.00E+00

Also are included in Table 3.5 are estimates for the IPD value for each chemical. These values assume a first order reaction rate and simple one step reaction mechanisms. These values should not be taken as official values for IPD. A more thorough examination of each compound's reaction kinetics would be necessary for determining true values of IPD. This, however, is beyond the scope of the current research. T_{onset}

values are also displayed. Four chemicals did not have onset temperatures within the temperature range considered and are indicated as such by N/A. Intermediate values and graphical determination of the activation energy can be found in Appendix B.

3.3 Interpretation of Results

The values for n_{maxn} vary widely for chemicals known to be very reactive (nitroethane, for example, would be ranked a 1 under n_{maxn}) and those known to be nonreactive (isopropyl alcohol would be a ranked a 3). Moreover, n_{maxn} is more susceptible to errors arising from testing conditions. Since n_{maxn} occurs most frequently at the end of a test, the maximum testing temperature can affect this quantity. The value for dn/dt_{maxn} is found almost exclusively at the beginning of an exotherm. Because of the length of time of the experiment, the presence of even the smallest air leaks will affect n_{maxn}. The gas generation rate, however, would not be significantly altered by a slow leak (less than 0.01 psi/min). As the gas generation potential is a multiple of n_{maxn}, it will be subject to the same errors as n_{maxn}. For these reasons it was determined that the gas generation rate will be used to estimate the gas generation hazard.

Table 3.6 lists the compounds in order of their gas generation rate. This could allow for a set of cut-offs to be made based solely on the gas generation potential. The cut-offs would be based on order of magnitude of the gas generation potential, and likely candidates for cut-offs are displayed in Table 3.7 and indicated by color in Table 3.6 as well.

Table 3.6
Gas Generation Rate Hazard Summary

Name	dn/dt_{maxn}
Manganese Carbonate	2.888E-04
Cumene	3.164E-04
Isoprene	1.183E-03
Polyethylene Glycol	1.194E-03
Nitrobenzene	1.938E-03
Water	3.437E-03
Polyvinyl Acetate	3.828E-03
Polyacrylic Acid	4.080E-03
Picoline	4.718E-03
Polyarylamide	5.663E-03
Isopropyl Alcohol	6.194E-03
Vinyl Acetate	7.848E-03
Styrene	9.674E-03
Acrylonitrile	9.841E-03
Nitroethane	1.297E-02
Methyl Methacrylate	1.352E-02
Tertbutyl Peroxide 1.3g – avg	2.166E-02
Hydroxylamine Chloride	5.756E-02
1, 2 – Dinitrobenzene	1.215E-01
Maleic Anhydride	2.144E-01
Cumene Hydroperoxide	3.558E-01
Hydrogen Peroxide - 12.5%	8.138E-01
2 - Butanone Peroxide	1.371E+00
Ethylene Oxide	1.404E+00
2, 4 – Dinitroaniline	9.404E+00

Table 3.7
Gas Generation Rate Hazard Proposed Cut-Offs

Rating	Range (1/min)
0	< 1.00E-03
1	1.00E-03 - 5.00E-03
2	5.00E-03 - 1.00E-02
3	1.00E-02 - 2.50E-01
4	> 1.00E+00

Although gas generation rate is an important consideration when determining overall instability, it should not be the sole factor. First, if chemicals are listed solely by gas generation rate, solvents such as water, isopropyl alcohol and picoline are considered to be more reactive than nitrobenzene. The solvents have gas generation solely from evaporation, whereas nitrobenzene undergoes an exothermic decomposition. As such, it should be considered more reactive.

Secondly, one of the reasons previously cited for conducting this research was that the current method of determining the NFPA instability rating did not include pressure generation in its criteria. As such, it is prudent to consider how decomposition temperature interacts with the gas generation rate to avoid making a similar omission. There are two different methods to incorporate thermal data. Knorr et al (2007) used temperature as the determining characteristic of thermal decomposition. IPD, however, is an accepted method of determining the thermal decomposition hazard. Both of these methods will be explored below.

Where available, the values for IPD were compared to literature values. Upon comparison, the approximations used do not appear to adequately represent the values for IPD. More analysis and likely further experimentation would need to be to determine the true kinetic parameters for each chemical. Moreover, chemicals such as polyvinyl acetate have IPD values of zero. If the IPD methodology is used, then the hazards from endothermic gas generation will continue to be under-ranked. For these reasons, the IPD values will not be used as a thermal component.

The onset temperature can be easily used as a measure of the thermal stability with a slight modification. Instead of defining the onset temperature as the temperature at which an exotherm begins, one could define it as the temperature at which any decomposition begins, whether it is an exothermic or endothermic reaction. With this modification, Figure 3.1 was created to determine likely regions for the NFPA rankings. The key indicates the current NFPA ranking, and the y axis is a logarithmic display. Water, picoline, and isopropyl alcohol do not appear on Figure 3.1 because they do not have onset temperatures.

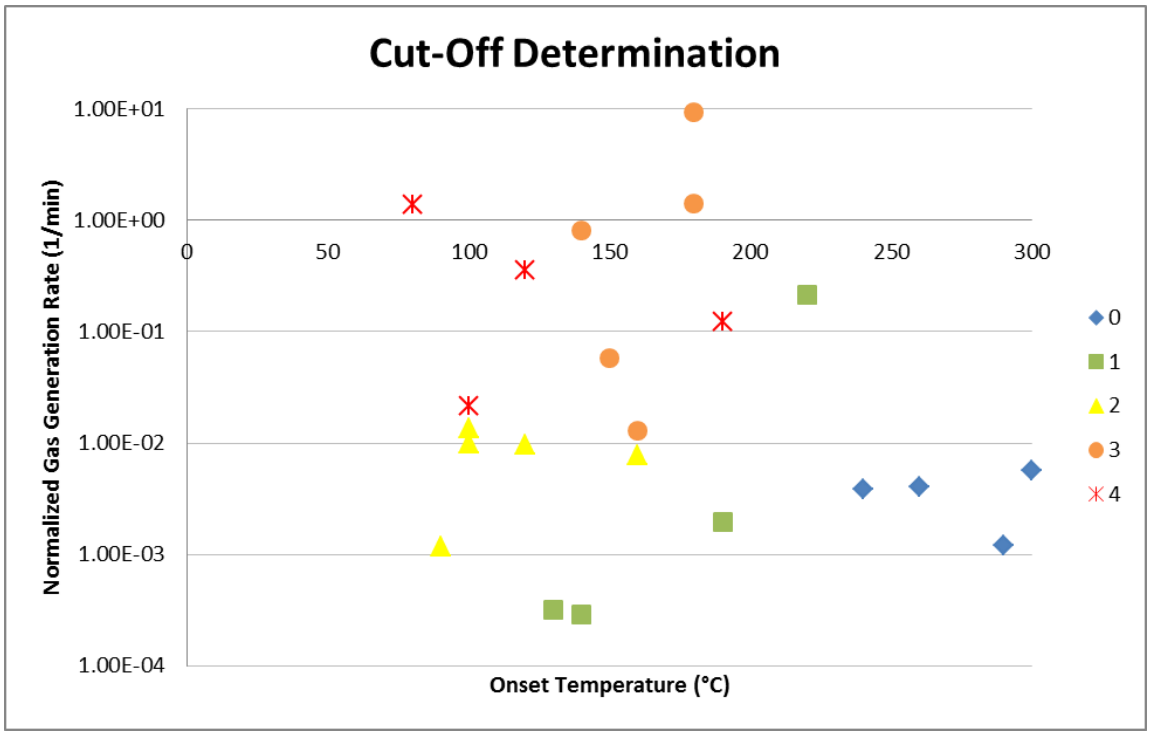

Fig. 3.1 Cut-Off Analysis - Onset Temperature and Gas Generation Rate

From Figure 3.1 it appears that cut-offs can be constructed at 130°C and 0.01 1/min. These cut-offs are displayed in Figure 3.2 and Table 3.8. Drawing lines at these cut-off points creates four different regions corresponding to the ratings 1-4. Low onset

temperature and high gas generation rates indicate the greatest instability, while chemicals with high T_{onset} and low dn/dt_{maxn} are the most stable. Since gas generation is needed for an explosion event, chemicals with high onset temperatures and high gas generation rates will be grouped into rating 3. Group 2 will include low onset temperature compounds with a low gas generation rate. Compounds that do not decompose in the temperature range under consideration are given the rating of 0.

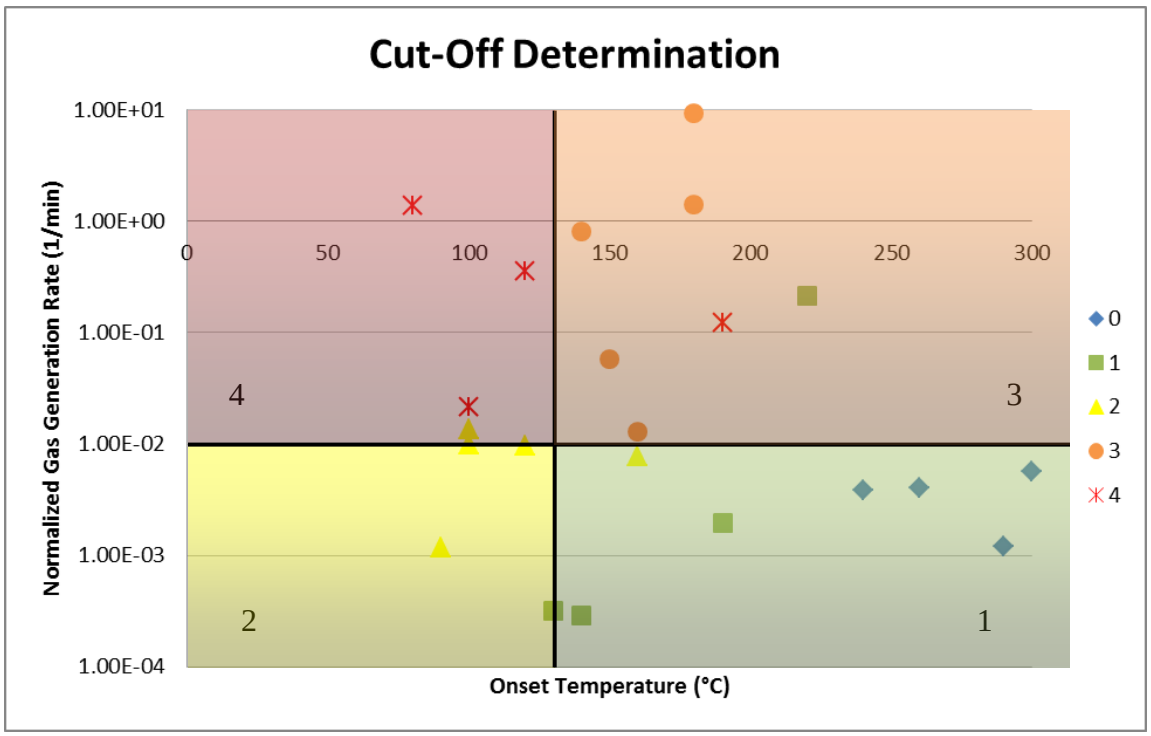

Fig. 3.2 – Cut-Off Determination

This proposed methodology displays good agreement with the previous NFPA ranking while incorporating the endothermic gas generation of the polymer groups. These polymer groups would be given a rating of 1. This is a reasonable rating as endothermic reactions in general should not pose as great a threat as compounds with strong exothermic behavior.

Table 3.8
New Rating Using Combined Methodology

Name	dn/dt_{maxn}	T_{onset}	Current NFPA Rating
Water	3.44E-03	0	0
Picoline	4.72E-03	0	0
Isopropyl Alcohol	6.19E-03	0	0
Polyarylamide	5.66E-03	300	0
Polyethylene Glycol	1.19E-03	290	0
Polyacrylic Acid	4.08E-03	260	0
Polyvinyl Acetate	3.83E-03	240	0
Nitrobenzene	1.94E-03	190	1
Vinyl Acetate	7.85E-03	160	2
Manganese Carbonate	2.89E-04	140	1
Cumene	3.16E-04	130	1
Styrene	9.67E-03	120	2
Acrylonitrile	9.84E-03	100	2
Isoprene	1.18E-03	90	2
Maleic Anhydride	2.14E-01	220	1
1, 2 - Dinitrobenzene	1.21E-01	190	4
Ethylene Oxide	1.40E+00	180	3
2, 4 - Dinitroaniline	9.40E+00	180	3
Nitroethane	1.30E-02	160	3
Hydroxylamine Chloride	5.76E-02	150	3
Hydrogen Peroxide - 12.5%	8.14E-01	140	3
Cumene Hydroperoxide	3.56E-01	120	4
Methyl Methacrylate	1.35E-02	100	2
Tertbutyl Peroxide 1.3g - avg	2.17E-02	100	4
2 - Butanone Peroxide	1.37E+00	80	4

The cut-offs were chosen such that the number of compounds belonging to each rating are approximately the same under each system (with the exception of the endothermic reactions). Table 3.8 lists the current NFPA rating, and Table 3.9 compares the number of compounds belonging to each rating under the current rating system and the proposed system. Sixteen out of twenty-five chemical ratings did not change under

the proposed methodology. Of the nine remaining chemicals, four of them are endothermic gas generators, one chemical (cumene) moved up a rating and two chemicals (1, 2 dinitrobenzene and vinyl acetate) moved down a rating. The two remaining chemicals (maleic anhydride and methyl methacrylate) moved up two spots. The increase in rank is due to large gas generation for both compounds. Further investigation into the instability of these compounds is likely warranted.

Table 3.9
Comparison of Rating Systems

Rating	Current number at this rating	Proposed number at this rating
0	7	3
1	4	7
2	5	4
3	5	7
4	4	4

To a certain extent, the boundaries for the different regions are arbitrary and could be varied slightly. The current IPD methodology for determining NFPA ratings acknowledges this point. The temperature value of 250°C was chosen as the temperature at which to calculate IPD specifically because it gave values that corresponded with accepted rating for the chemicals considered. The proposed methodology meets this criterion as discussed above.

4. CONCLUSIONS AND RECOMMENDATIONS

4.1 Conclusions

This thesis examined the problems associated with defining instability solely in terms of exothermic decomposition, or more specifically the hazards associated with not taking into account endothermic reactions that produce significant gaseous components. To this end, 25 chemicals were tested for the amount of gas generated, the gas generation rate, and the gas generation product. The onset temperature and IPD of each chemical were also explored as a measure of thermal instability. The definition for onset temperature was expanded to include the temperature at which any decomposition reaction began, not just an exothermic reaction.

It was determined that the onset temperature and the gas generation rate were the most suitable measures for the instability of each chemical. These parameters were graphed and divided into quadrants corresponding to the NFPA ratings 1 through 4. Compounds that did not decompose in the temperature range examined were given the rating of zero. Compounds with low onset temperature and high gas generation rates were assigned the rating of 4, while chemicals with high T_{onset} and low dn/dt_{maxn} were assigned a value of 1. Chemicals with high onset temperatures and high gas generation rates were grouped into rating 3. Group 2 included low onset temperature compounds with a low gas generation rate. The cut-offs used to define these regions were 130°C for the onset temperature and 0.01 (1/min) for the gas generation rate.

This methodology was found to provide good agreement with the current NFPA 704 Instability rating while taking into consideration those compounds that endothermicly release gases. Out of 25 compounds, 19 ratings did not change. Four of the chemicals are endothermic gas generators, one chemical (cumene) moved up a rating and two chemicals (1, 2 dinitrobenzene and vinyl acetate) moved down a rating. Maleic anhydride and methyl methacrylate moved up two spots. These two compounds had much higher gas generation rates than the other chemicals within their former group.

4.2 Recommendations

The following is a list of recommendations for the use of the information contained in this thesis, as well as suggestions for future work in the area of instability ratings.

This thesis contains a thorough and consistent data set for a wide range of compounds. While the vast majority of these chemicals are mid-molecular weight organic compounds, they comprise a diverse set of functional groups and chemistries. Future researchers could use this data set as a starting point when conducting more focused research—for example, exploring nitrated compounds or peroxides in detail.

Many of the compounds in this study were only tested once. As such, there may be some benefit to repeating some of the experiments in this thesis for replication purposes, especially those compounds that are border cases or that have drastically different ratings under the proposed methodology. Future students may want to pursue a more rigorous equation of state or more detailed kinetic analysis.

Access to APTAC equipment is quite rare and few companies operate such a device. It is therefore prudent to determine another means of obtaining the same information using equipment that is readily available. Other calorimeters (such as ARC or closed cell Dewar calorimeters for example) should be tested and a methodology established so that a wide range of chemical producers can test and establish accurate ratings. While it is always advisable to thoroughly test new chemicals, it would be useful to have a means of obtaining the needed onset temperature and molar generation rate. While ASTM CHETAH can be used to predict the onset temperature, detailed modeling and analysis would need to be done to construct software to predict the molar generation rate.

At the same time, it is suggested that smaller sample cells be utilized. This will allow smaller samples to be tested more quickly. Moreover, this should allow less expensive and less time-consuming determination of the gas generation rate and onset temperature. Finally, it may be prudent to switch to testing at atmospheric pressure instead of at elevated pressure, again to lower costs and provide an easier method of testing.

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APPENDIX A

The following is the data used in the normalization study. Each chemical is listed followed by pertinent information in four summary tables. Normal experiment parameters were used except where indicated. Each chemical is accompanied by five graphs. These graphs are the profiles for normalized gas generation, normalized gas generation rate, temperature and pressure, temperature and pressure rate, and rate constant determination.

A.1 Tertbutyl Peroxide 1.3g lg – 1

Table A.1
Material Properties - Tertbutyl Peroxide 1.3g lg – 1

Property	Value
m_s (g)	1.33
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.2
Cell Properties - Tertbutyl Peroxide 1.3g lg – 1

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	22.80

Table A.3
IPD Properties - Tertbutyl Peroxide 1.3g lg – 1

Property	Value
A (1/s)	8.411E+06
E_A (J/(mol*K))	8.472E+04
T_{onset} (°C)	100
T_{max} (°C)	165
ΔH (J/g)	2221.
IPD (W/ml)	51.65

Table A.4
Gas Properties - Tertbutyl Peroxide 1.3g lg – 1

Property	Value
n_{max} (mol)	1.979E-02
dn/dt_{max} (mol/min)	9.426E-05
n_{maxn}	2.176E+00
dn/dt_{maxn} (1/min)	1.036E-02
GGP (1/min)	2.255E-02

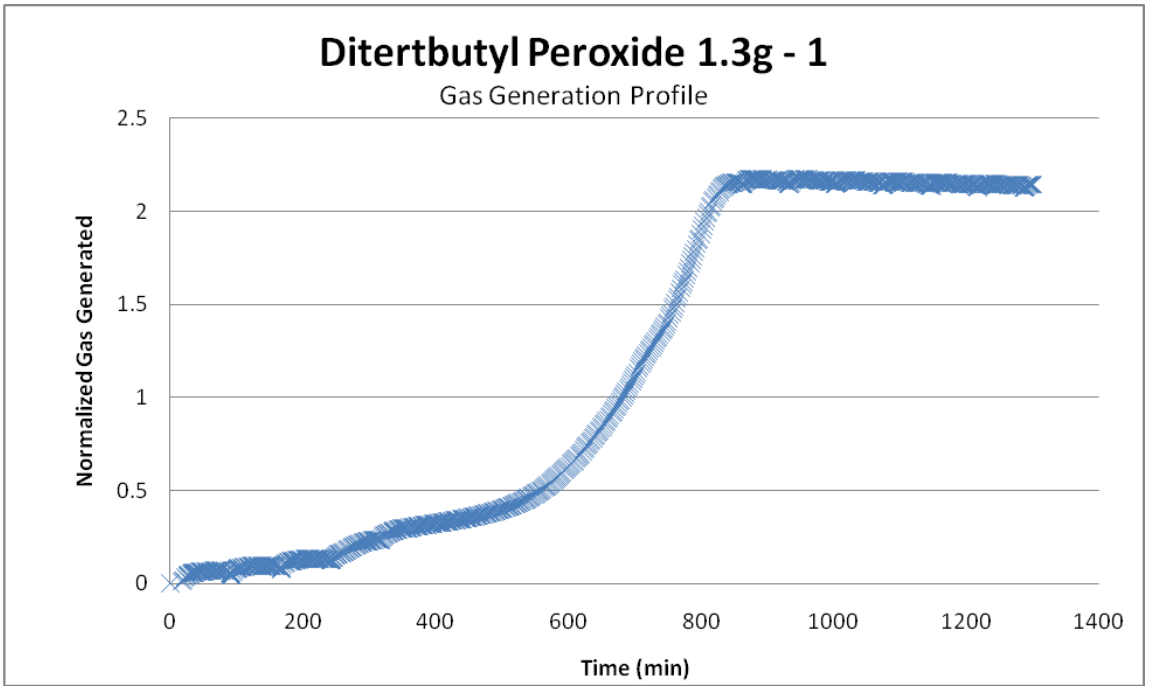

Fig. A.1 Normalized Gas Generation - Tertbutyl Peroxide 1.3g lg – 1

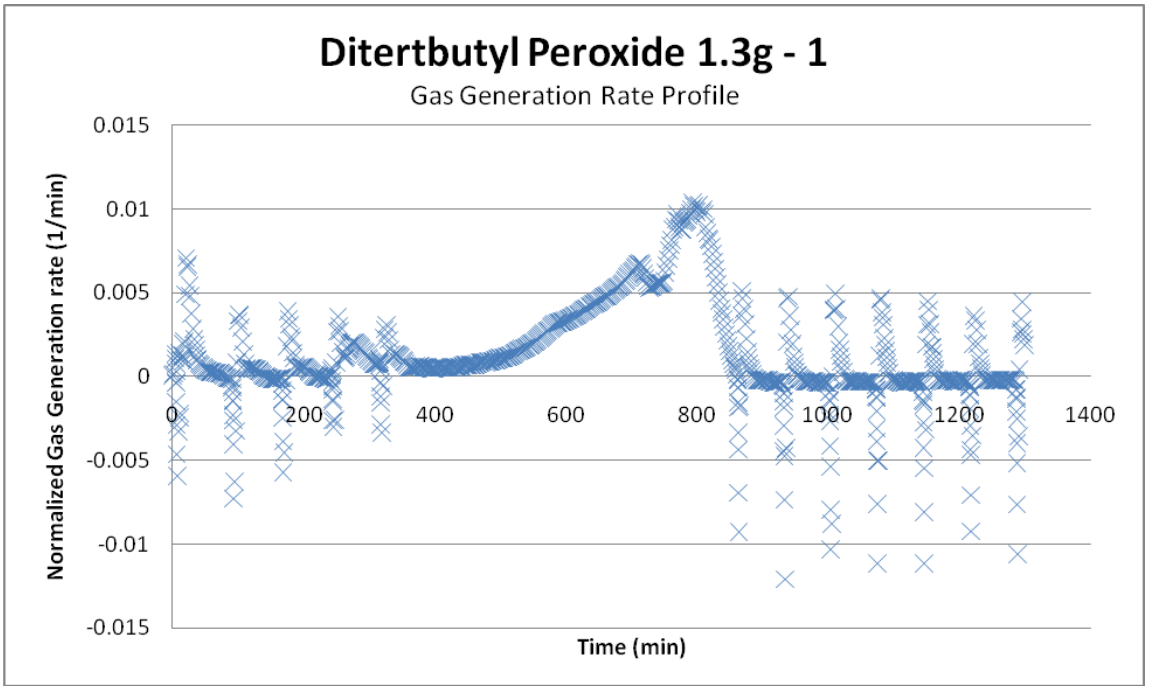

Fig. A.2 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g lg – 1

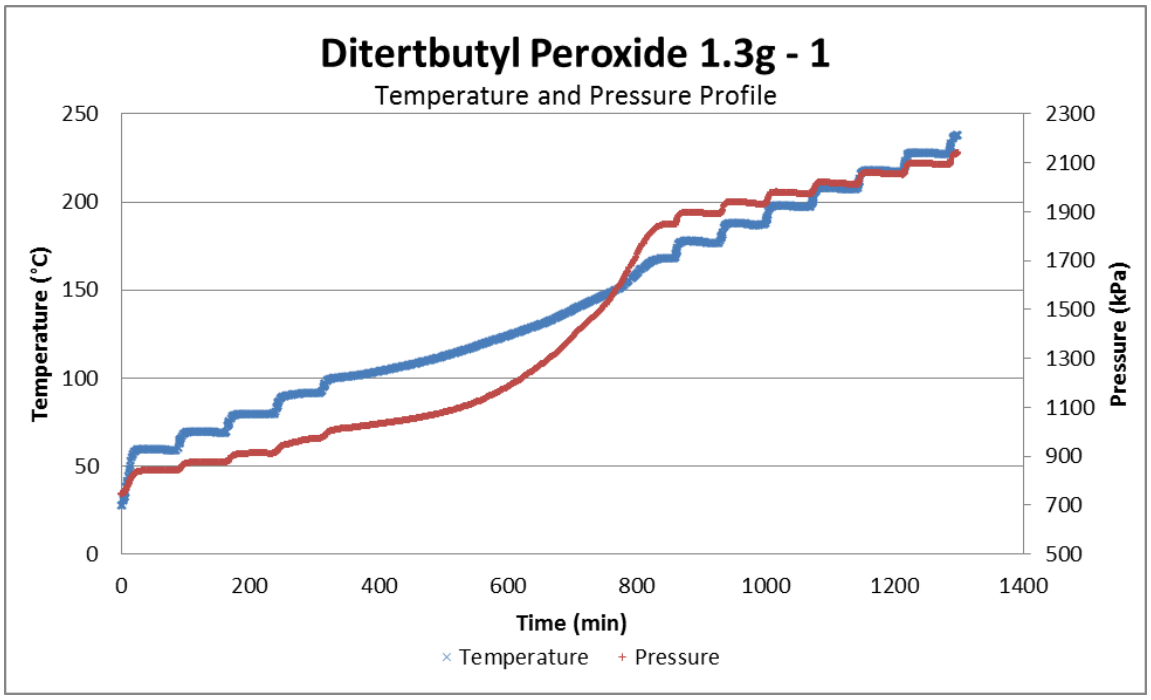

Fig. A.3 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g lg – 1

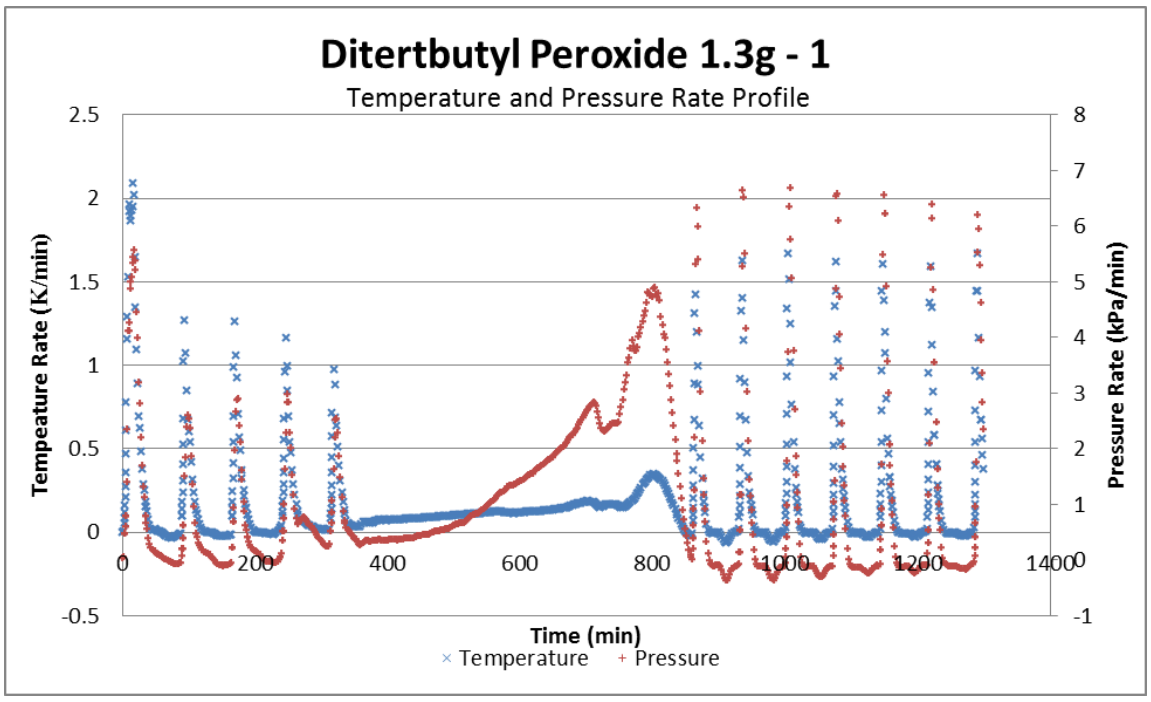

Fig. A.4 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g lg – 1

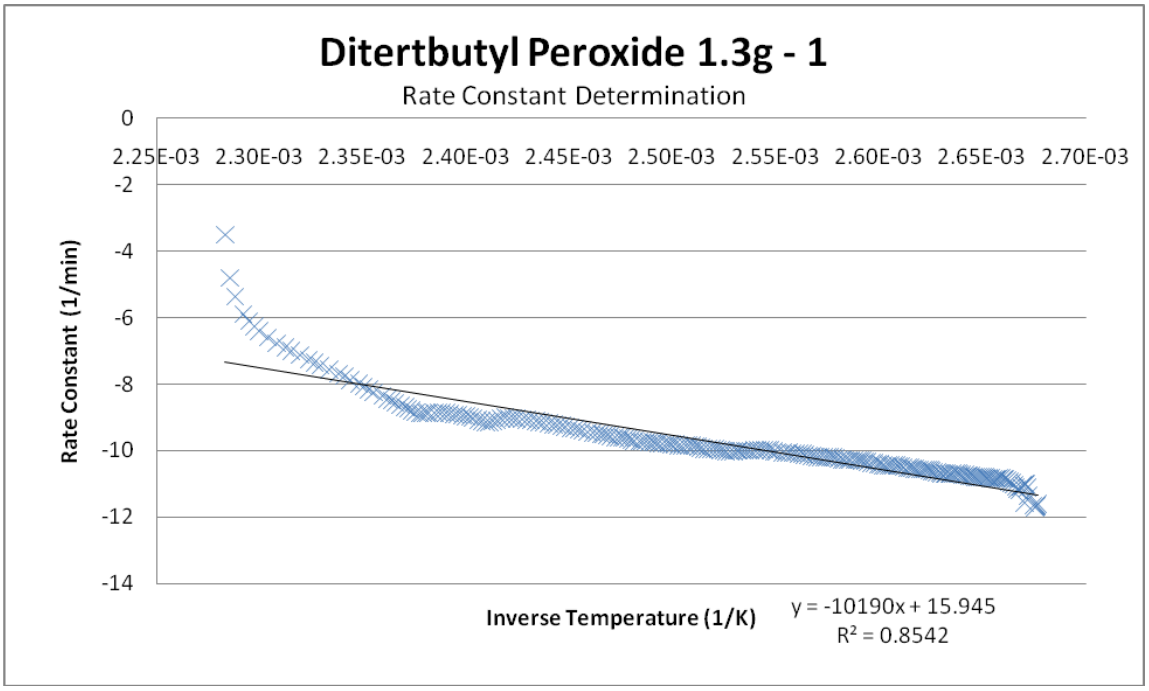

Fig. A.5 Rate Constant Determination - Tertbutyl Peroxide 1.3g lg – 1

A.2 Tertbutyl Peroxide 1.3g lg – 2

Table A.5
Material Properties - Tertbutyl Peroxide 1.3g lg – 2

Property	Value
m_s (g)	1.36
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.6
Cell Properties - Tertbutyl Peroxide 1.3g lg – 2

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	22.32

Table A.7
IPD Properties - Tertbutyl Peroxide 1.3g lg – 2

Property	Value
A (1/s)	9.704E+06
E_A (J/(mol*K))	8.497E+04
T_{onset} (°C)	100
T_{max} (°C)	177
ΔH (J/g)	2576.
IPD (W/ml)	65.38

Table A.8
Gas Properties - Tertbutyl Peroxide 1.3g lg – 2

Property	Value
n_{max} (mol)	2.154E-02
dn/dt_{max} (mol/min)	2.059E-04
n_{maxn}	2.316E+00
dn/dt_{maxn} (1/min)	2.213E-02
GGP (1/min)	5.127E-02

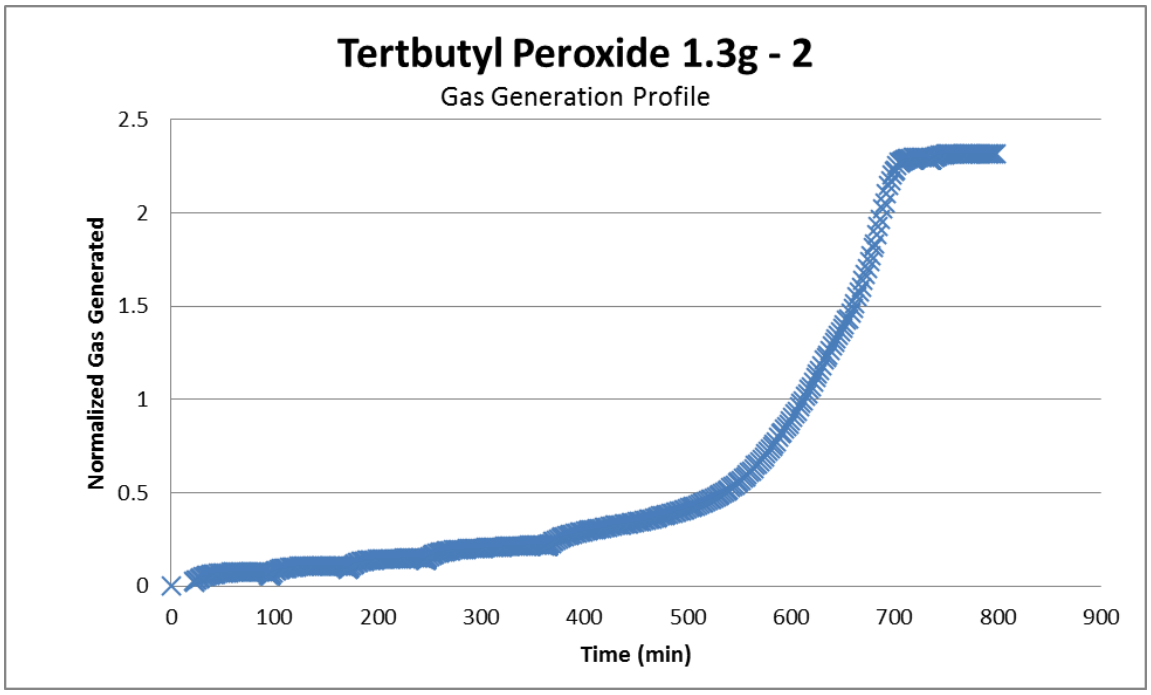

Fig. A.6 Normalized Gas Generation - Tertbutyl Peroxide 1.3g lg – 2

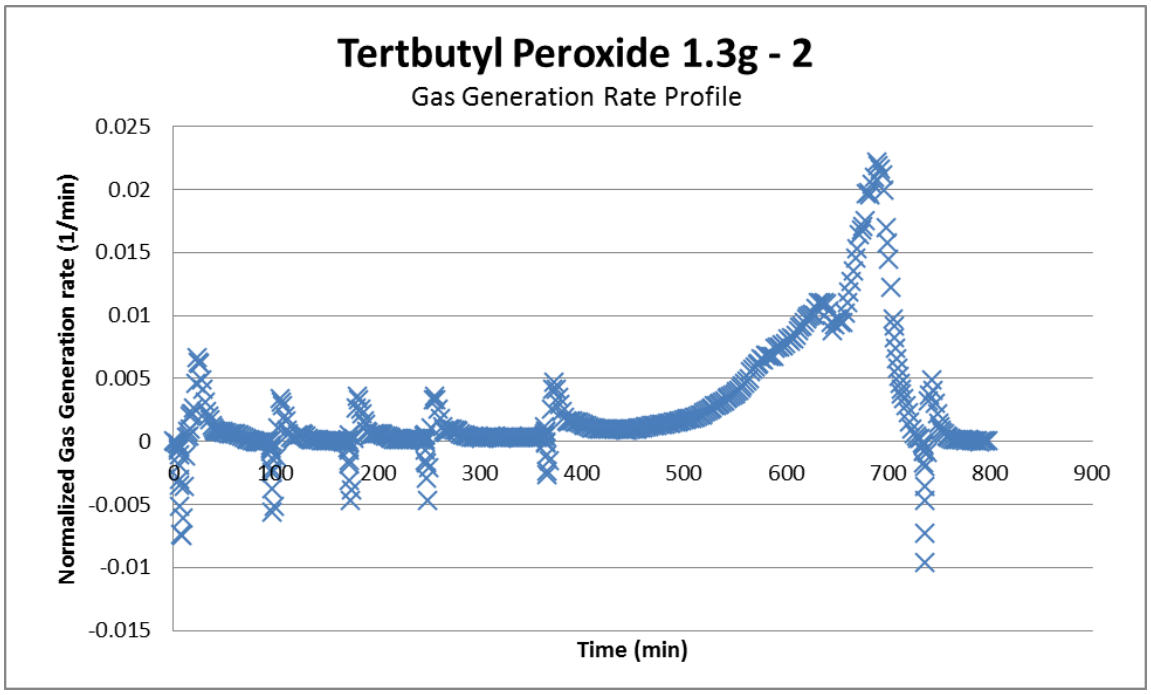

Fig. A.7 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g lg – 2

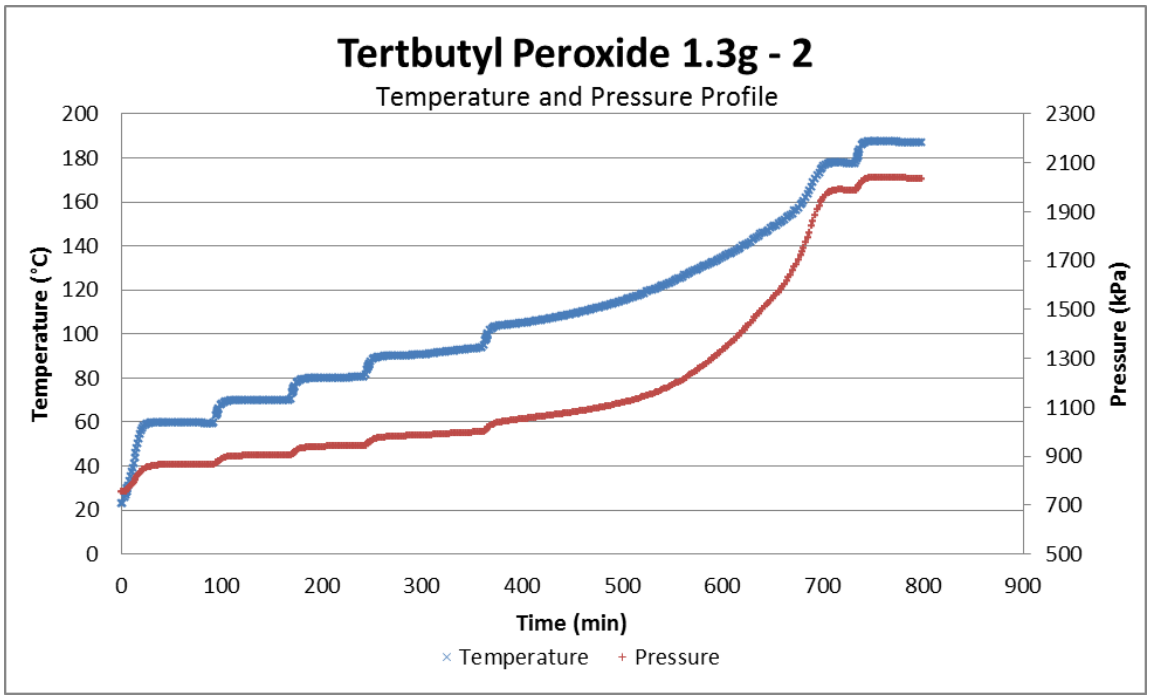

Fig. A.8 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g lg – 2

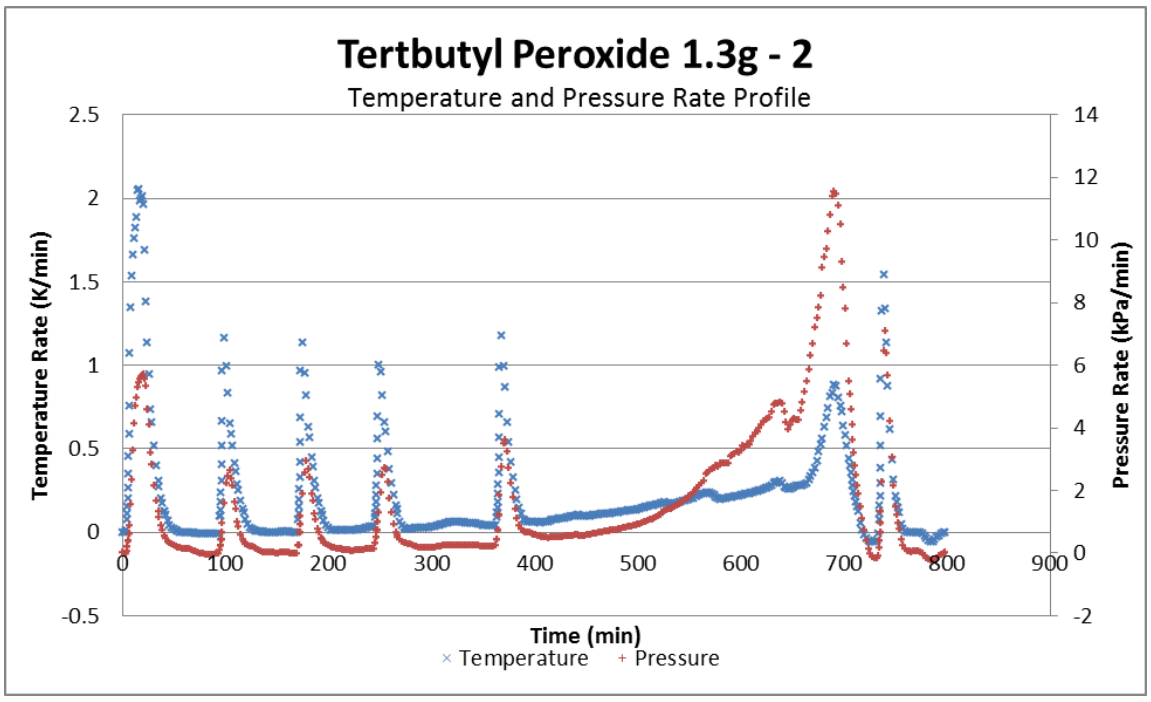

Fig. A.9 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g lg – 2

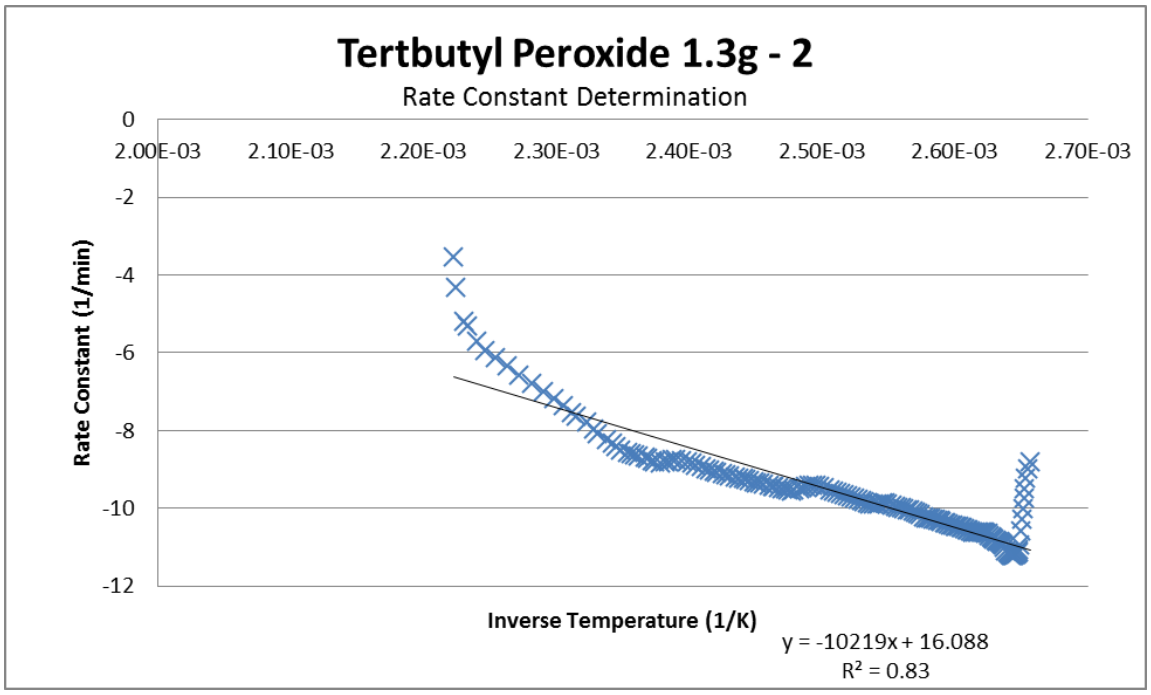

Fig. A.10 Rate Constant Determination - Tertbutyl Peroxide 1.3g lg – 2

A.3 Tertbutyl Peroxide 1.3g lg – 3

Table A.9
Material Properties - Tertbutyl Peroxide 1.3g lg – 3

Property	Value
m_s (g)	1.34
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.10
Cell Properties - Tertbutyl Peroxide 1.3g lg – 3

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	22.637

Table A.11
IPD Properties - Tertbutyl Peroxide 1.3g lg – 3

Property	Value
A (1/s)	7.500E+07
E_A (J/(mol*K))	9.159E+04
T_{onset} (°C)	100
T_{max} (°C)	178
ΔH (J/g)	2647.
IPD (W/ml)	113.17

Table A.12
Gas Properties - Tertbutyl Peroxide 1.3g lg – 3

Property	Value
n_{max} (mol)	2.112E-02
dn/dt_{max} (mol/min)	2.431E-04
n_{maxn}	2.304E+00
dn/dt_{maxn} (1/min)	2.653E-02
GGP (1/min)	6.112E-02

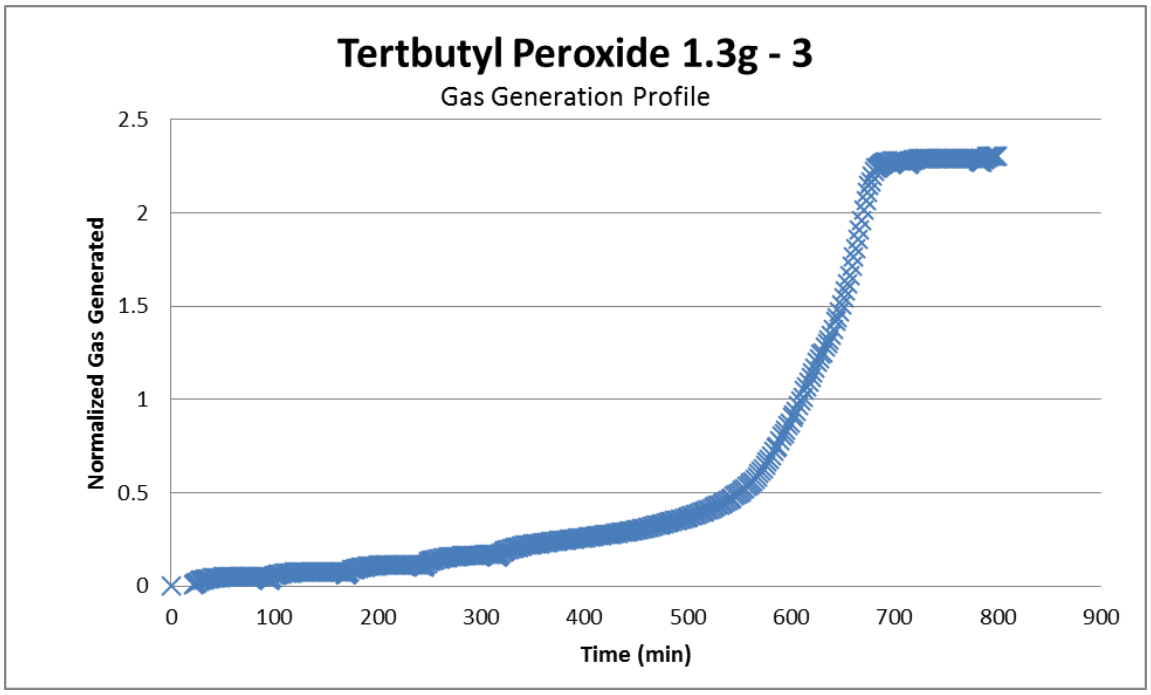

Fig. A.11 Normalized Gas Generation - Tertbutyl Peroxide 1.3g lg – 3

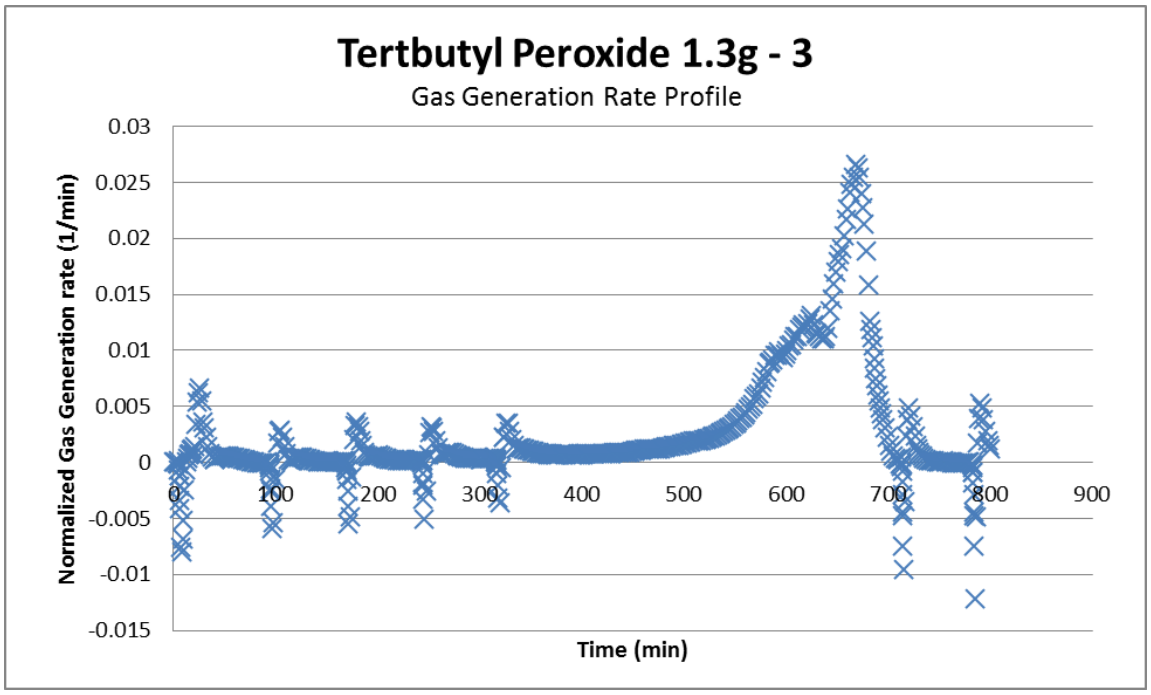

Fig. A.12 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g lg – 3

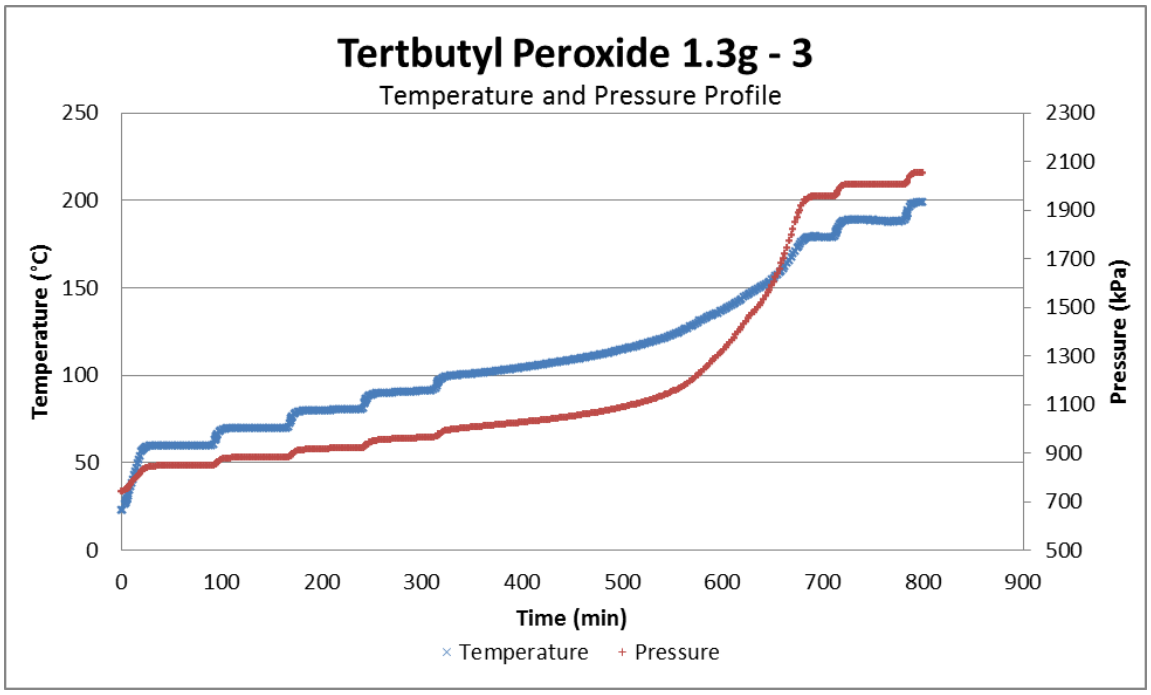

Fig. A.13 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g lg – 3

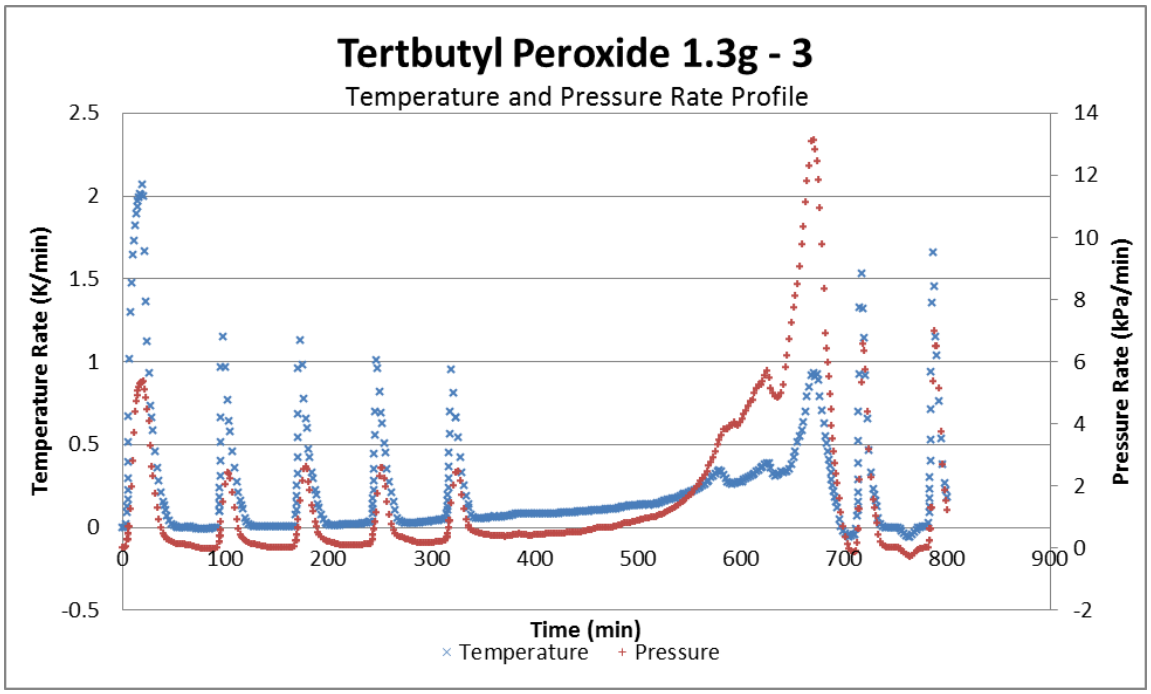

Fig. A.14 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g lg – 3

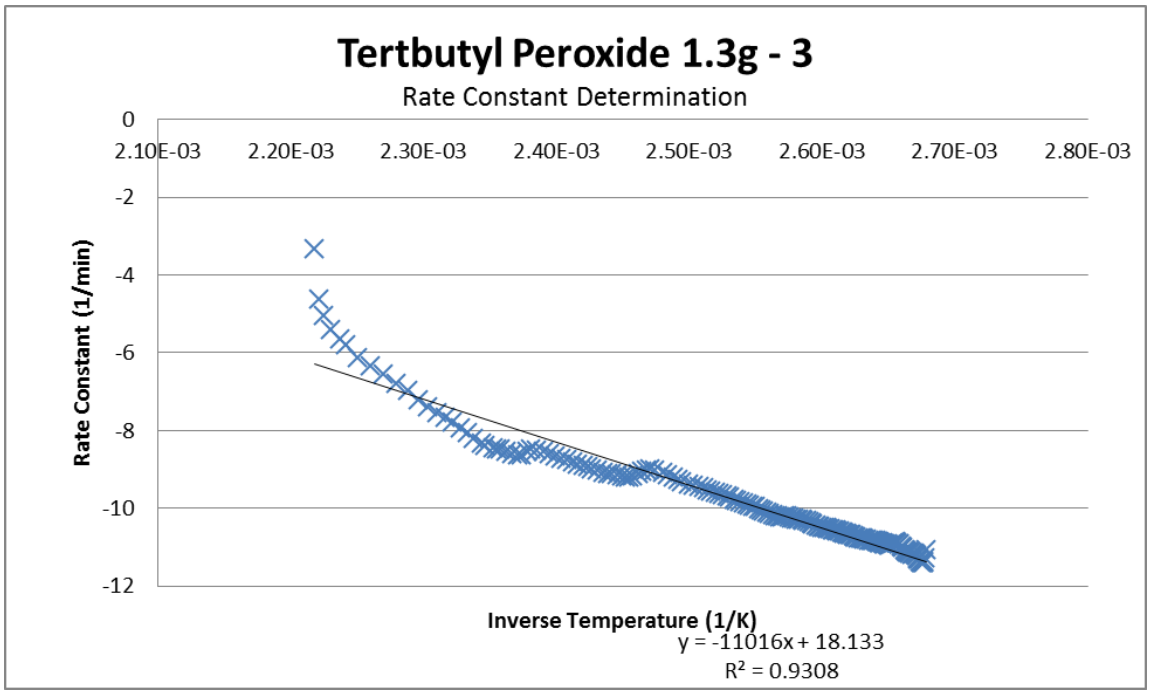

Fig. A.15 Rate Constant Determination - Tertbutyl Peroxide 1.3g lg – 3

A.4 Tertbutyl Peroxide 1.3g lg – 4

Table A.13
Material Properties - Tertbutyl Peroxide 1.3g lg – 4

Property	Value
m_s (g)	1.36
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.14
Cell Properties - Tertbutyl Peroxide 1.3g lg – 4

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	22.32

Table A.15
IPD Properties - Tertbutyl Peroxide 1.3g lg – 4

Property	Value
A (1/s)	6.013E+07
E_A (J/(mol*K))	9.093E+04
T_{onset} (°C)	100
T_{max} (°C)	178
ΔH (J/g)	2610.
IPD (W/ml)	104.23

Table A.16
Gas Properties - Tertbutyl Peroxide 1.3g lg – 4

Property	Value
n_{max} (mol)	1.839E-02
dn/dt_{max} (mol/min)	2.001E-04
n_{maxn}	1.977E+00
dn/dt_{maxn} (1/min)	2.152E-02
GGP (1/min)	4.254E-02

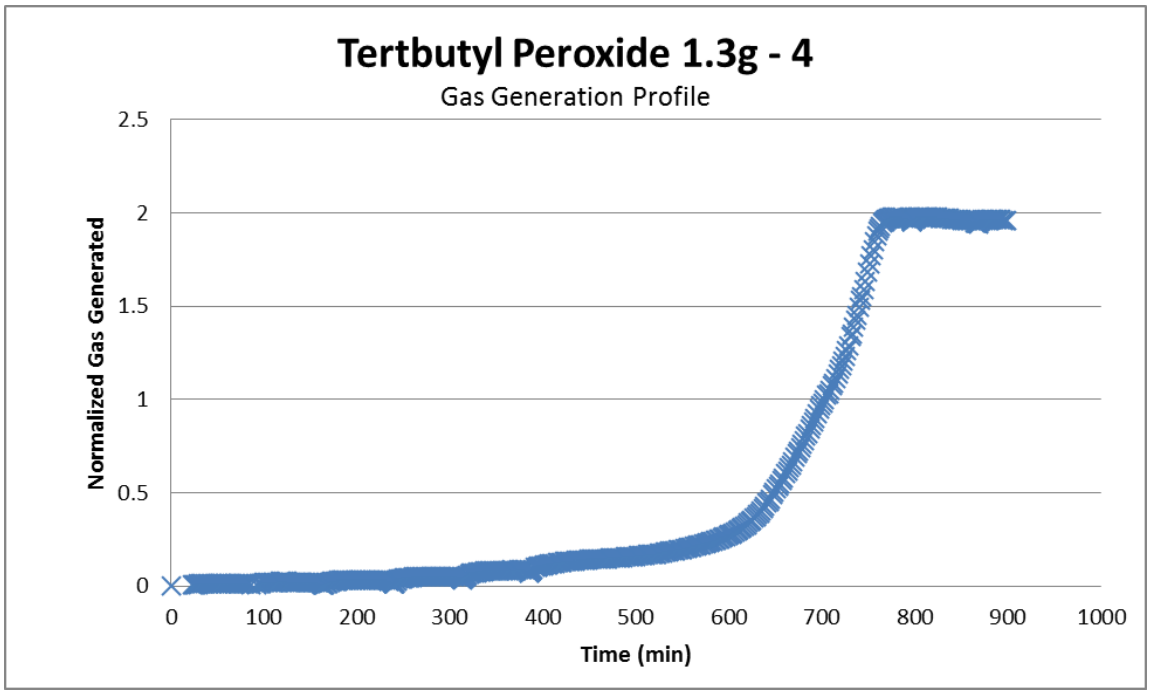

Fig. A.16 Normalized Gas Generation - Tertbutyl Peroxide 1.3g lg – 4

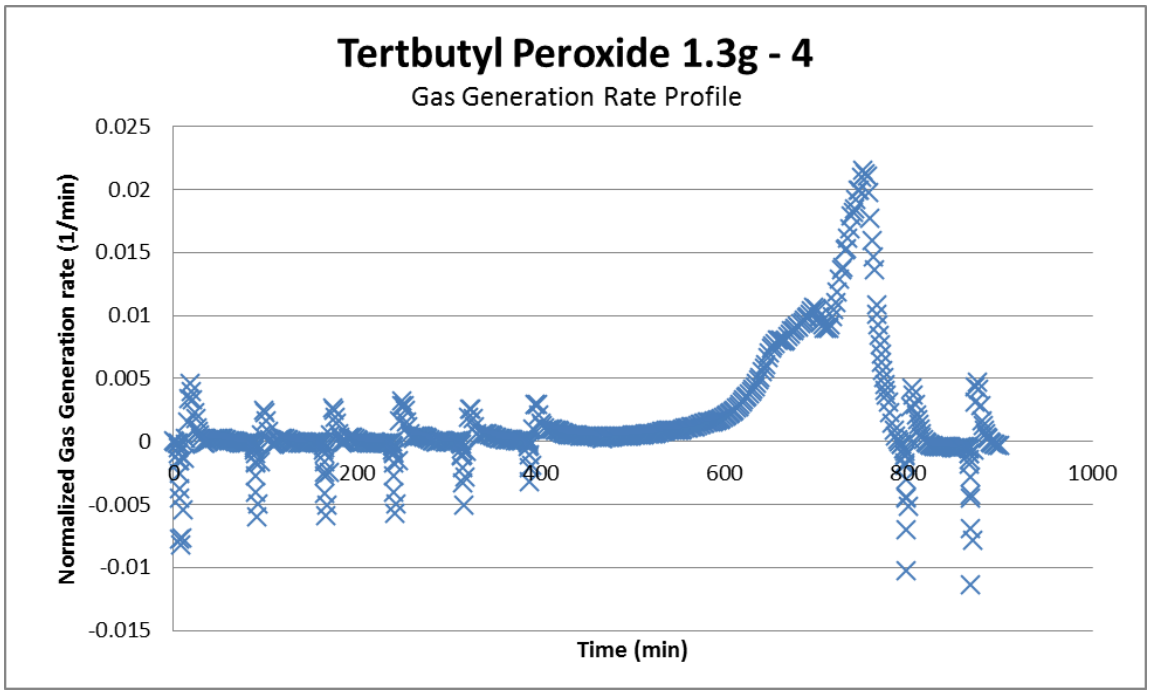

Fig. A.17 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g lg – 4

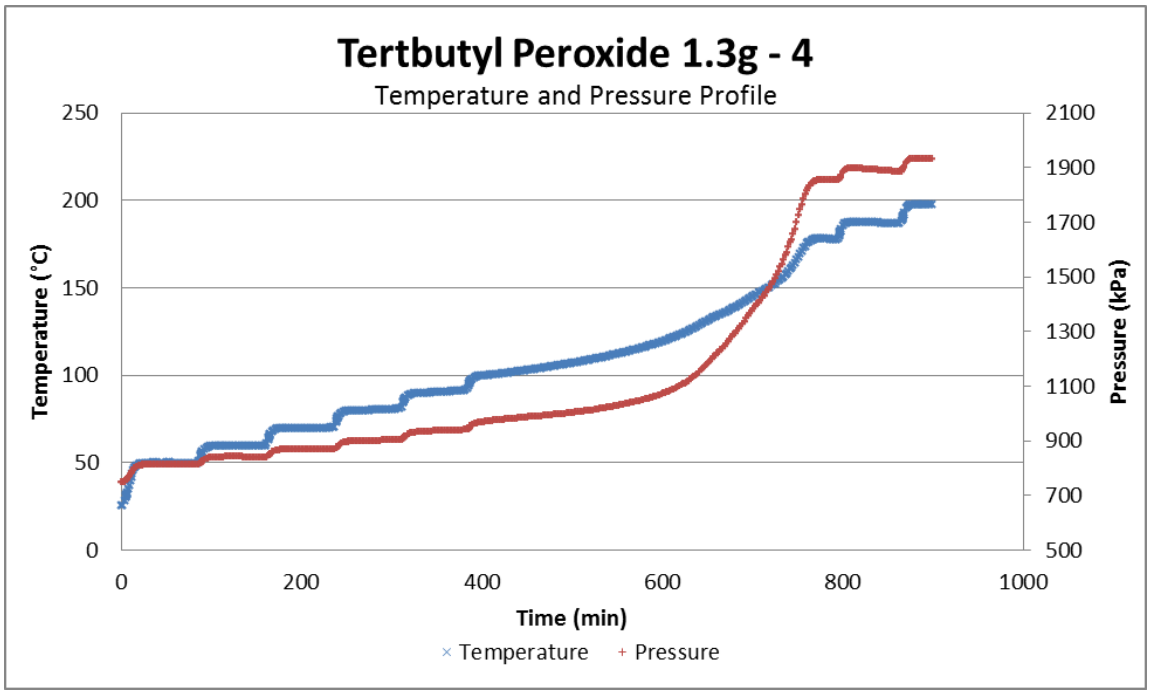

Fig. A.18 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g lg – 4

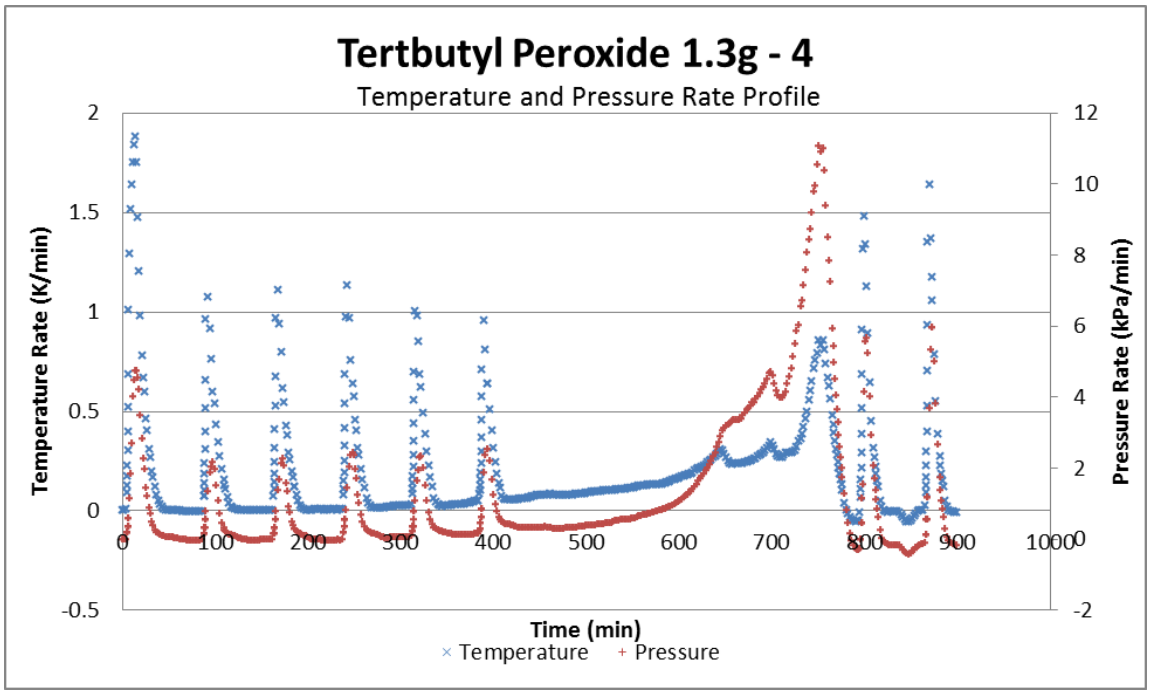

Fig. A.19 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g lg – 4

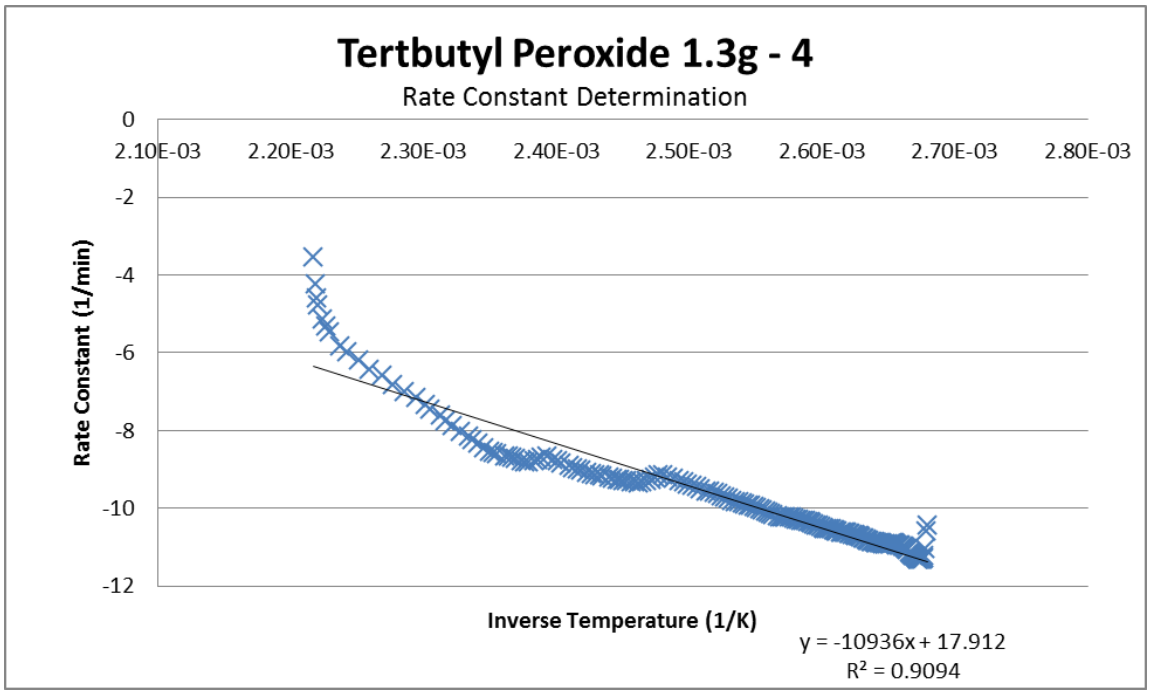

Fig. A.20 Rate Constant Determination - Tertbutyl Peroxide 1.3g lg – 4

A.5 Tertbutyl Peroxide 1.3g lg – 5

Table A.17
Material Properties - Tertbutyl Peroxide 1.3g lg – 5

Property	Value
m_s (g)	1.38
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.18
Cell Properties - Tertbutyl Peroxide 1.3g lg – 5

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	22.01

Table A.19
IPD Properties - Tertbutyl Peroxide 1.3g lg – 5

Property	Value
A (1/s)	8.052E+07
E_A (J/(mol*K))	9.187E+04
T_{onset} (°C)	100
T_{max} (°C)	177
ΔH (J/g)	2540.
IPD (W/ml)	109.49

Table A.20
Gas Properties - Tertbutyl Peroxide 1.3g lg – 5

Property	Value
n_{max} (mol)	2.100E-02
dn/dt_{max} (mol/min)	2.620E-04
n_{maxn}	2.225E+00
dn/dt_{maxn} (1/min)	2.776E-02
GGP (1/min)	6.178E-02

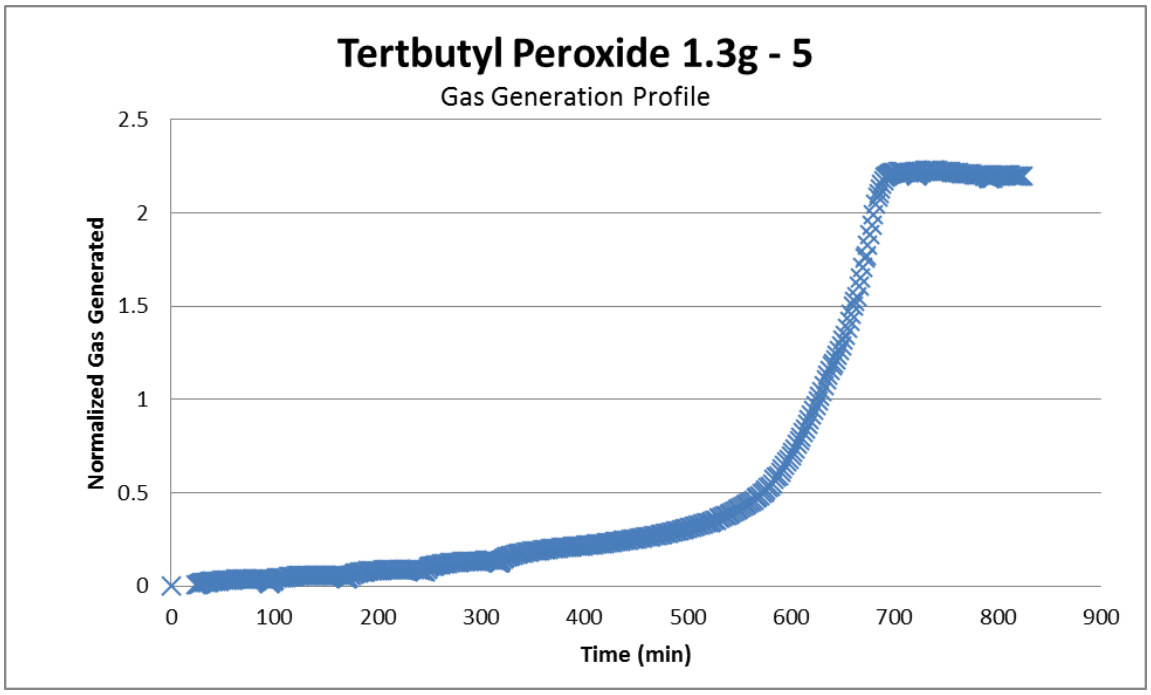

Fig. A.21 Normalized Gas Generation - Tertbutyl Peroxide 1.3g lg – 5

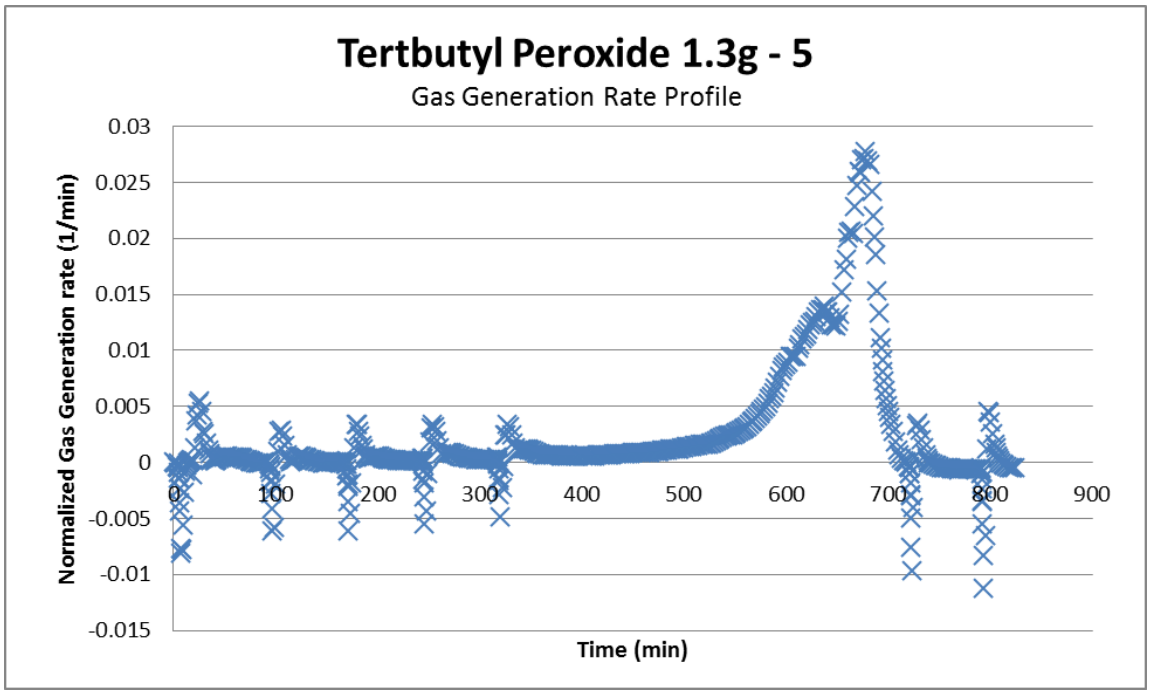

Fig. A.22 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g lg – 5

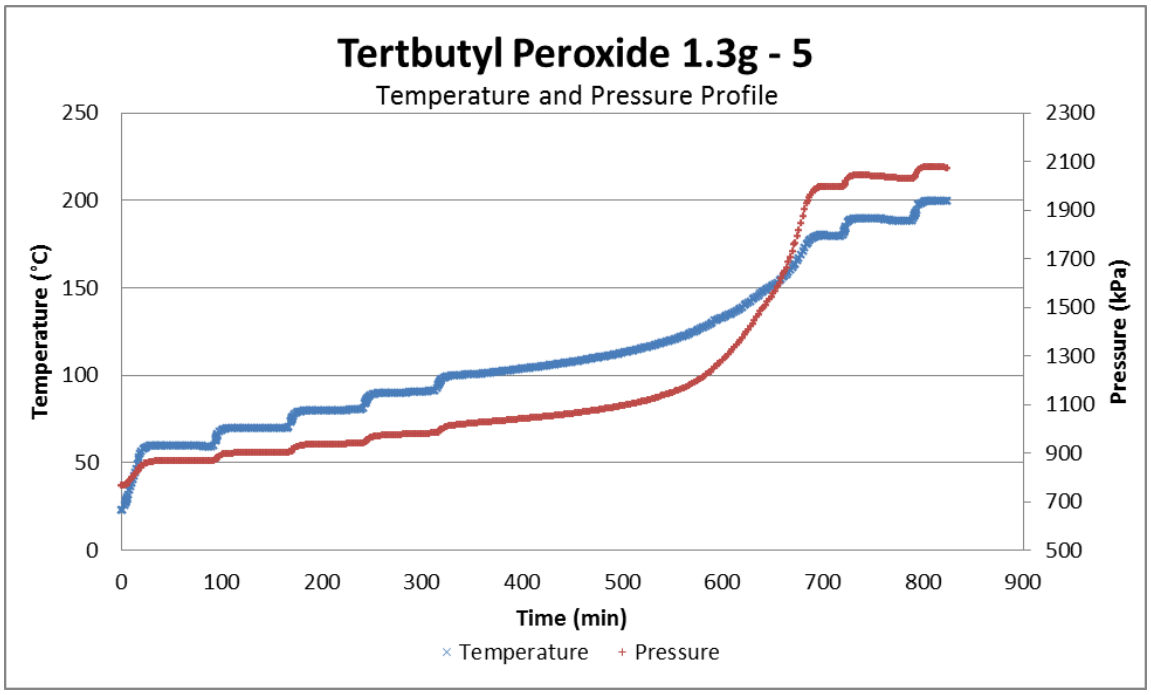

Fig. A.23 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g lg – 5

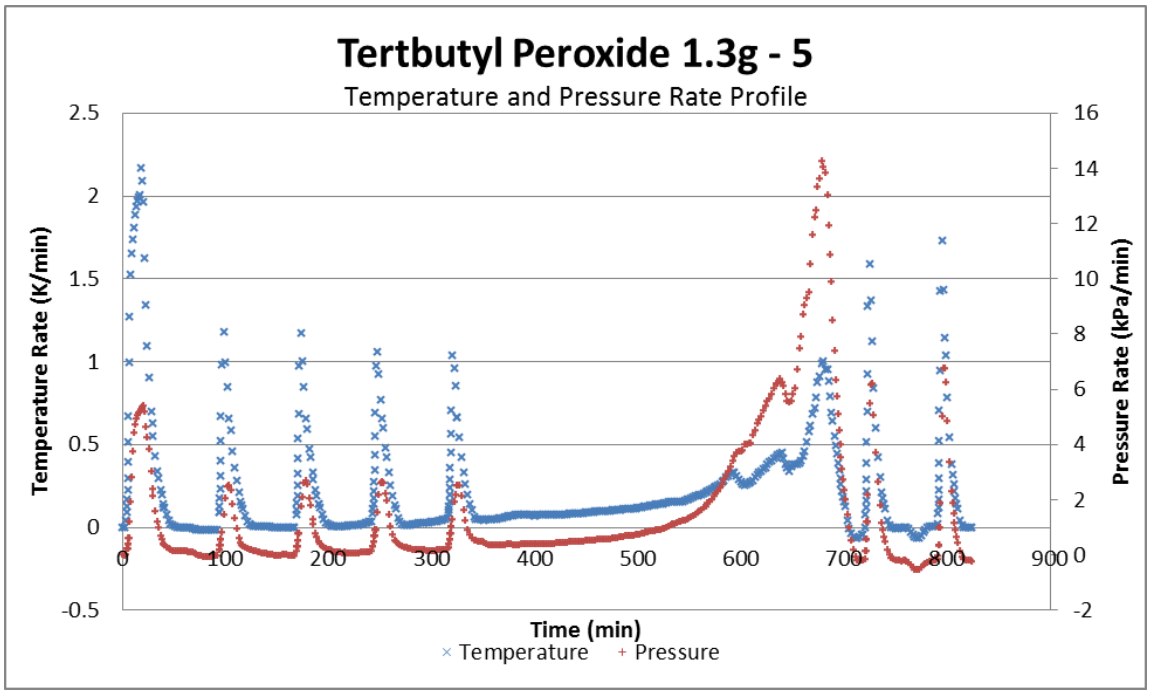

Fig. A.24 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g lg – 5

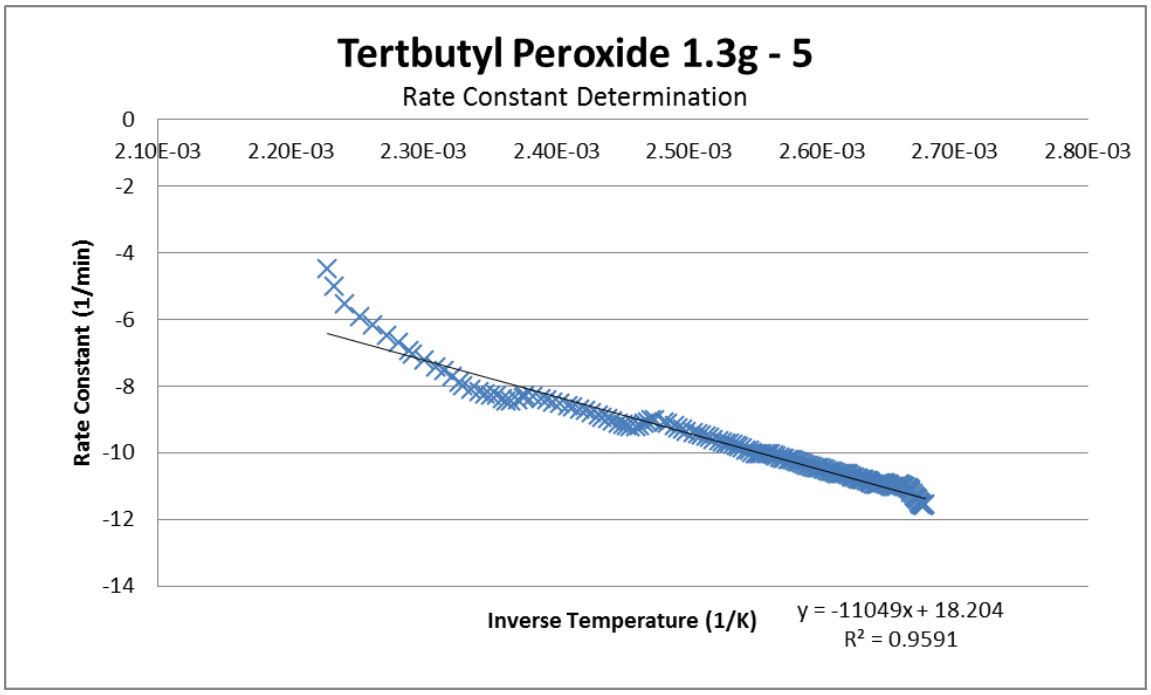

Fig. A.25 Rate Constant Determination - Tertbutyl Peroxide 1.3g lg – 5

A.6 Tertbutyl Peroxide 1.3g – md

Table A.21
Material Properties - Tertbutyl Peroxide 1.3g - md

Property	Value
m_s (g)	1.36
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.22
Cell Properties - Tertbutyl Peroxide 1.3g - md

Property	Value
m_{cell} (g)	35.21
V_{cell} (mL)	43.68
φ	15.51

Table A.23
IPD Properties - Tertbutyl Peroxide 1.3g - md

Property	Value
A (1/s)	2.715E+09
E_A (J/(mol*K))	1.024E+05
T_{onset} (°C)	90
T_{max} (°C)	200
ΔH (J/g)	2557.
IPD (W/ml)	327.91

Table A.24
Gas Properties - Tertbutyl Peroxide 1.3g - md

Property	Value
n_{max} (mol)	1.824E-02
dn/dt_{max} (mol/min)	2.590E-03
n_{maxn}	1.961E+00
dn/dt_{maxn} (1/min)	2.784E-01
GGP (1/min)	5.460E-01

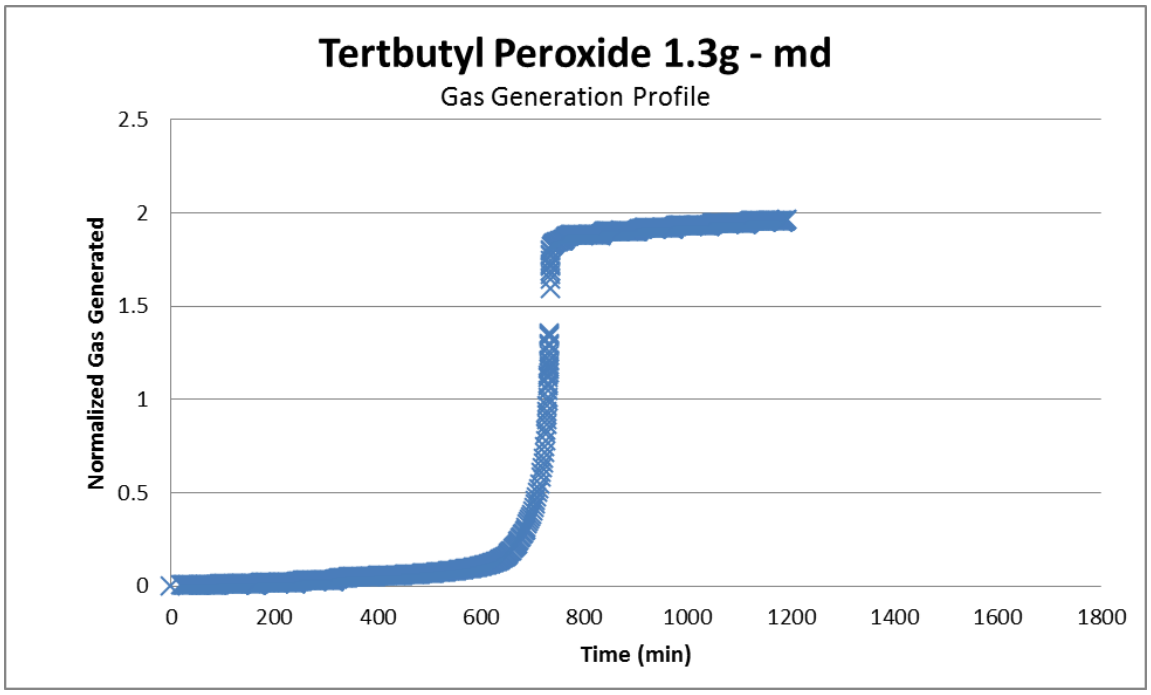

Fig. A.26 Normalized Gas Generation - Tertbutyl Peroxide 1.3g - md

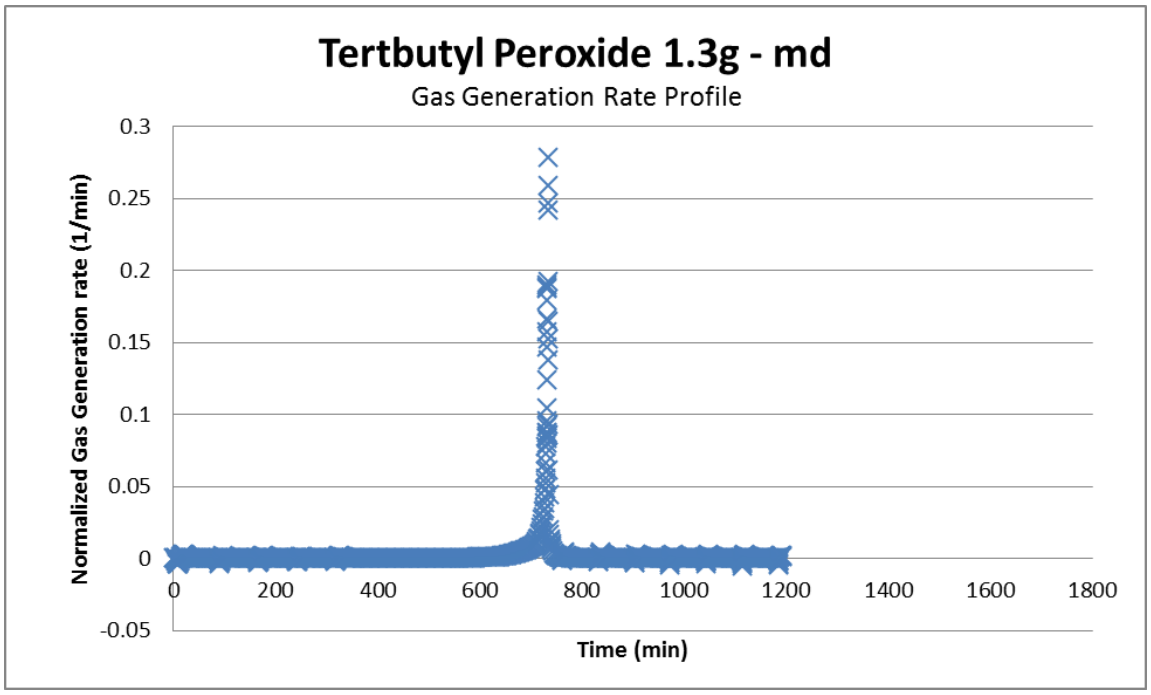

Fig. A.27 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g - md

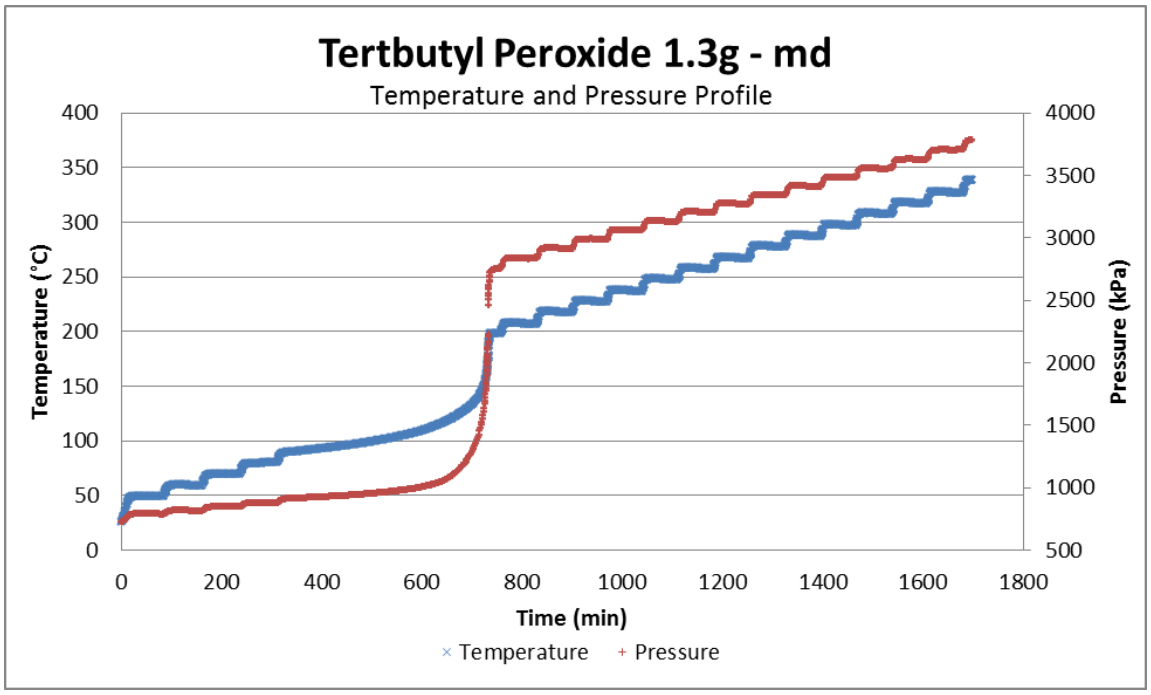

Fig. A.28 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g - md

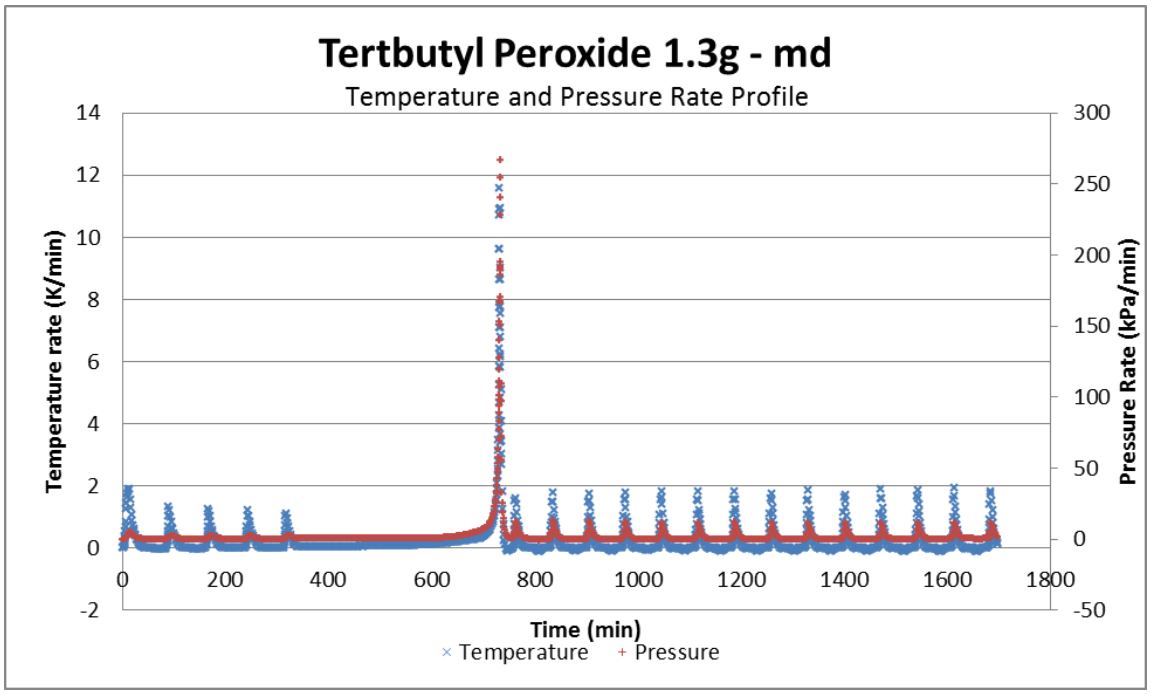

Fig. A.29 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g - md

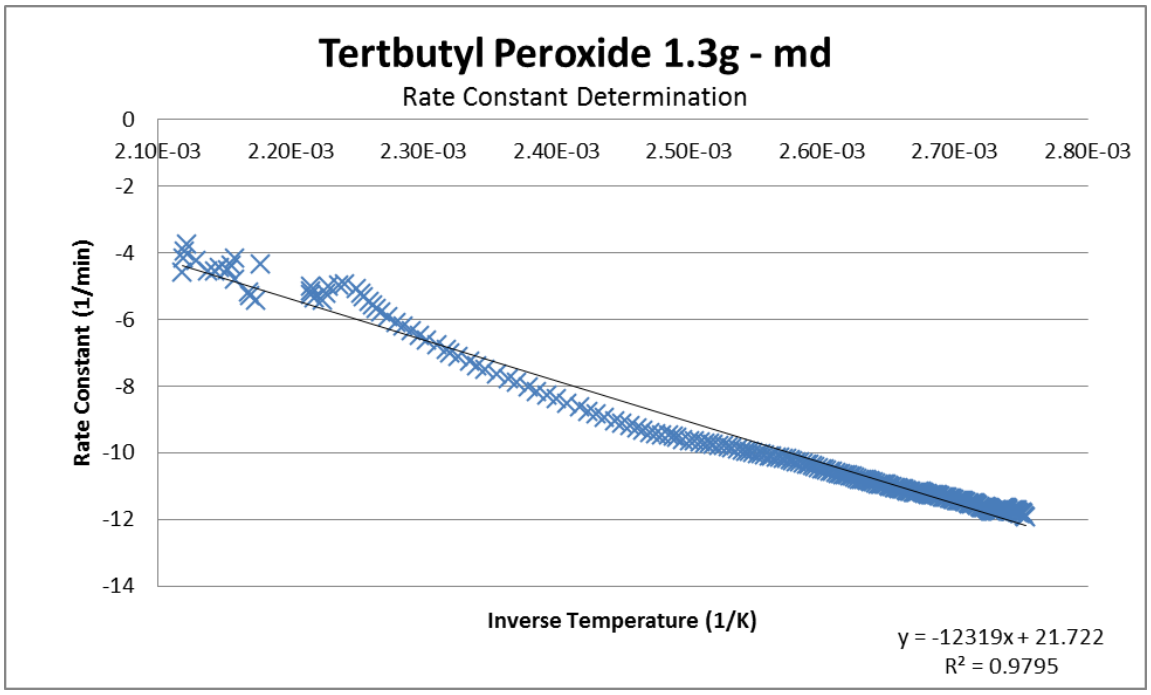

Fig. A.30 Rate Constant Determination - Tertbutyl Peroxide 1.3g - md

A.7 Tertbutyl Peroxide 1.3g – sm

Table A.25
Material Properties - Tertbutyl Peroxide 1.3g - sm

Property	Value
m_s (g)	1.32
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.26
Cell Properties - Tertbutyl Peroxide 1.3g - sm

Property	Value
m_{cell} (g)	23.19
V_{cell} (mL)	31.02
φ	10.84

Table A.27
IPD Properties - Tertbutyl Peroxide 1.3g - sm

Property	Value
A (1/s)	1.869E+10
E_A (J/(mol*K))	1.066E+05
T_{onset} (°C)	80
T_{max} (°C)	198
ΔH (J/g)	1918.
IPD (W/ml)	648.52

Table A.28
Gas Properties - Tertbutyl Peroxide 1.3g - sm

Property	Value
n_{max} (mol)	1.645E-02
dn/dt_{max} (mol/min)	5.030E-02
n_{maxn}	1.823E+00
dn/dt_{maxn} (1/min)	5.572E+00
GGP (1/min)	1.016E+01

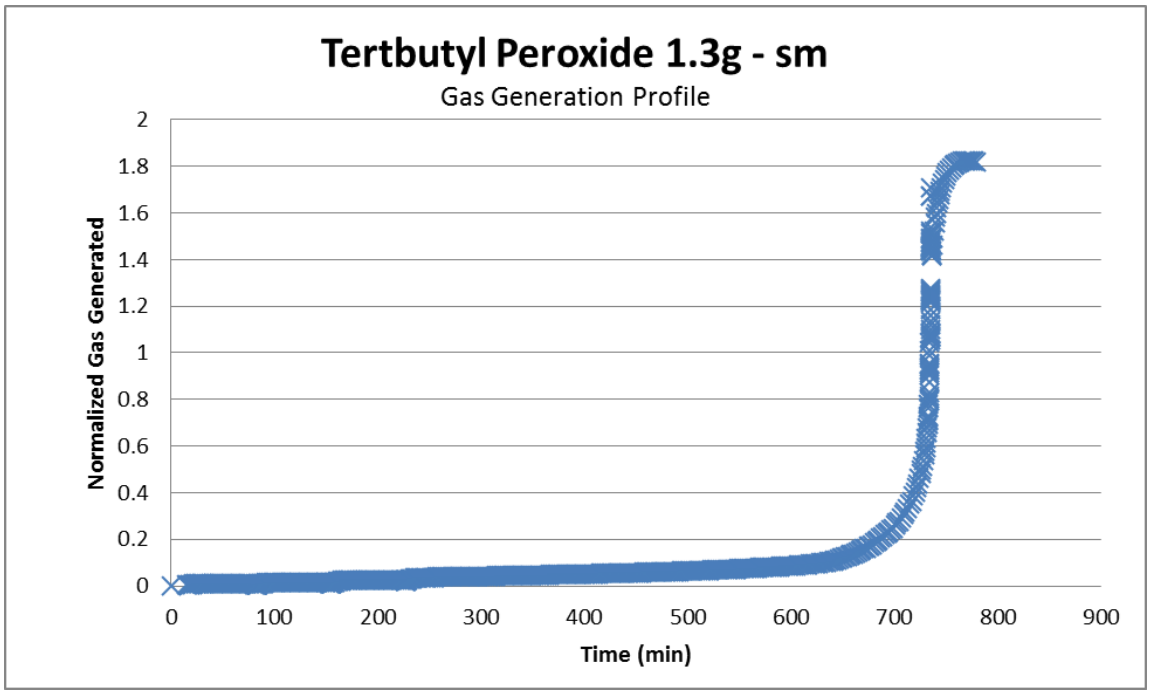

Fig. A.31 Normalized Gas Generation - Tertbutyl Peroxide 1.3g - sm

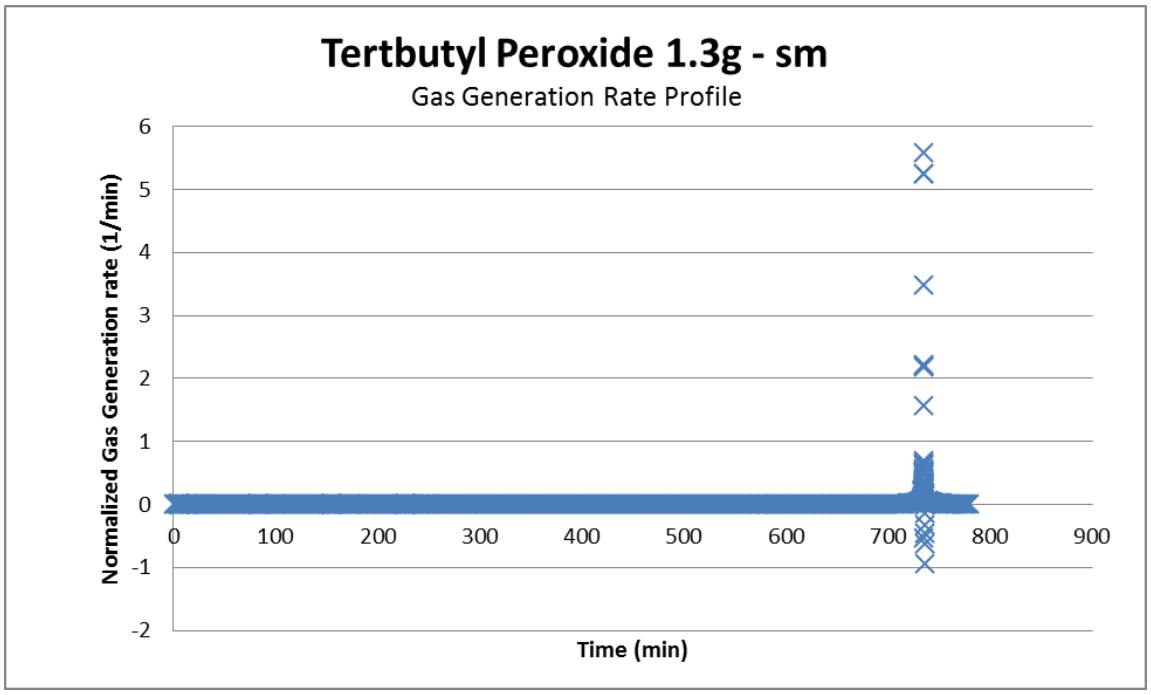

Fig. A.32 Normalized Gas Generation Rate - Tertbutyl Peroxide 1.3g - sm

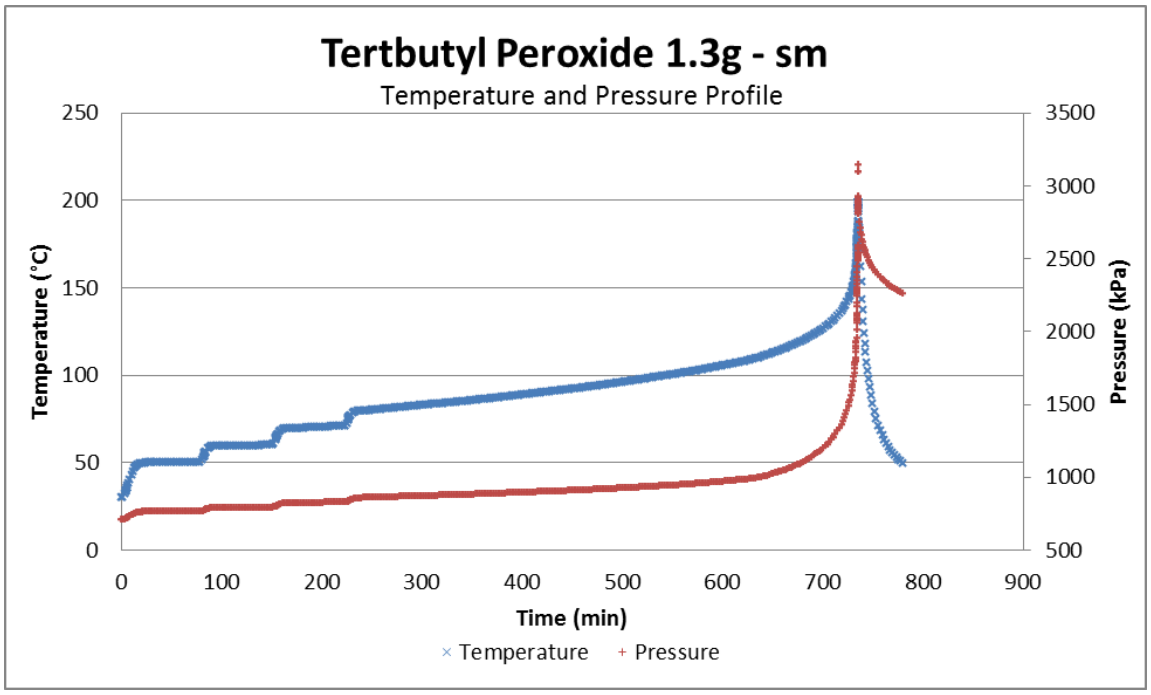

Fig. A.33 Temperature and Pressure Profiles - Tertbutyl Peroxide 1.3g - sm

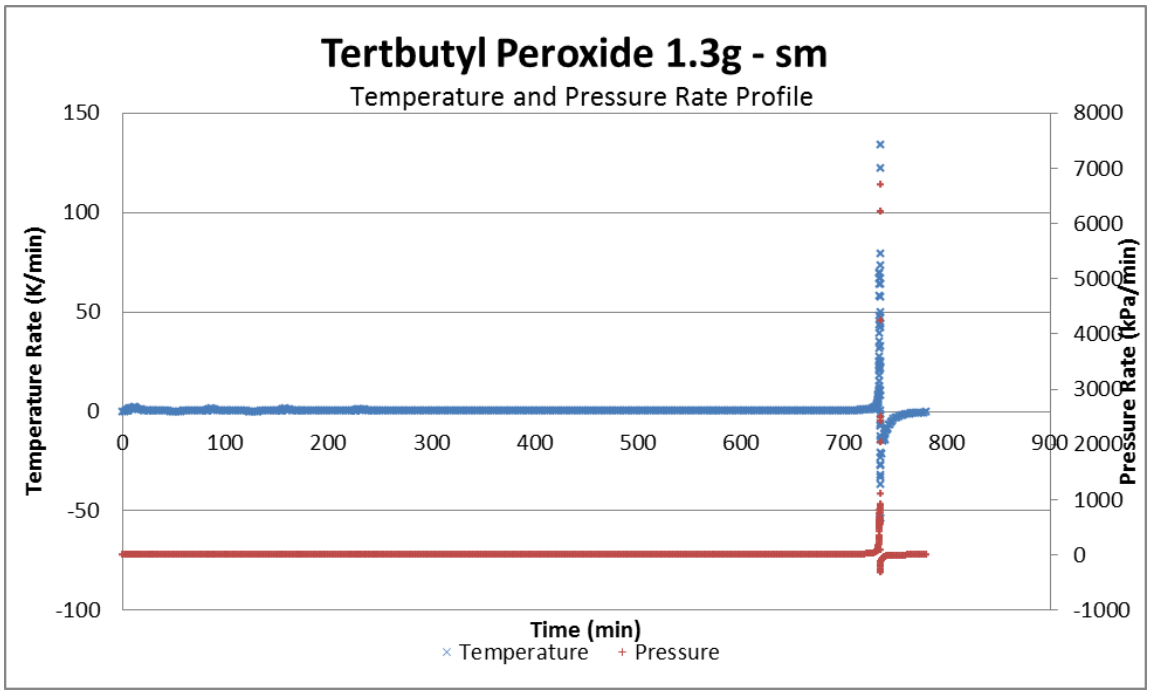

Fig. A.34 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 1.3g - sm

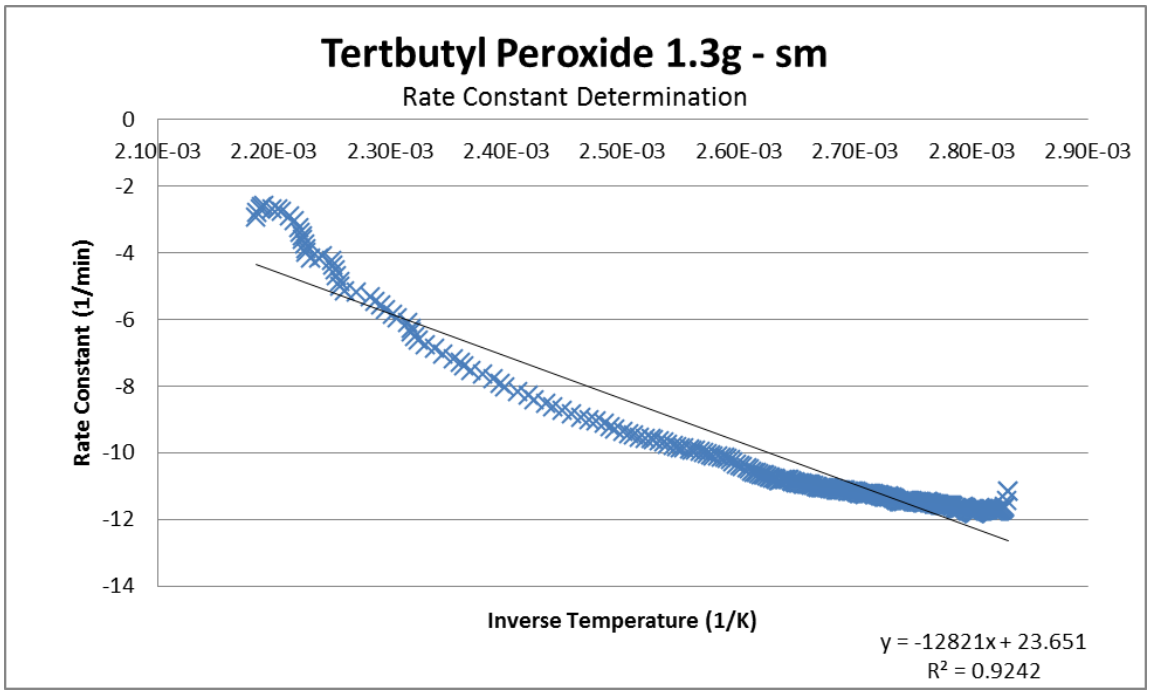

Fig. A.35 Rate Constant Determination - Tertbutyl Peroxide 1.3g - sm

A.8 Tertbutyl Peroxide 3g – lg

Table A.29
Material Properties - Tertbutyl Peroxide 3g - lg

Property	Value
m_s (g)	3.17
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.30
Cell Properties - Tertbutyl Peroxide 3g - lg

Property	Value
m_{cell} (g)	55.42
V_{cell} (mL)	92.69
φ	10.80

Table A.31
IPD Properties - Tertbutyl Peroxide 3g - lg

Property	Value
A (1/s)	8.928E+27
E_A (J/(mol*K))	2.257E+05
T_{onset} (°C)	80
T_{max} (°C)	198
ΔH (J/g)	1910.
IPD (W/ml)	3.949E+08

Table A.32
Gas Properties - Tertbutyl Peroxide 3g - lg

Property	Value
n_{max} (mol)	1.702E-02
dn/dt_{max} (mol/min)	1.004E-04
n_{maxn}	7.853E-01
dn/dt_{maxn} (1/min)	4.631E-03
GGP (1/min)	3.636E-03

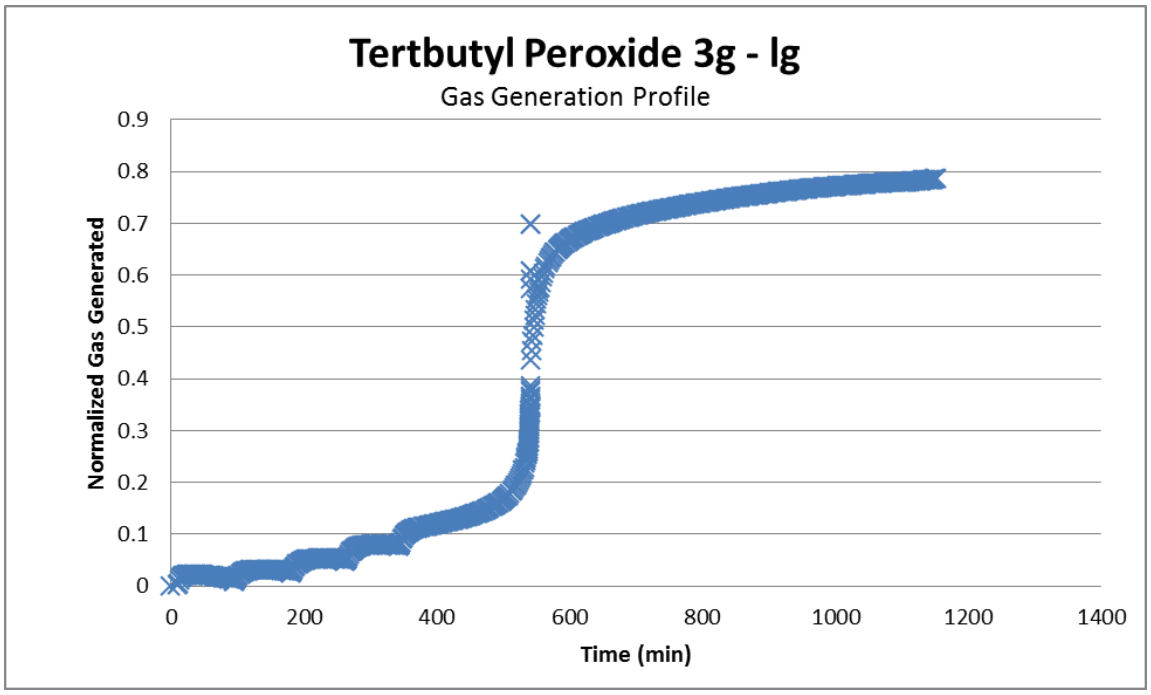

Fig. A.36 Normalized Gas Generation - Tertbutyl Peroxide 3g - lg

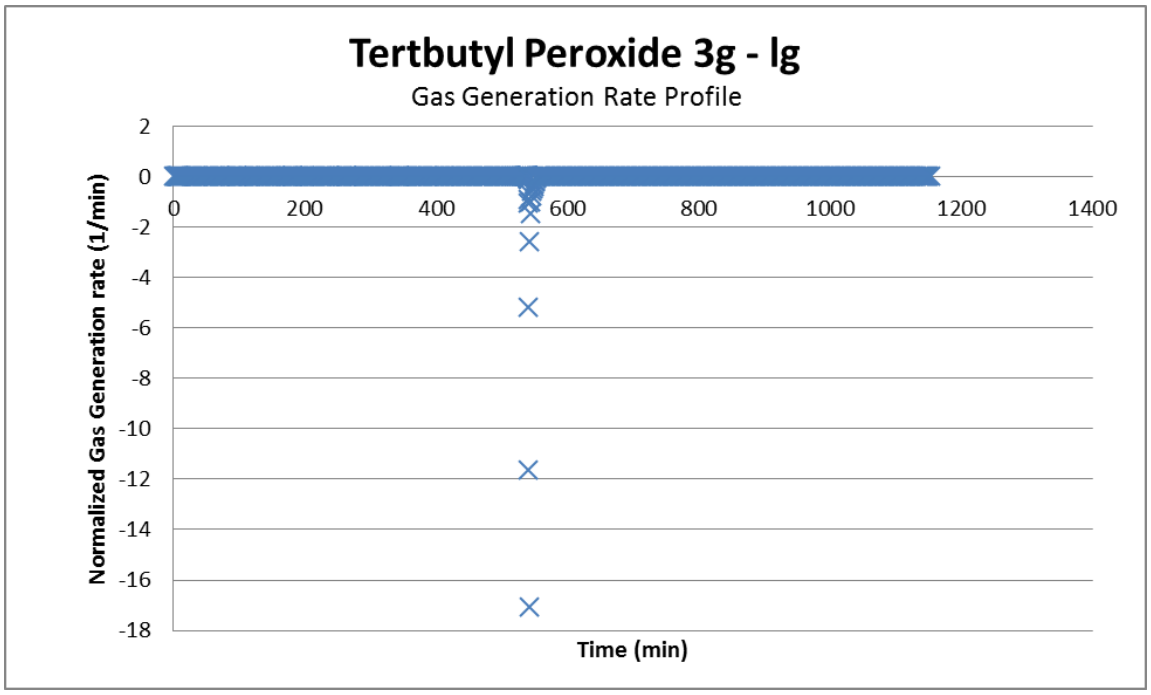

Fig. A.37 Normalized Gas Generation Rate - Tertbutyl Peroxide 3g - lg

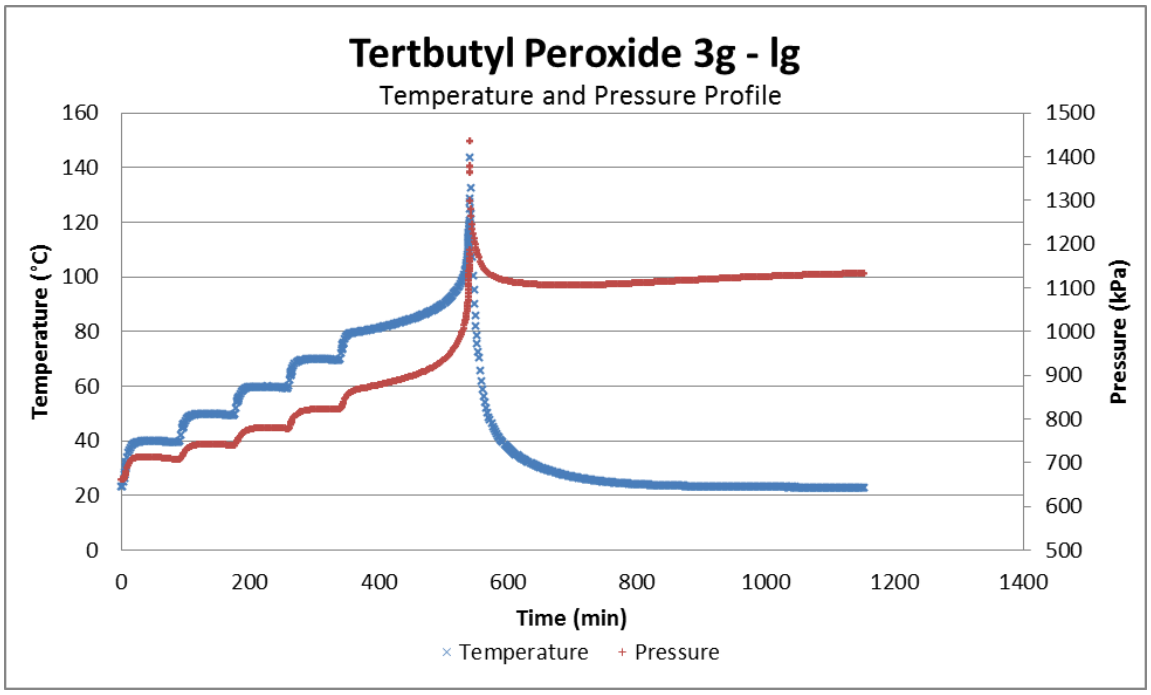

Fig. A.38 Temperature and Pressure Profiles - Tertbutyl Peroxide 3g - lg

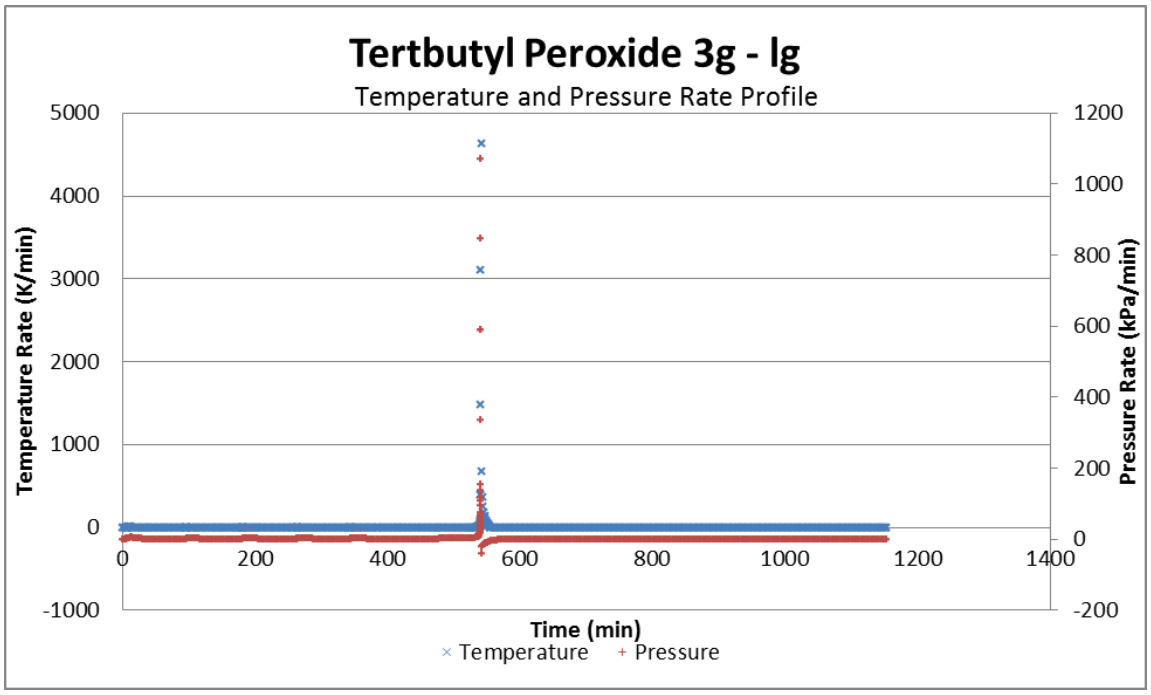

Fig. A.39 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 3g - lg

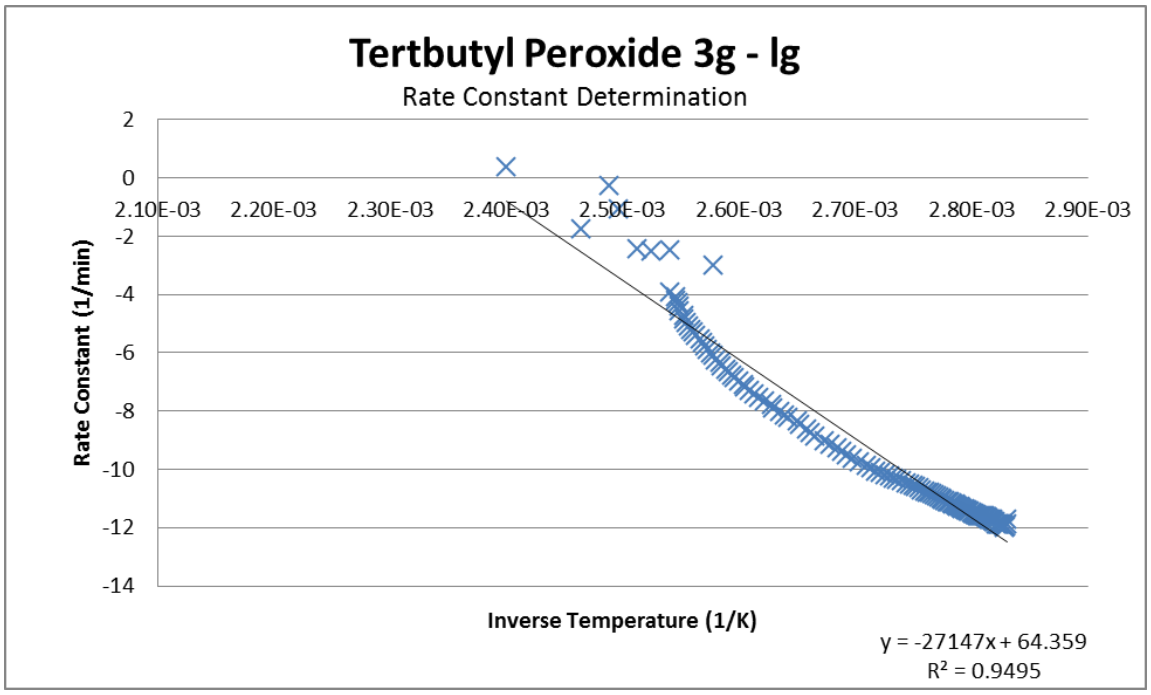

Fig. A.40 Rate Constant Determination - Tertbutyl Peroxide 3g - lg

A.9 Tertbutyl Peroxide 3g – md

Table A.33
Material Properties - Tertbutyl Peroxide 3g - md

Property	Value
m_s (g)	3.19
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.34
Cell Properties - Tertbutyl Peroxide 3g - md

Property	Value
m_{cell} (g)	38.8
V_{cell} (mL)	42.15
φ	7.816

Table A.35
IPD Properties - Tertbutyl Peroxide 3g - md

Property	Value
A (1/s)	4.569E+15
E_A (J/(mol*K))	1.488E+05
T_{onset} (°C)	100
T_{max} (°C)	220
ΔH (J/g)	1406.
IPD (W/ml)	7116.

Table A.36
Gas Properties - Tertbutyl Peroxide 3g - md

Property	Value
n_{max} (mol)	2.033E-02
dn/dt_{max} (mol/min)	5.475E-02
n_{maxn}	9.319E-01
dn/dt_{maxn} (1/min)	2.510E+00
GGP (1/min)	2.339E+00

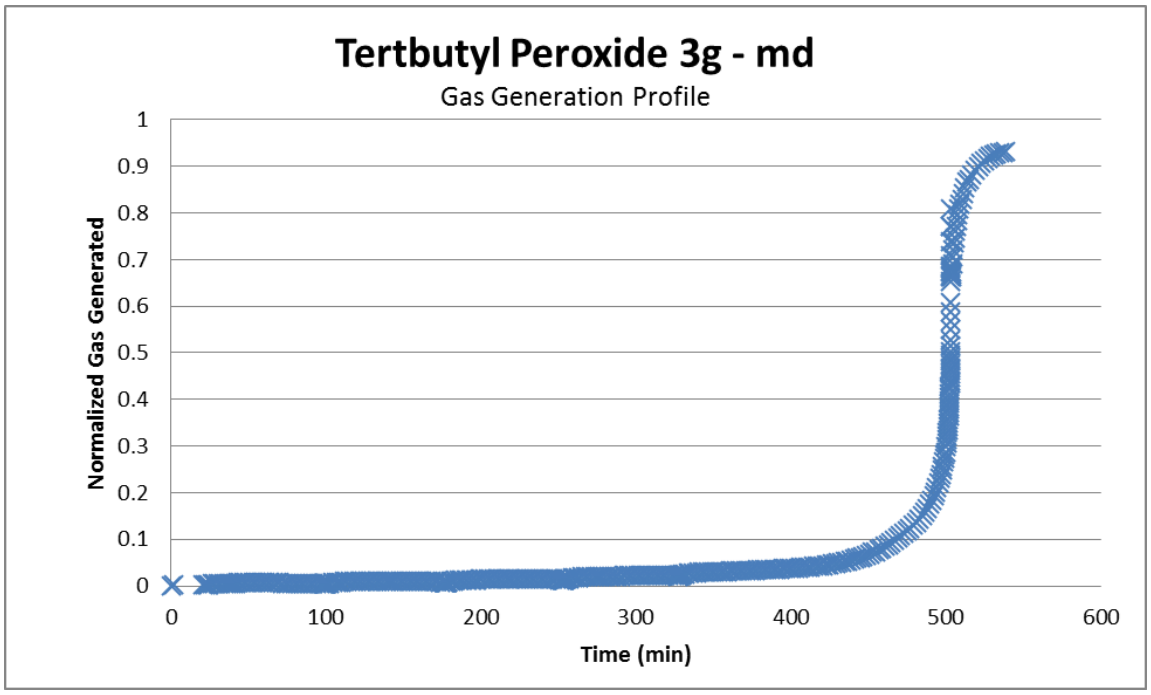

Fig. A.41 Normalized Gas Generation - Tertbutyl Peroxide 3g - md

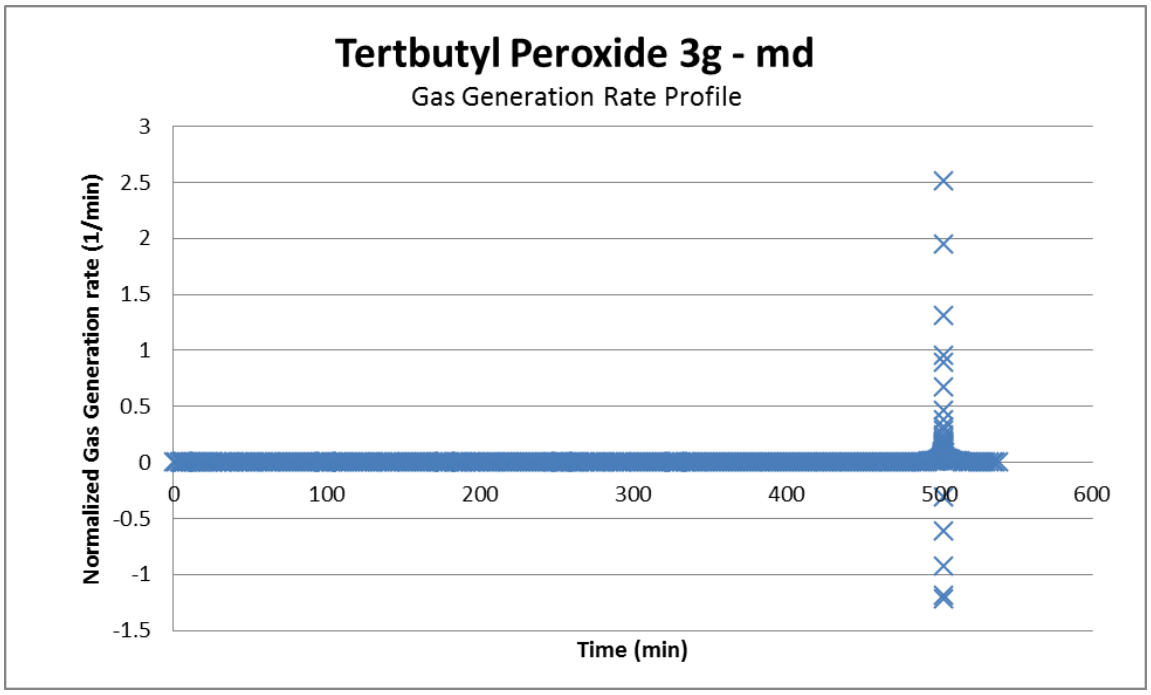

Fig. A.42 Normalized Gas Generation Rate - Tertbutyl Peroxide 3g - md

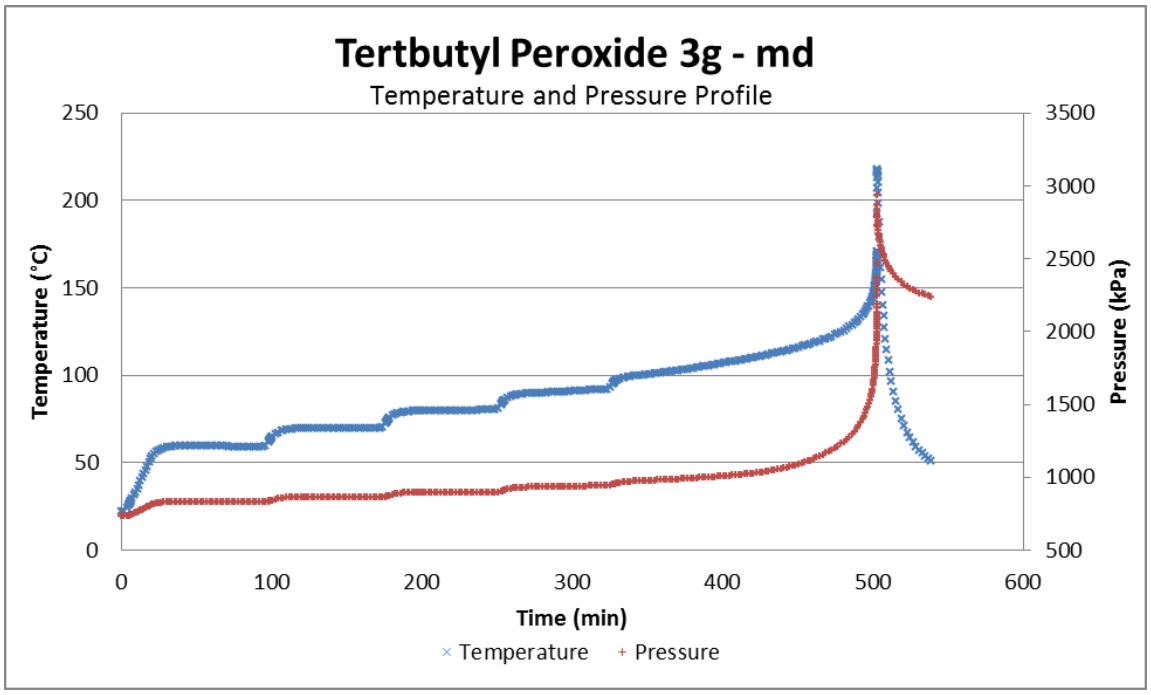

Fig. A.43 Temperature and Pressure Profiles - Tertbutyl Peroxide 3g - md

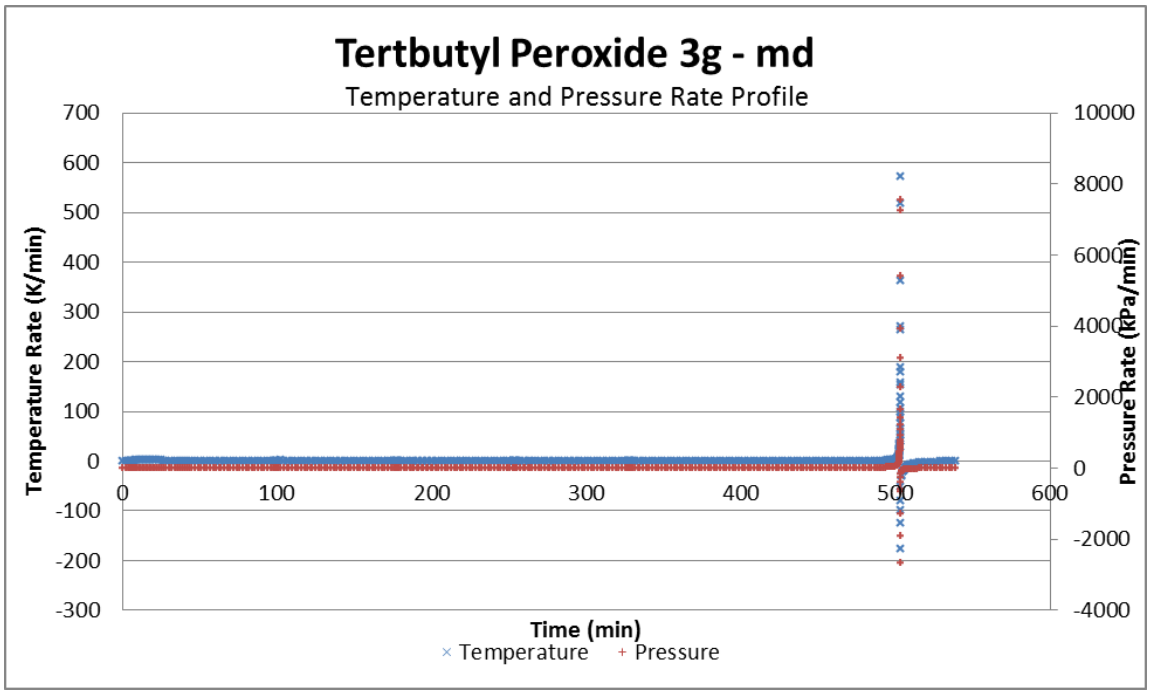

Fig. A.44 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 3g - md

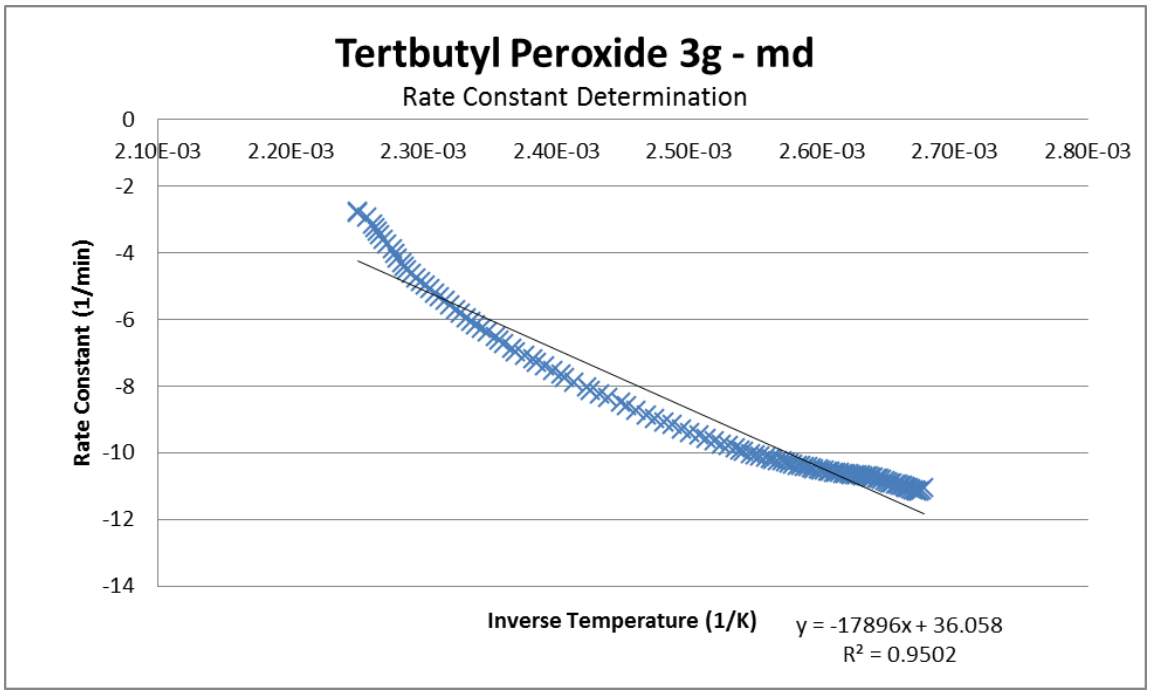

Fig. A.45 Rate Constant Determination - Tertbutyl Peroxide 3g - md

A.10 Tertbutyl Peroxide 0.5g - lg

Table A.36
Material Properties - Tertbutyl Peroxide 0.5g - lg

Property	Value
m_s (g)	0.53
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.37
Cell Properties - Tertbutyl Peroxide 0.5g - lg

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	55.71

Table A.38
IPD Properties - Tertbutyl Peroxide 0.5g - lg

Property	Value
A (1/s)	1.269E+03
E_A (J/(mol*K))	5.670E+04
T_{onset} (°C)	120
T_{max} (°C)	170
ΔH (J/g)	4175.
IPD (W/ml)	9.195

Table A.39
Gas Properties - Tertbutyl Peroxide 0.5g - lg

Property	Value
n_{max} (mol)	5.323E-03
dn/dt_{max} (mol/min)	5.975E-05
n_{maxn}	1.469E+00
dn/dt_{maxn} (1/min)	1.648E-02
GGP (1/min)	2.421E-02

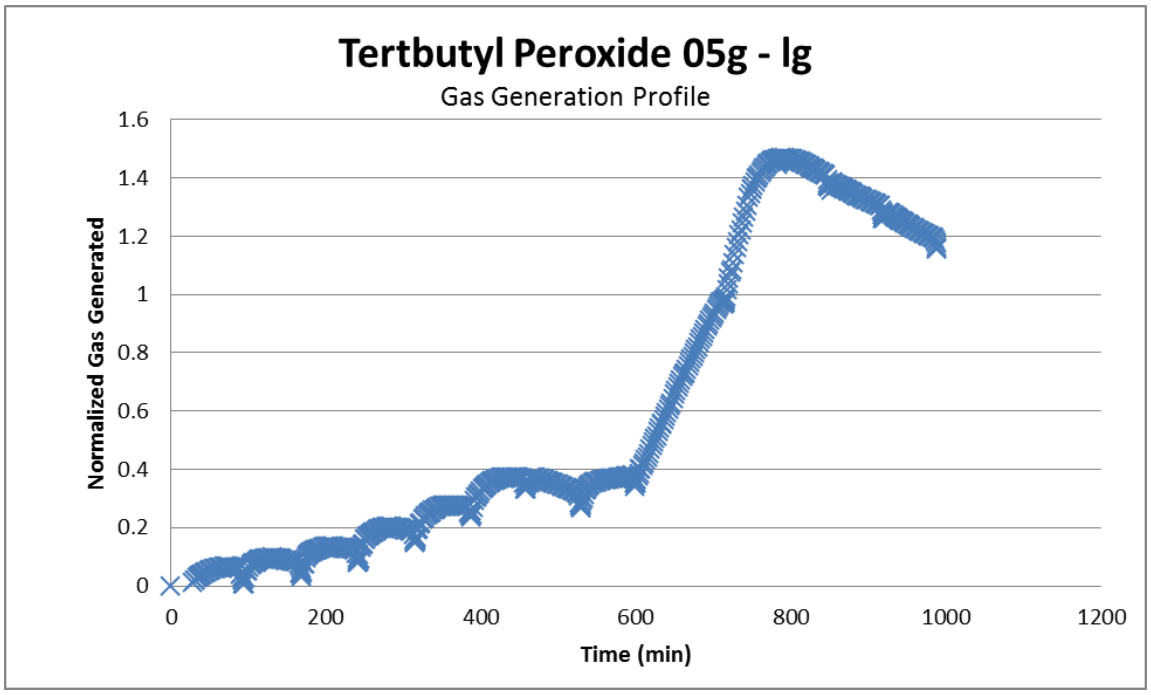

Fig. A.46 Normalized Gas Generation - Tertbutyl Peroxide 0.5g - lg

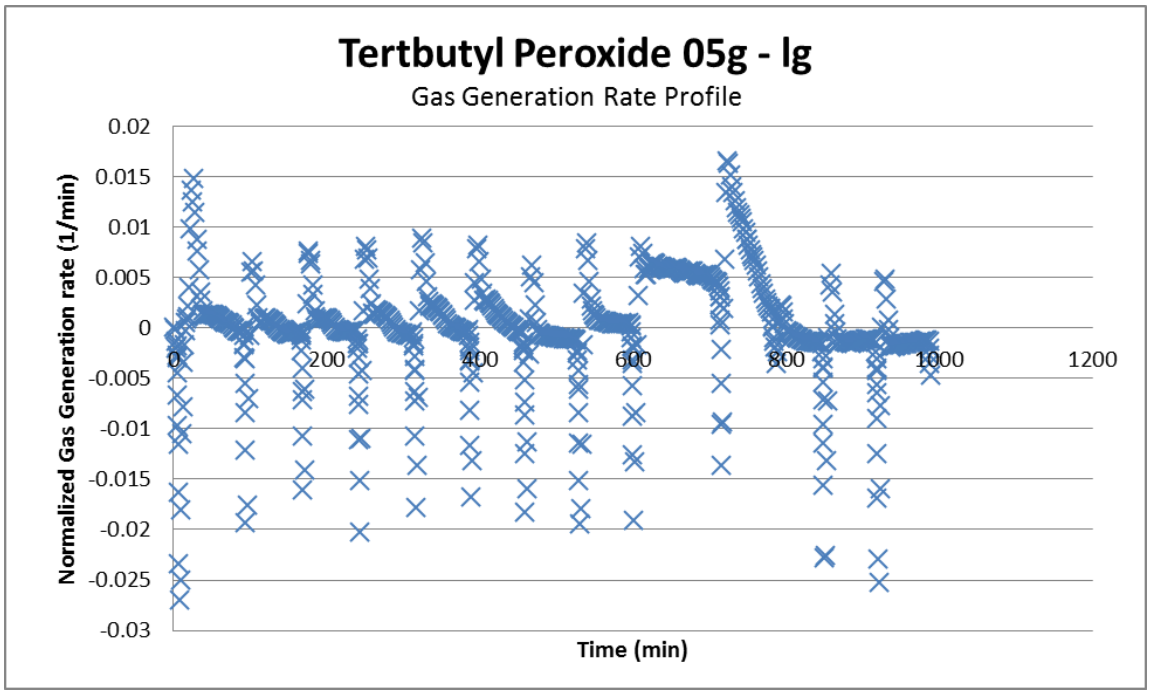

Fig. A.47 Normalized Gas Generation Rate - Tertbutyl Peroxide 0.5g - lg

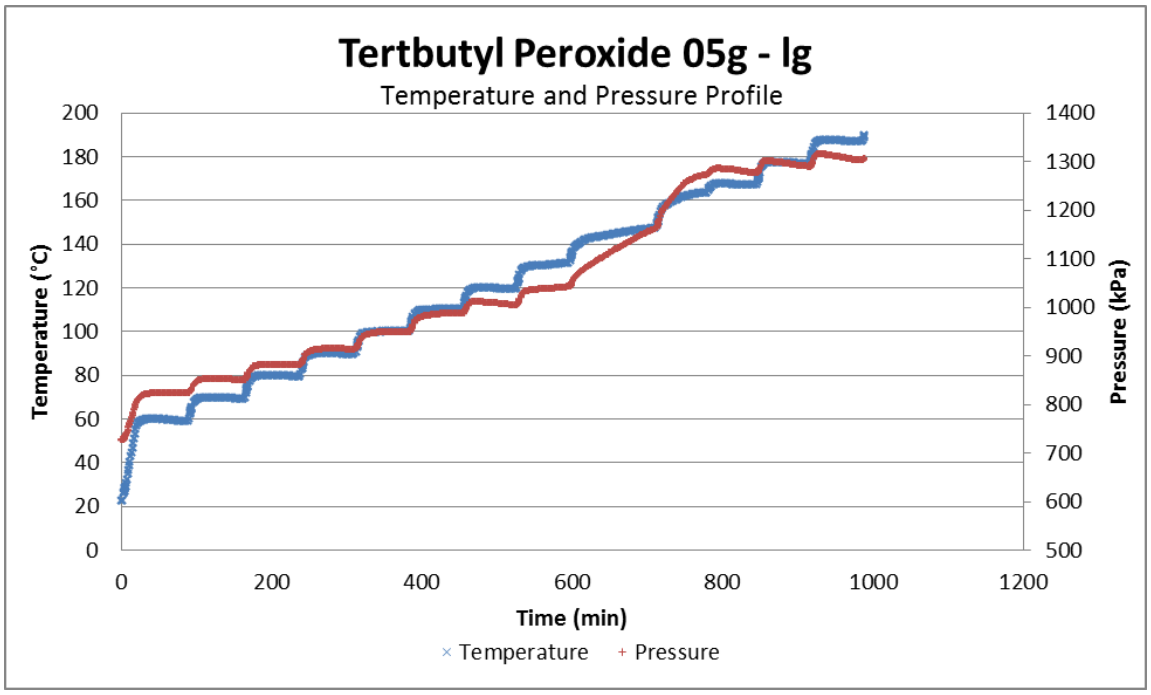

Fig. A.48 Temperature and Pressure Profiles - Tertbutyl Peroxide 0.5g - lg

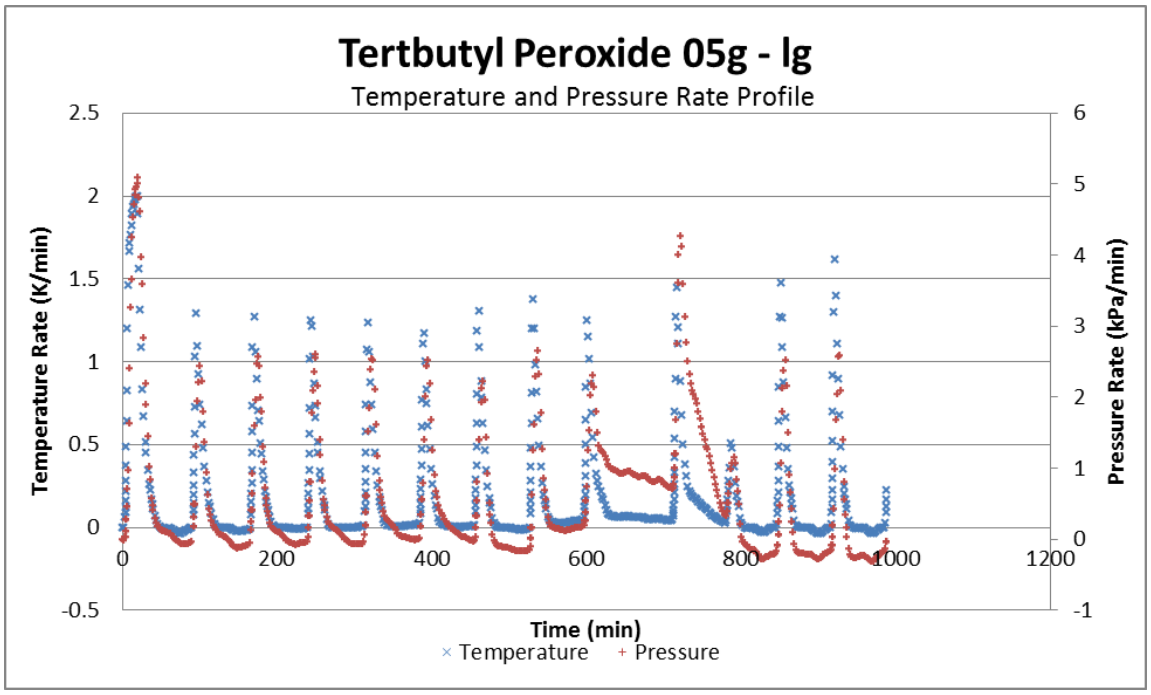

Fig. A.49 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 0.5g - lg

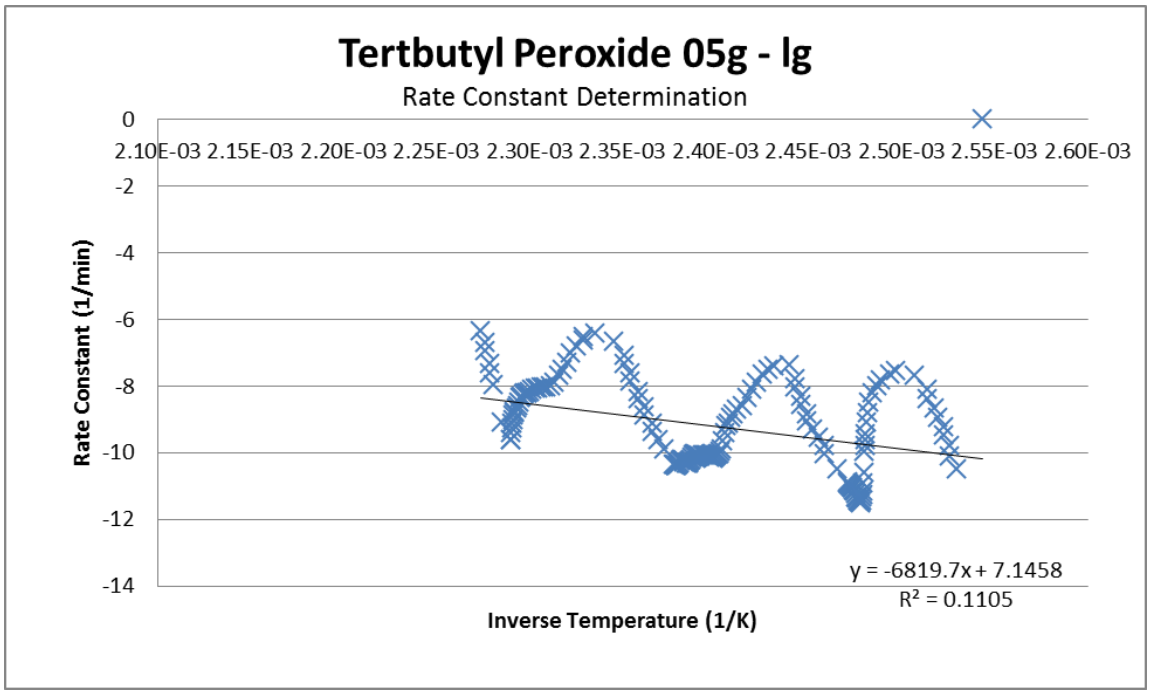

Fig. A.50 Rate Constant Determination - Tertbutyl Peroxide 0.5g - lg

A.11 Tertbutyl Peroxide 0.5g - md

Table A.40
Material Properties - Tertbutyl Peroxide 0.5g - md

Property	Value
m_s (g)	0.5
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.41
Cell Properties - Tertbutyl Peroxide 0.5g - md

Property	Value
m_{cell} (g)	35.96
V_{cell} (mL)	42.09
φ	41.30

Table A.43
IPD Properties - Tertbutyl Peroxide 0.5g - md

Property	Value
A (1/s)	2.786E+09
E_A (J/(mol*K))	9.938E+04
T_{onset} (°C)	90
T_{max} (°C)	140
ΔH (J/g)	3095.
IPD (W/ml)	820.12

Table A.44
Gas Properties - Tertbutyl Peroxide 0.5g - md

Property	Value
n_{max} (mol)	7.093E-03
dn/dt_{max} (mol/min)	4.772E-05
n_{maxn}	2.075E+00
dn/dt_{maxn} (1/min)	1.396E-02
GGP (1/min)	2.895E-02

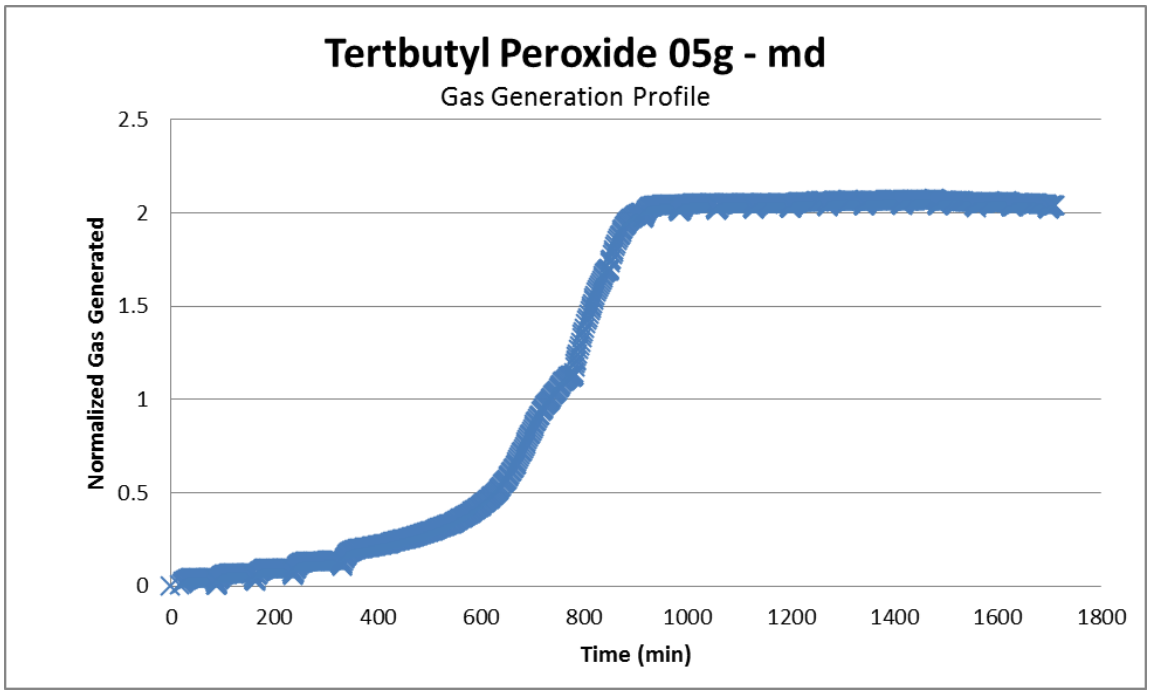

Fig. A.51 Normalized Gas Generation - Tertbutyl Peroxide 0.5g - md

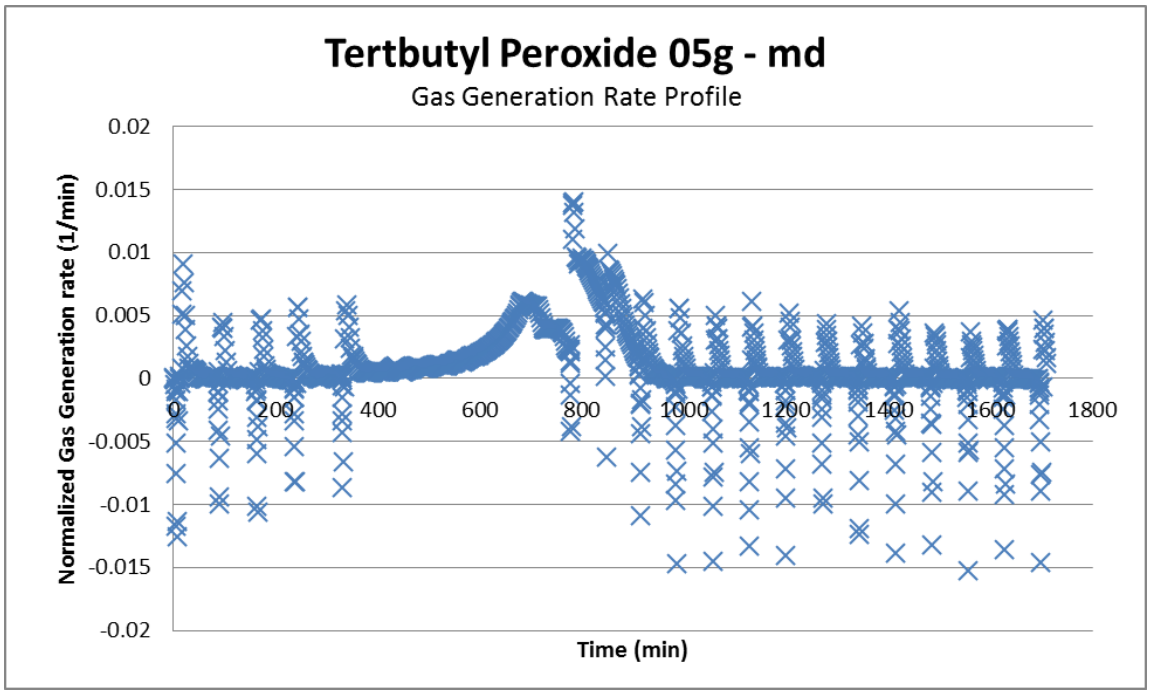

Fig. A.52 Normalized Gas Generation Rate - Tertbutyl Peroxide 0.5g - md

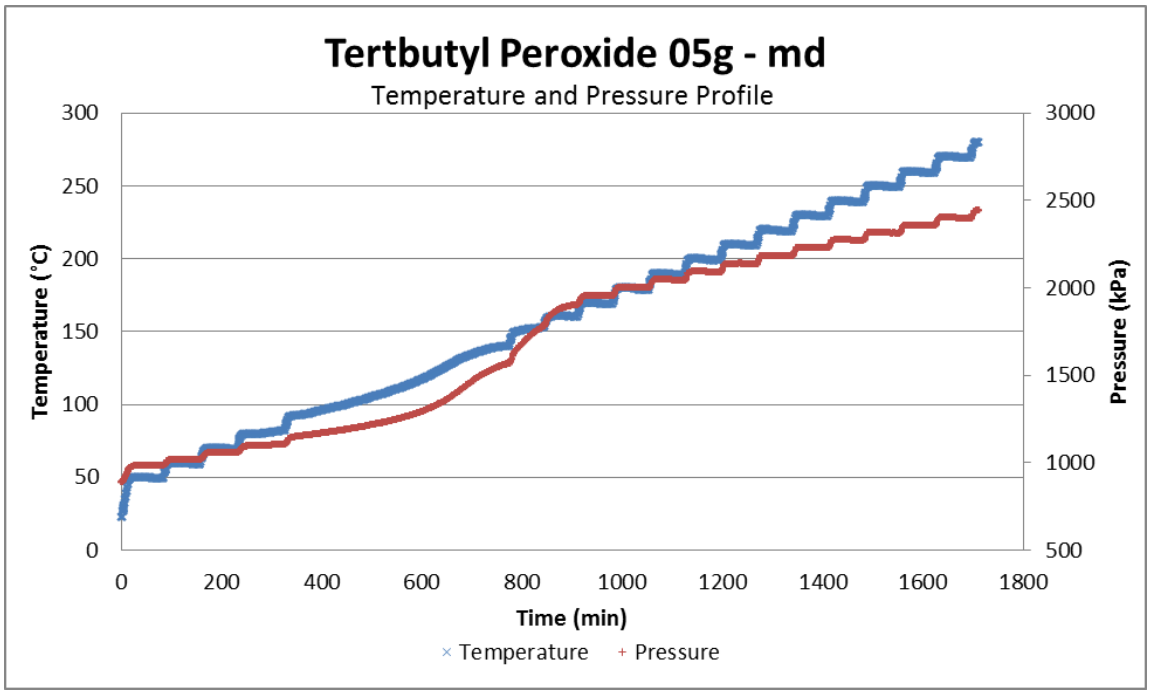

Fig. A.53 Temperature and Pressure Profiles - Tertbutyl Peroxide 0.5g - md

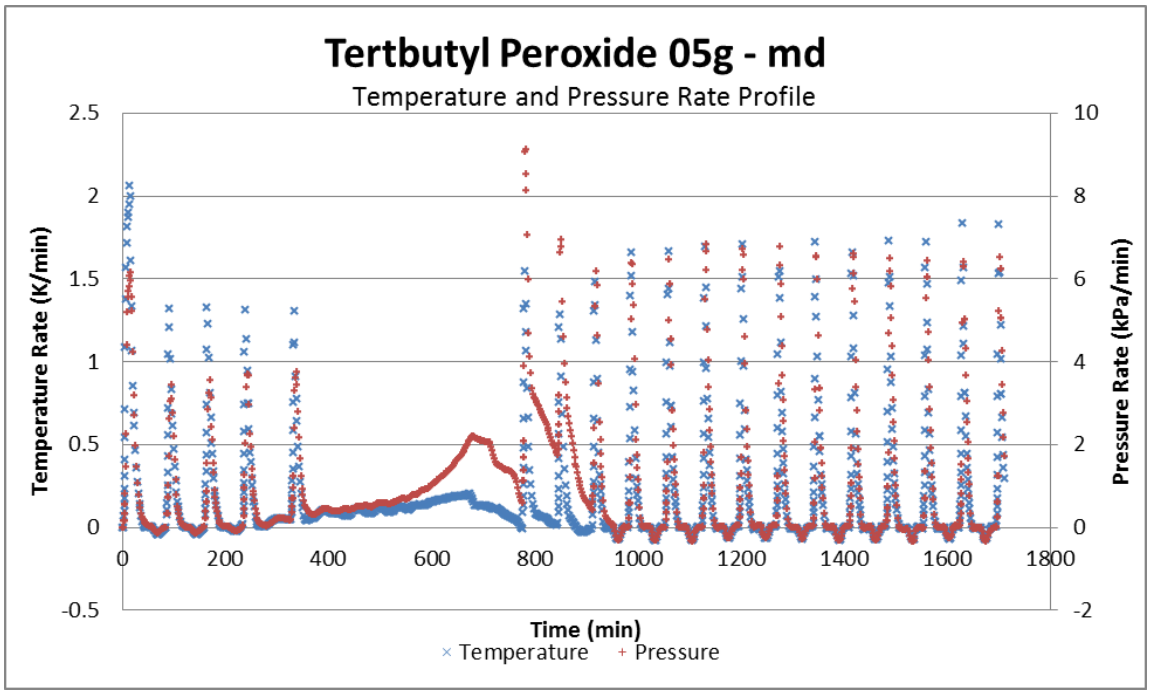

Fig. A.54 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 0.5g - md

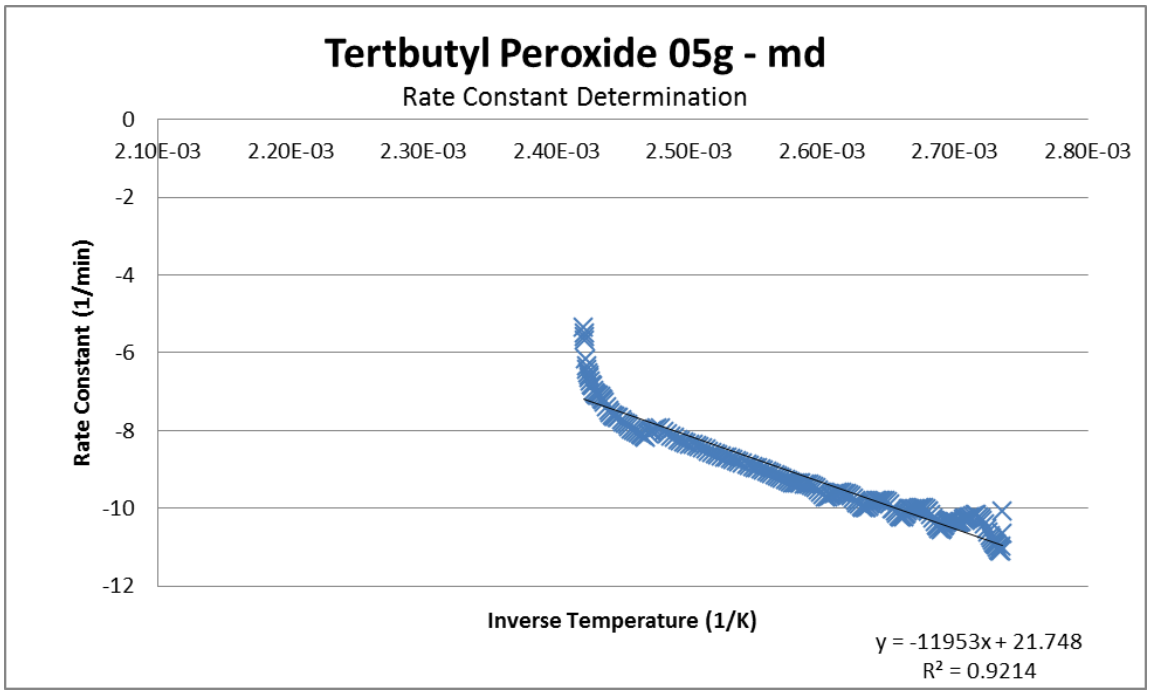

Fig. A.55 Rate Constant Determination - Tertbutyl Peroxide 0.5g - md

A.12 Tertbutyl Peroxide 0.5g - sm

Table A.45
Material Properties - Tertbutyl Peroxide 0.5g - sm

Property	Value
m_s (g)	0.52
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.46
Cell Properties - Tertbutyl Peroxide 0.5g - sm

Property	Value
m_{cell} (g)	23.65
V_{cell} (mL)	30.87
φ	26.47

Table A.47
IPD Properties - Tertbutyl Peroxide 0.5g - sm

Property	Value
A (1/s)	2.728E+06
E_A (J/(mol*K))	7.917E+04
T_{onset} (°C)	90
T_{max} (°C)	150
ΔH (J/g)	2382.
IPD (W/ml)	64.39

Table A.48
Gas Properties - Tertbutyl Peroxide 0.5g - sm

Property	Value
n_{max} (mol)	6.204E-03
dn/dt_{max} (mol/min)	4.961E-05
n_{maxn}	1.745E+00
dn/dt_{maxn} (1/min)	1.395E-02
GGP (1/min)	2.434E-02

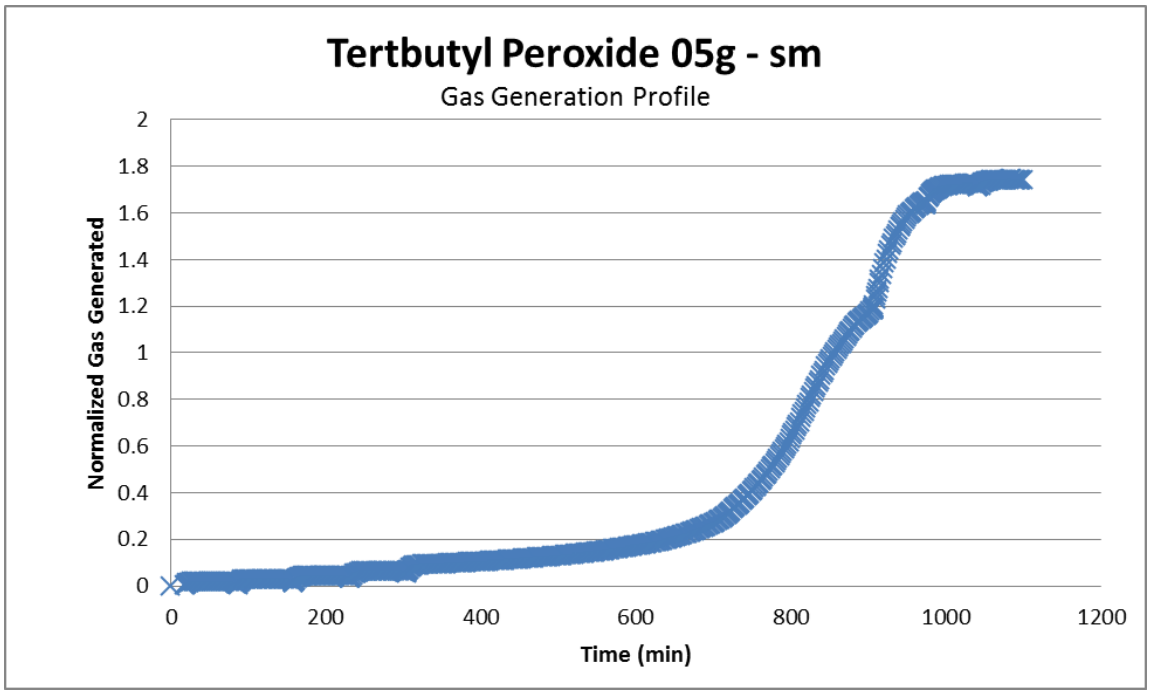

Fig. A.56 Normalized Gas Generation - Tertbutyl Peroxide 0.5g - sm

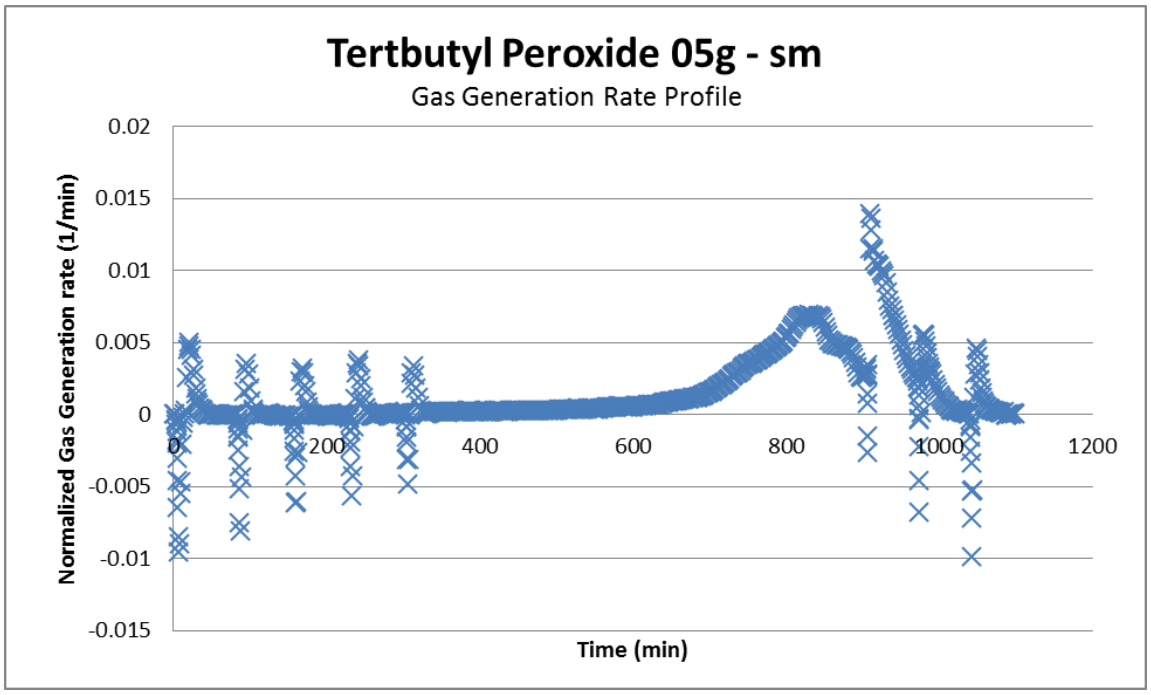

Fig. A.57 Normalized Gas Generation Rate - Tertbutyl Peroxide 0.5g - sm

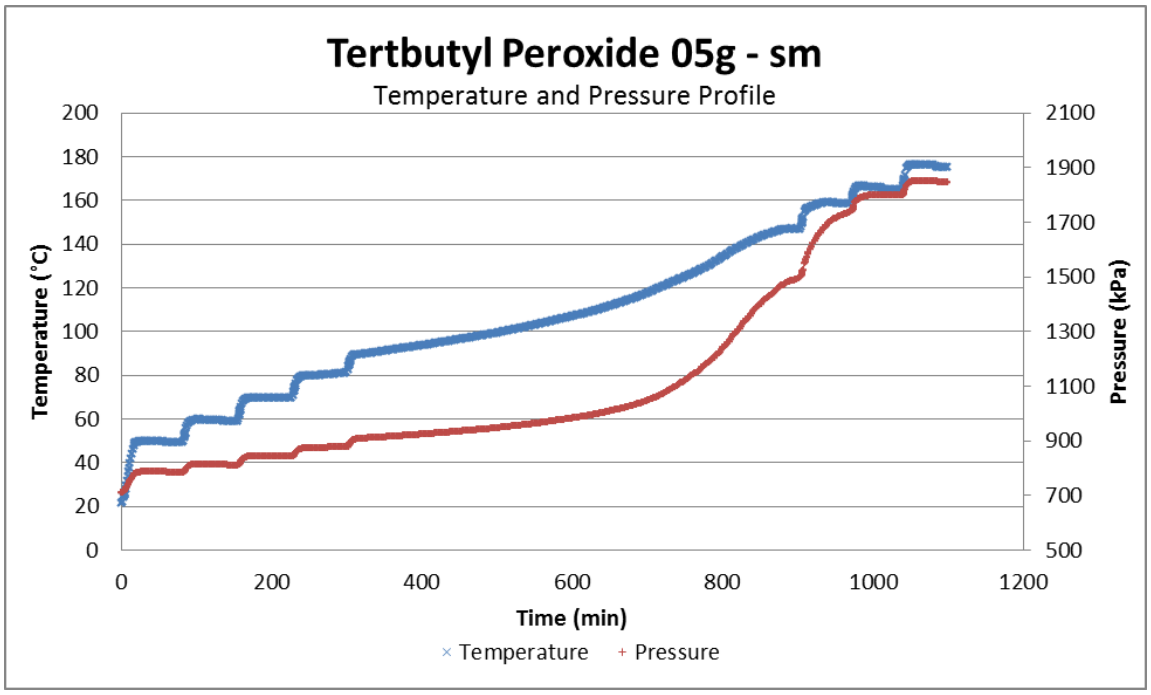

Fig. A.58 Temperature and Pressure Profiles - Tertbutyl Peroxide 0.5g - sm

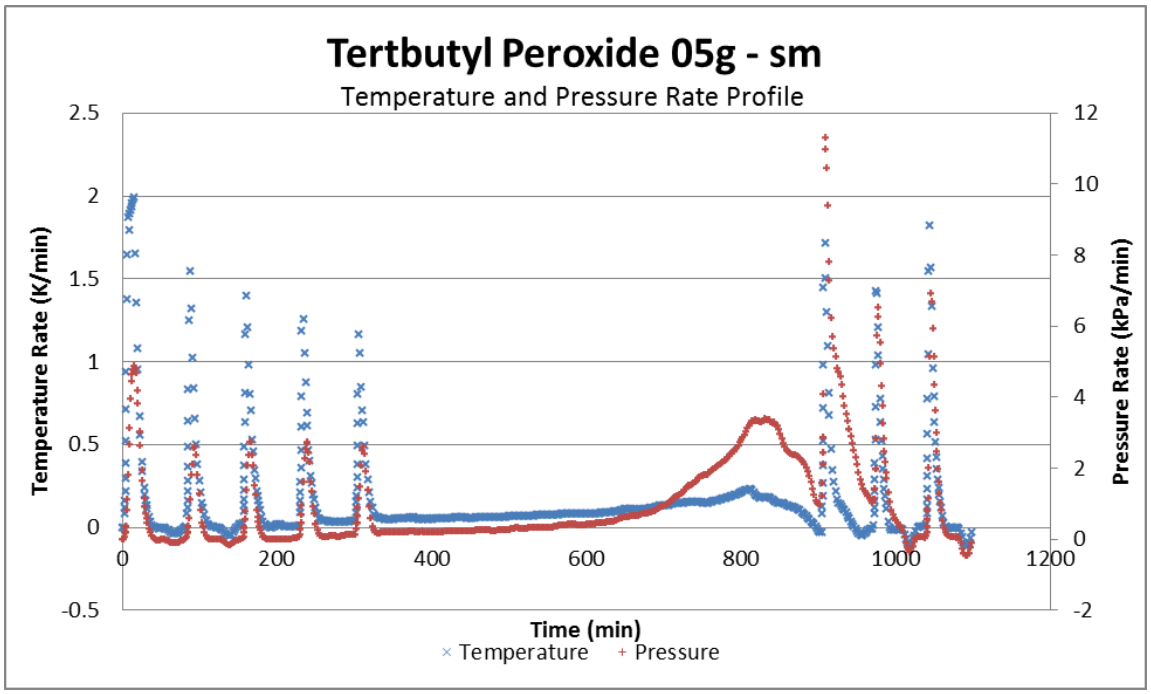

Fig. A.59 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 0.5g - sm

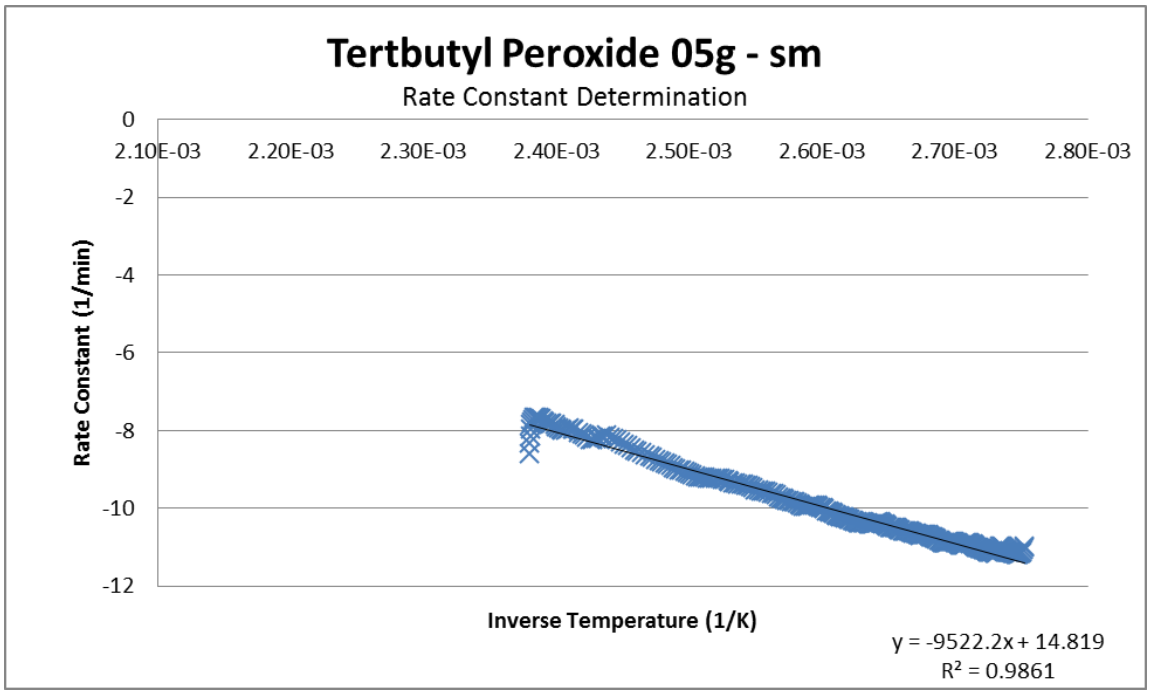

Fig. A.60 Rate Constant Determination - Tertbutyl Peroxide 0.5g - sm

A.13 Tertbutyl Peroxide 6g – lg

Table A.49
Material Properties - Tertbutyl Peroxide 6g - lg

Property	Value
m_s (g)	6.2
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.50
Cell Properties - Tertbutyl Peroxide 6g - lg

Property	Value
m_{cell} (g)	52.54
V_{cell} (mL)	93.30
φ	5.749

Table A.51
IPD Properties - Tertbutyl Peroxide 6g - lg

Property	Value
A (1/s)	7.547E+22
E_A (J/(mol*K))	1.877E+05
T_{onset} (°C)	80
T_{max} (°C)	160
ΔH (J/g)	689.4
IPD (W/ml)	7.452E+06

Table A.52
Gas Properties - Tertbutyl Peroxide 6g - lg

Property	Value
n_{max} (mol)	2.226E-02
dn/dt_{max} (mol/min)	2.779E-02
n_{maxn}	5.250E-01
dn/dt_{maxn} (1/min)	6.553E-01
GGP (1/min)	3.441E-01

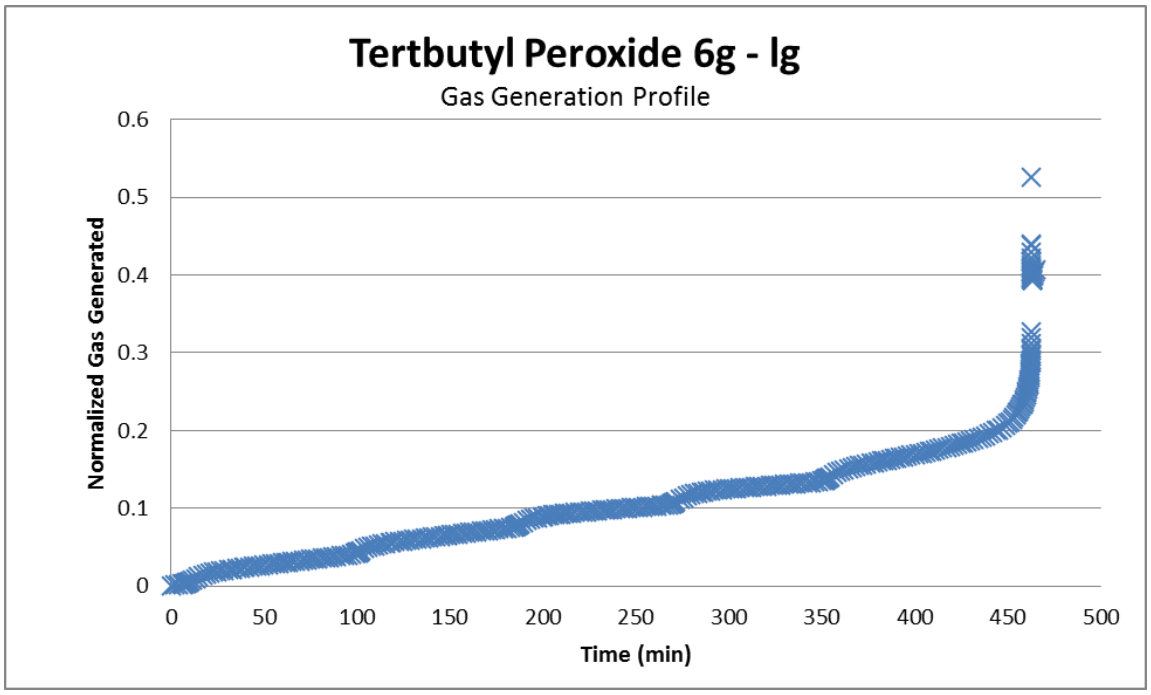

Fig. A.61 Normalized Gas Generation - Tertbutyl Peroxide 6g - lg

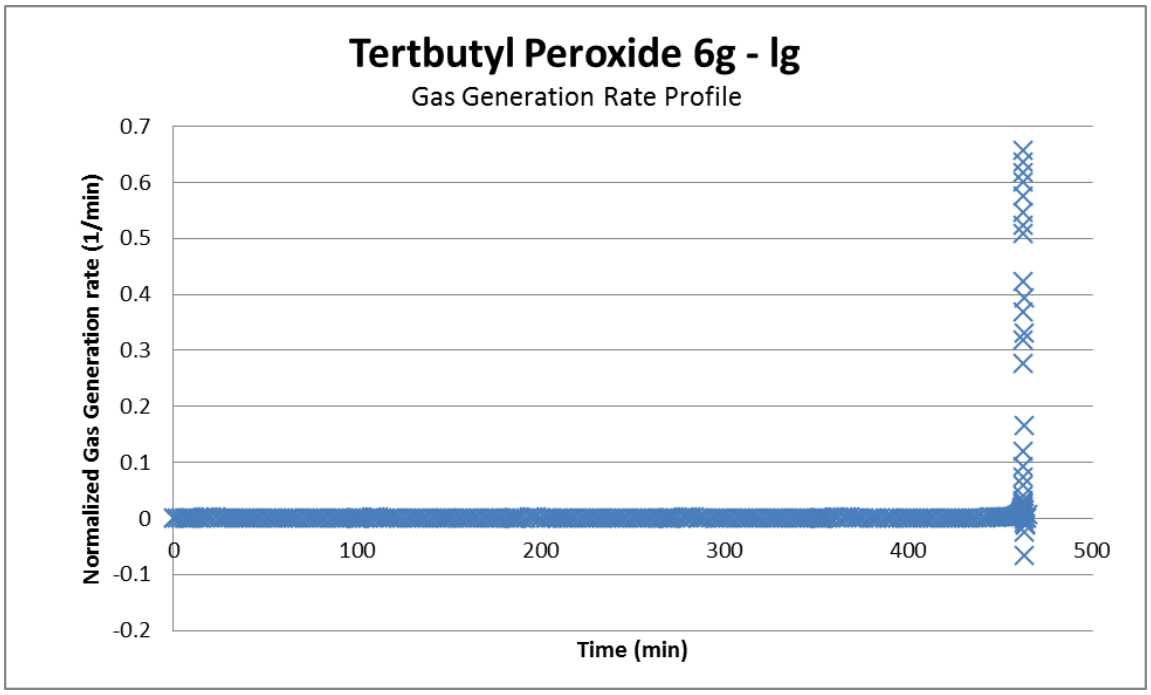

Fig. A.62 Normalized Gas Generation Rate - Tertbutyl Peroxide 6g - lg

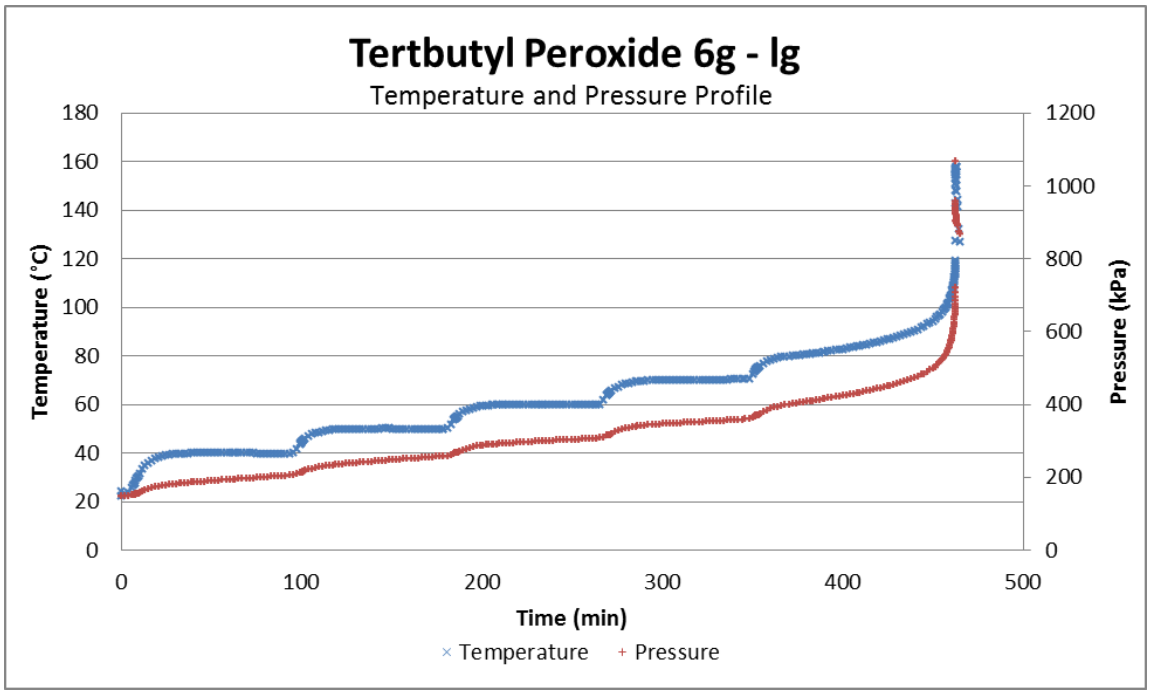

Fig. A.63 Temperature and Pressure Profiles - Tertbutyl Peroxide 6g - lg

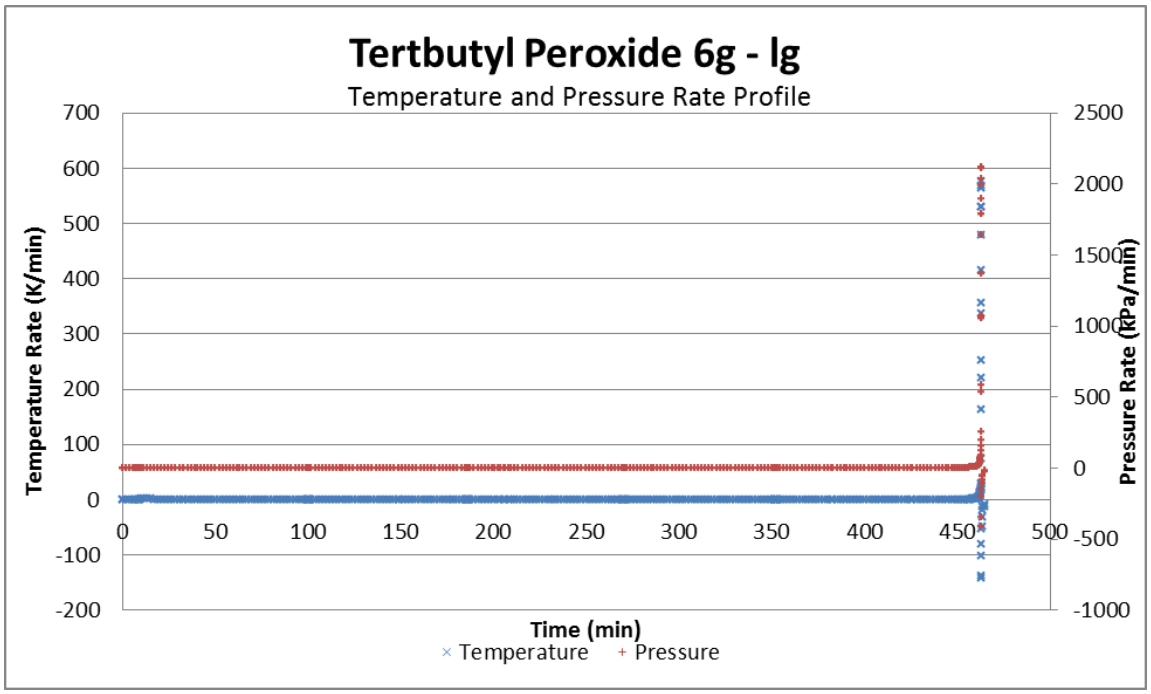

Fig. A.64 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 6g - lg

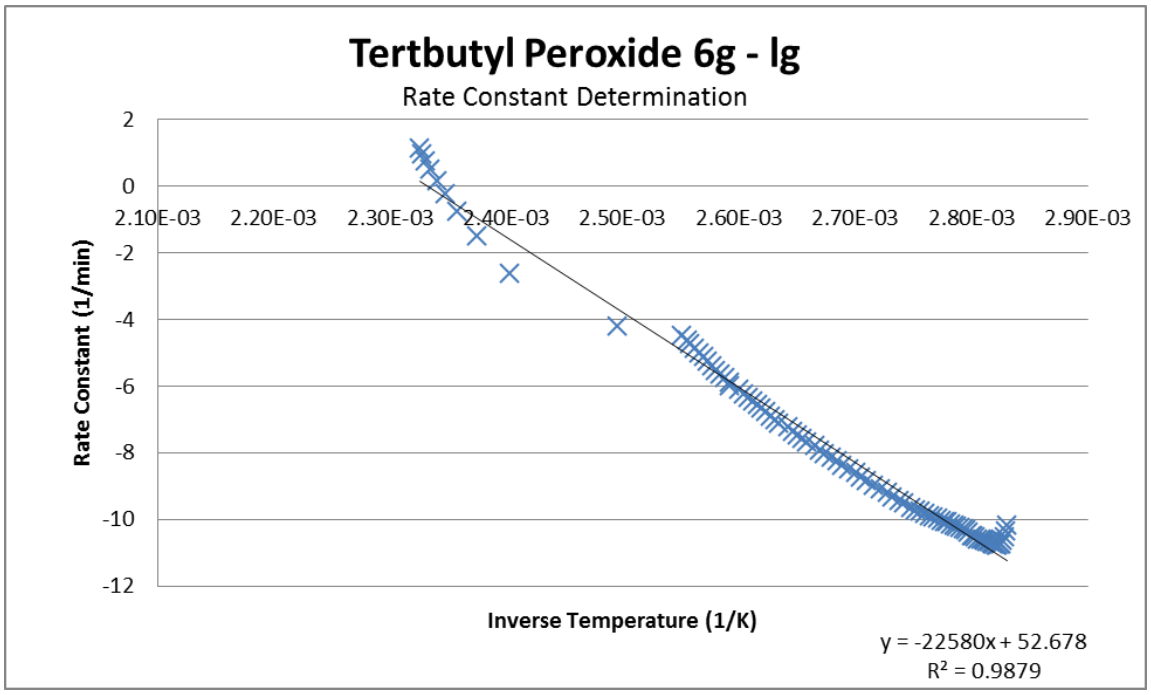

Fig. A.65 Rate Constant Determination - Tertbutyl Peroxide 6g - lg

A.14 Tertbutyl Peroxide 0.9g - lg

Table A.53
Material Properties - Tertbutyl Peroxide 0.9g - lg

Property	Value
m_s (g)	0.93
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.54
Cell Properties - Tertbutyl Peroxide 0.9g - lg

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	32.18

Table A.55
IPD Properties - Tertbutyl Peroxide 0.9g - lg

Property	Value
A (1/s)	3.795E+09
E_A (J/(mol*K))	1.052E+05
T_{onset} (°C)	100
T_{max} (°C)	160
ΔH (J/g)	2894.
IPD (W/ml)	274.0

Table A.56
Gas Properties - Tertbutyl Peroxide 0.9g - lg

Property	Value
n_{max} (mol)	1.000E-02
dn/dt_{max} (mol/min)	7.707E-05
n_{maxn}	1.573E+00
dn/dt_{maxn} (1/min)	1.212E-02
GGP (1/min)	1.906E-02

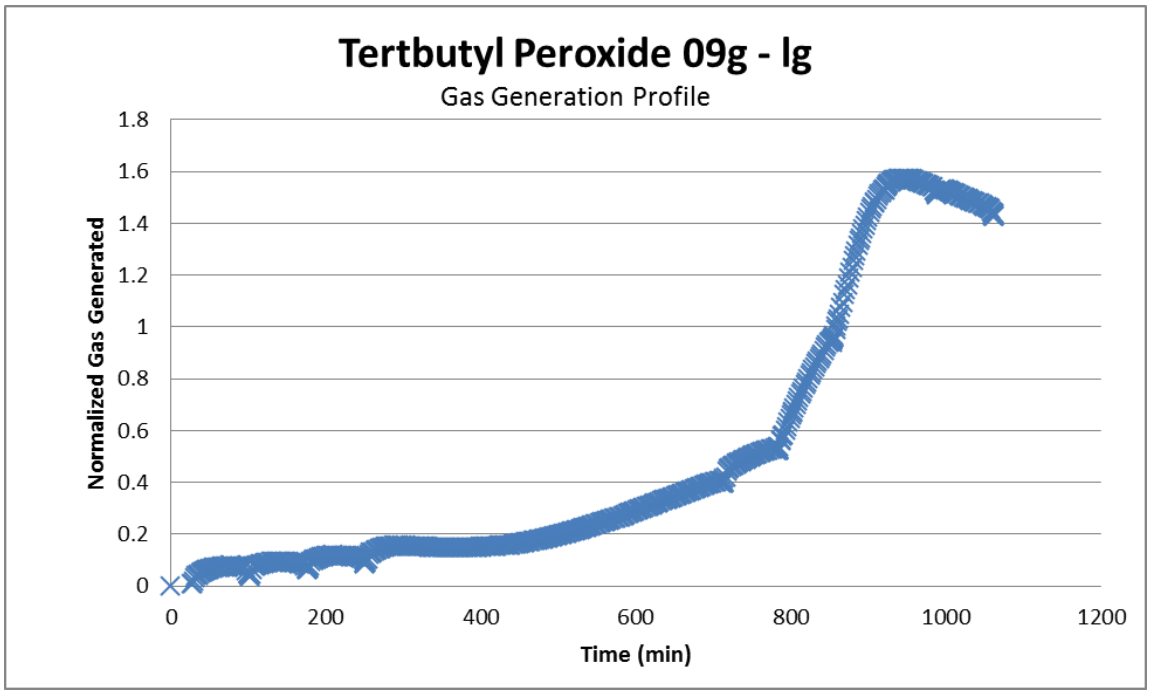

Fig. A.66 Normalized Gas Generation - Tertbutyl Peroxide 0.9g - lg

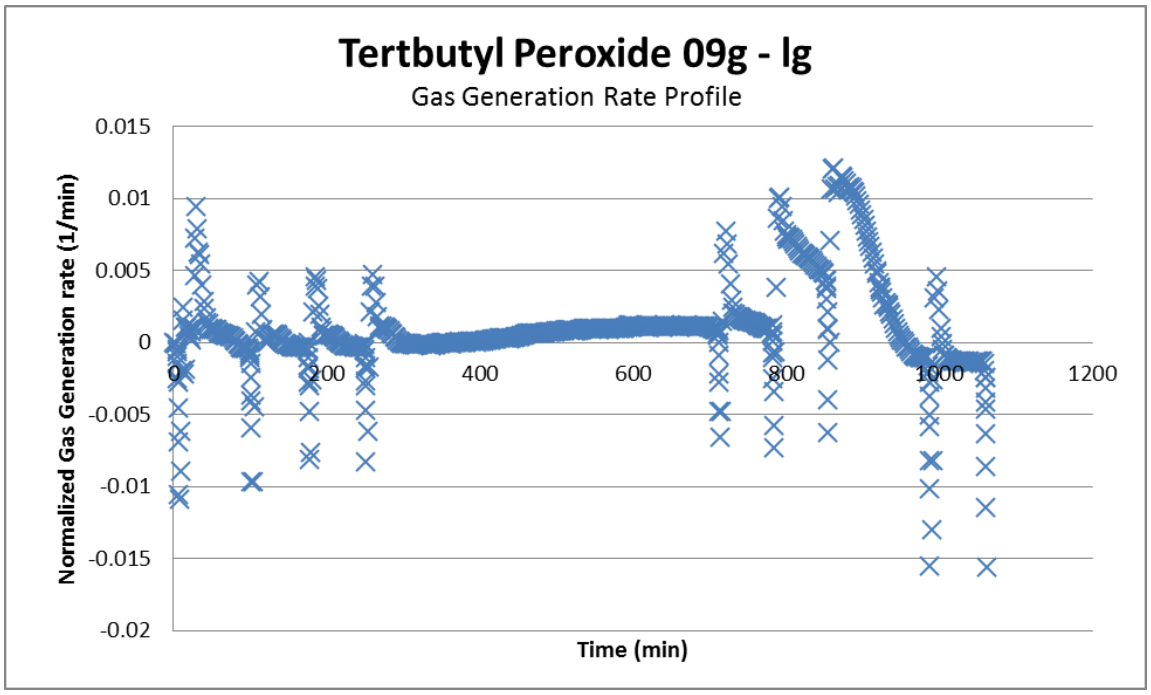

Fig. A.67 Normalized Gas Generation Rate - Tertbutyl Peroxide 0.9g - lg

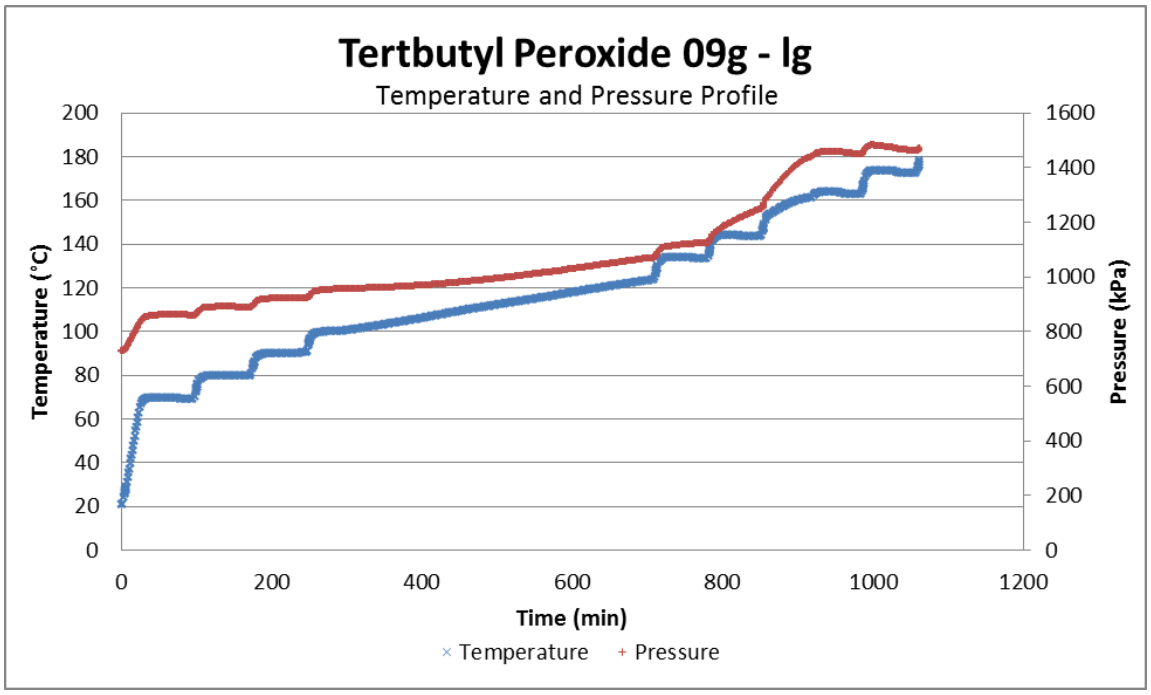

Fig. A.68 Temperature and Pressure Profiles - Tertbutyl Peroxide 0.9g - lg

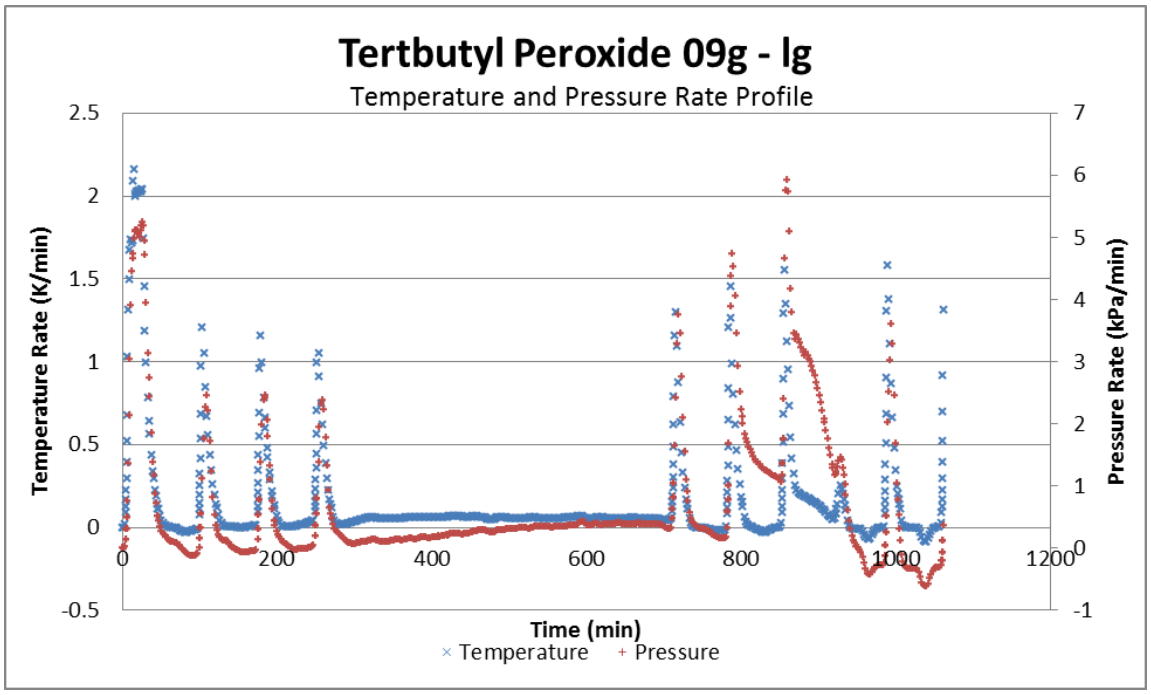

Fig. A69 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 0.9g - lg

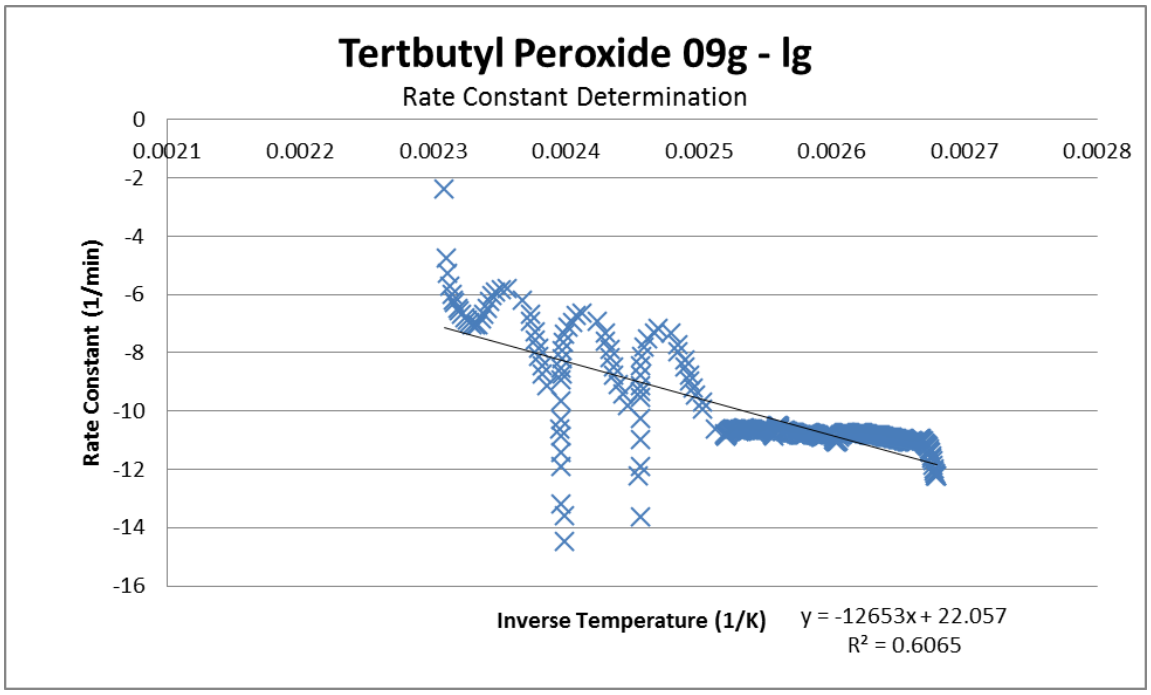

Fig. A.70 Rate Constant Determination - Tertbutyl Peroxide 0.9g - lg

A.15 Tertbutyl Peroxide 18g - lg

Table A.57
Material Properties - Tertbutyl Peroxide 18g - lg

Property	Value
m_s (g)	17.99
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table A.58
Cell Properties - Tertbutyl Peroxide 18g - lg

Property	Value
m_{cell} (g)	53.01
V_{cell} (mL)	93.99
φ	2.651

Table A.59
IPD Properties - Tertbutyl Peroxide 18g - lg

Property	Value
A (1/s)	5.917E+14
E_A (J/(mol*K))	1.327E+05
T_{onset} (°C)	80
T_{max} (°C)	220
ΔH (J/g)	556.4
IPD (W/ml)	1.473E+04

Table A.60
Gas Properties - Tertbutyl Peroxide 18g - lg

Property	Value
n_{max} (mol)	5.840E-02
dn/dt_{max} (mol/min)	8.854E-02
n_{maxn}	4.747E-01
dn/dt_{maxn} (1/min)	7.197E-01
GGP (1/min)	3.417E-01

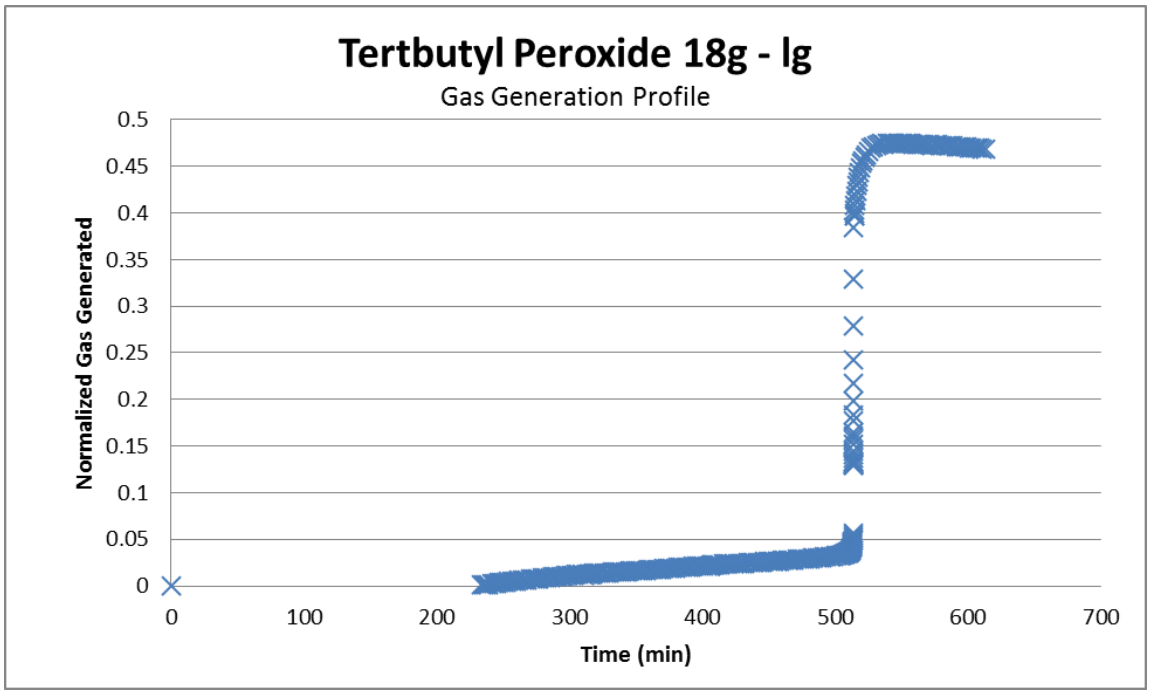

Fig. A.71 Normalized Gas Generation - Tertbutyl Peroxide 18g - lg

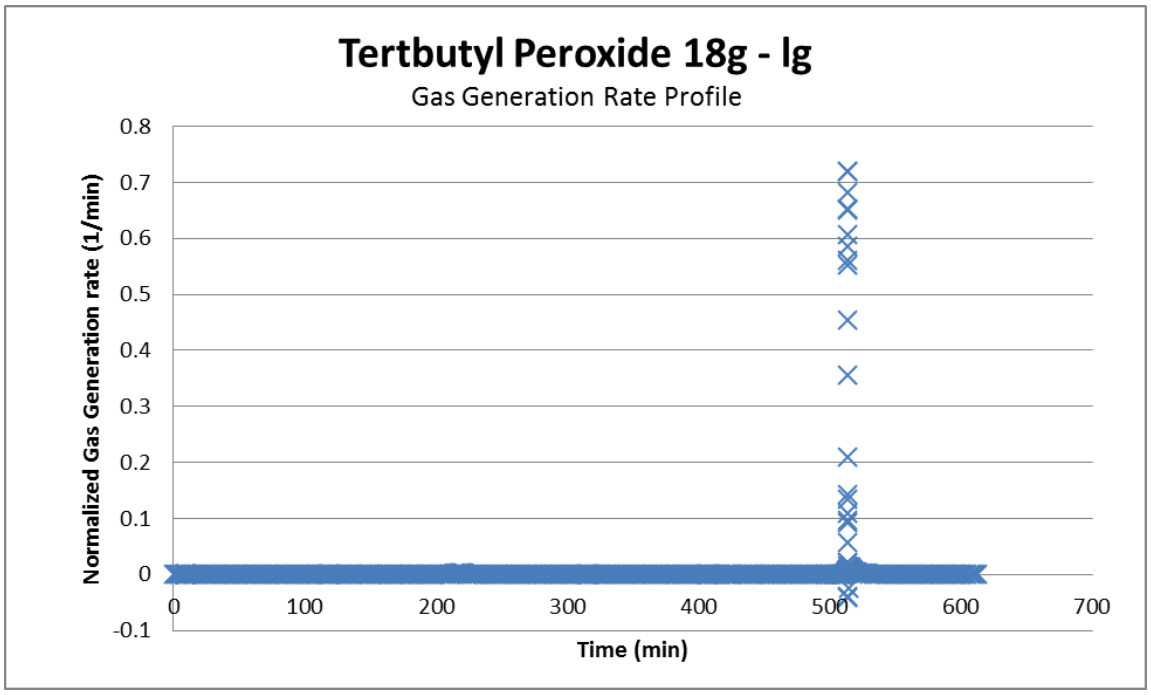

Fig. A.72 Normalized Gas Generation Rate - Tertbutyl Peroxide 18g - lg

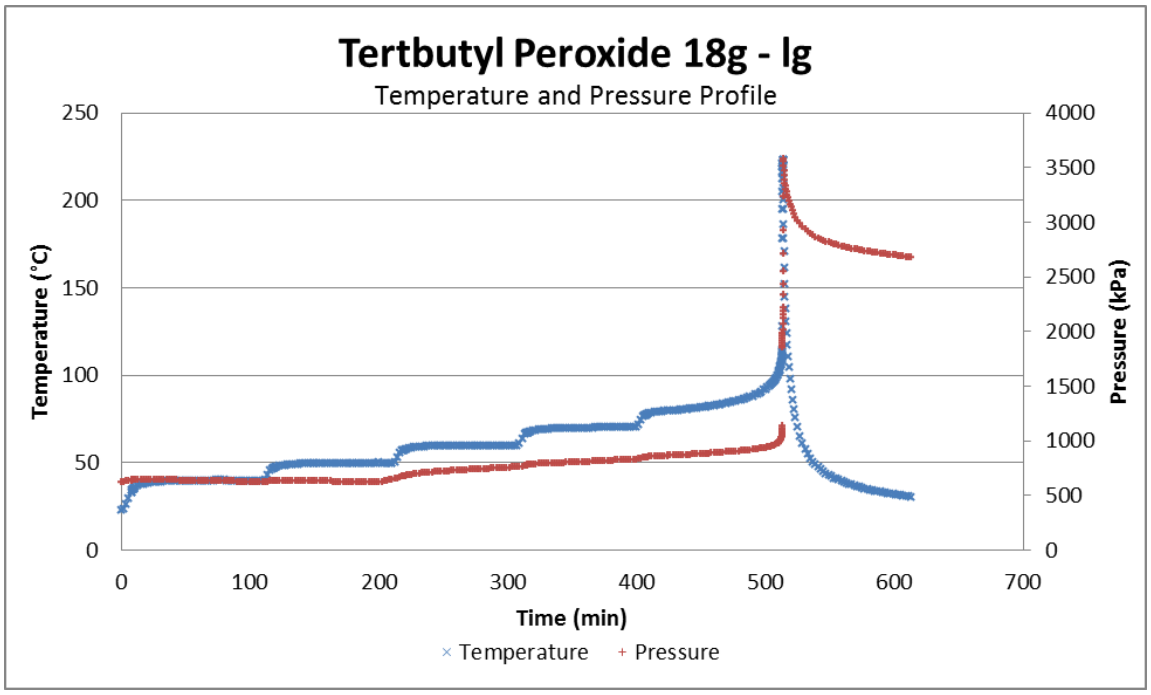

Fig. A.73 Temperature and Pressure Profiles - Tertbutyl Peroxide 18g - lg

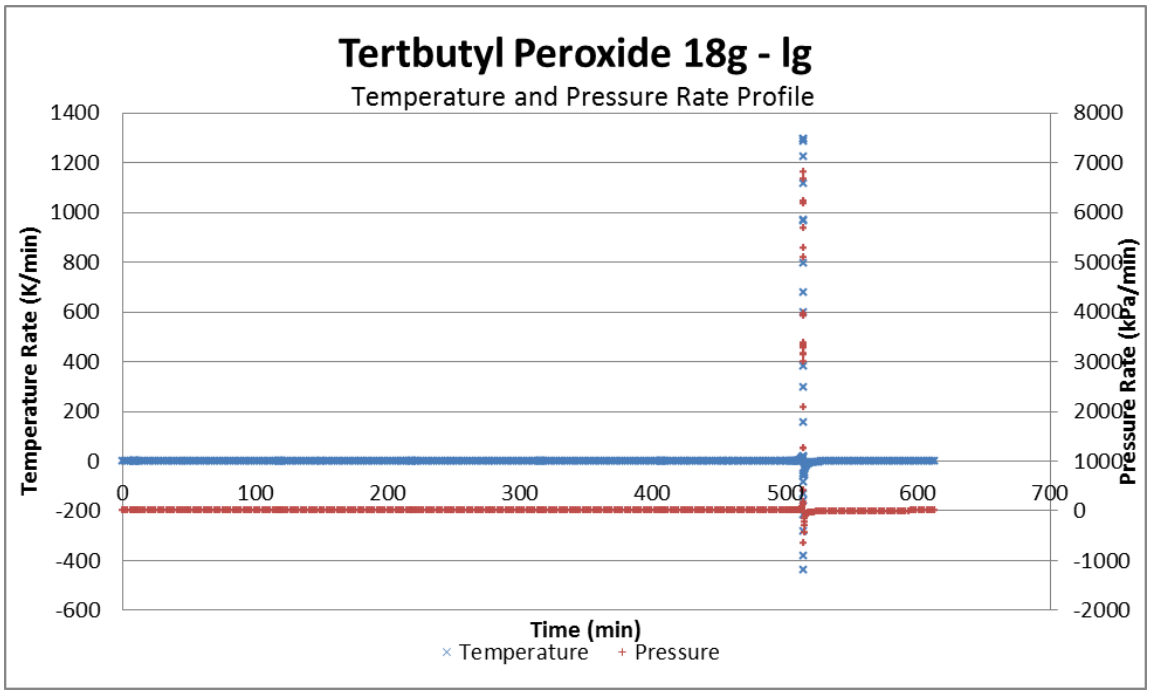

Fig. A.74 Temperature and Pressure Rate Profiles - Tertbutyl Peroxide 18g - lg

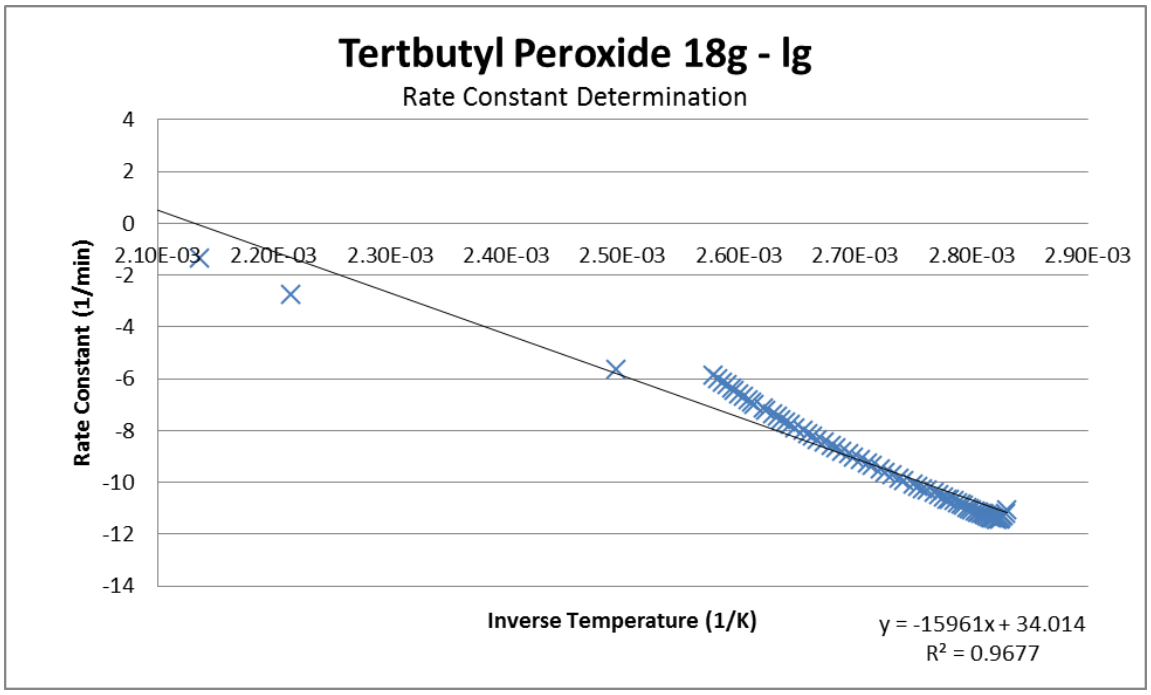

Fig. A.75 Rate Constant Determination - Tertbutyl Peroxide 18g - lg

APPENDIX B

The following is the data used in the main study to determine cutoffs. Each chemical is listed followed by pertinent information in four summary tables. Normal experiment parameters were used except where indicated. Each chemical is accompanied by five graphs. These graphs are the profiles for normalized gas generation, normalized gas generation rate, temperature and pressure, temperature and pressure rate, and rate constant determination.

B.1 1, 2 - Dinitrobenzene

Table B.1
Material Properties - 1, 2 - Dinitrobenzene

Property	Value
m_s (g)	0.83
ρ_s (g/mL)	1.31
C_s (J/(g*K))	1.192
MW (g/mol)	168.107

Table B.1
Cell Properties - 1, 2 - Dinitrobenzene

Property	Value
m_{cell} (g)	50.87
V_{cell} (mL)	97.53
φ	44.19

Table B.1
IPD Properties - 1, 2 - Dinitrobenzene

Property	Value
A (1/s)	1.086E+02
E_A (J/(mol*K))	6.676E+04
T_{onset} (°C)	190
T_{max} (°C)	410
ΔH (J/g)	1.158E+04
IPD (W/ml)	0.3564

Table B.1
Gas Properties - 1, 2 - Dinitrobenzene

Property	Value
n_{max} (mol)	6.910E-03
dn/dt_{max} (mol/min)	5.998E-04
n_{maxn}	1.399E+00
dn/dt_{maxn} (1/min)	1.215E-01
GGP (1/min)	1.700E-01

Note – This compound exhibited an explosion event.

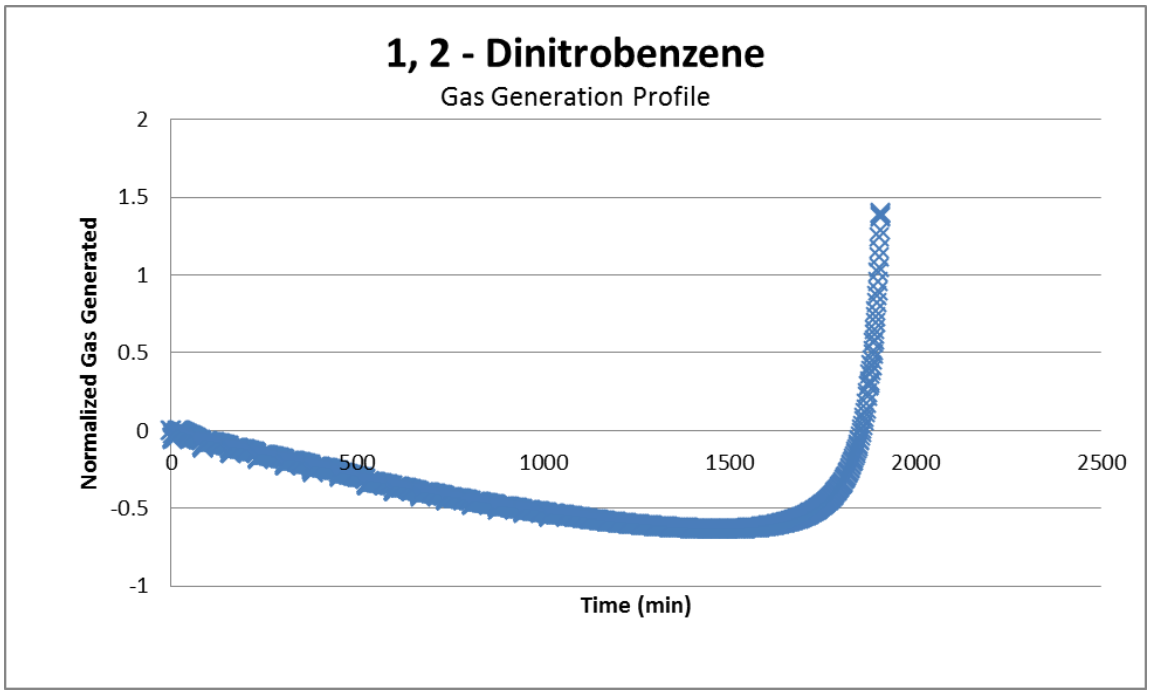

Fig. B.1 Normalized Gas Generation - 1, 2 - Dinitrobenzene

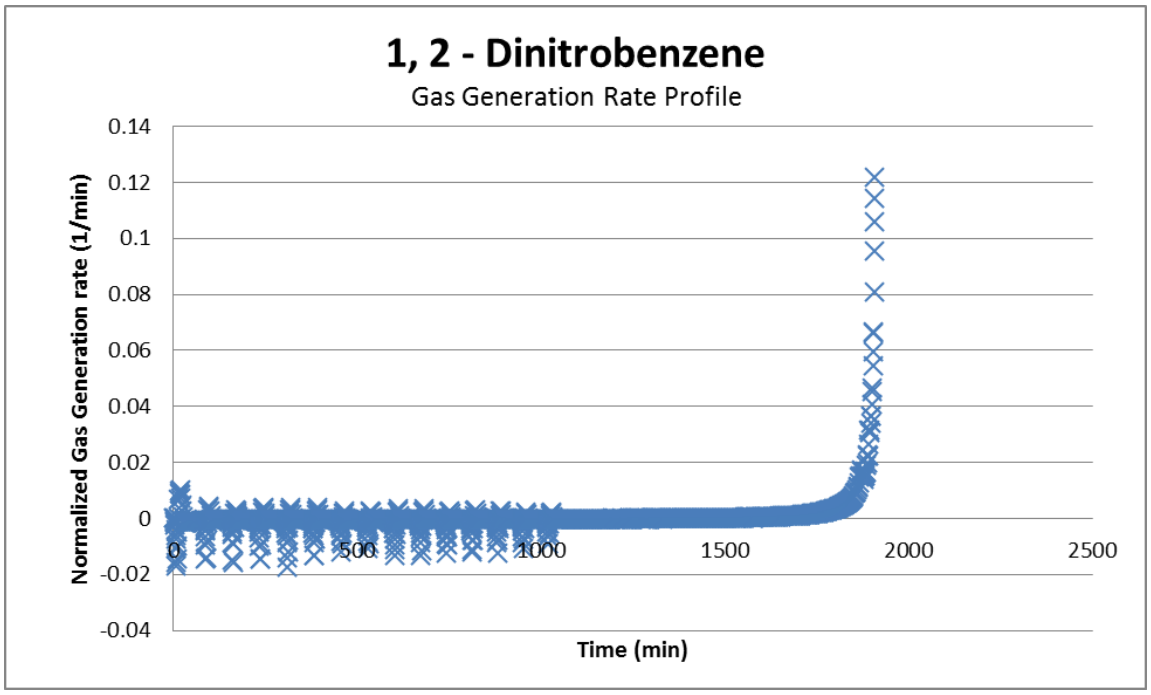

Fig. B.2 Normalized Gas Generation Rate - 1, 2 - Dinitrobenzene

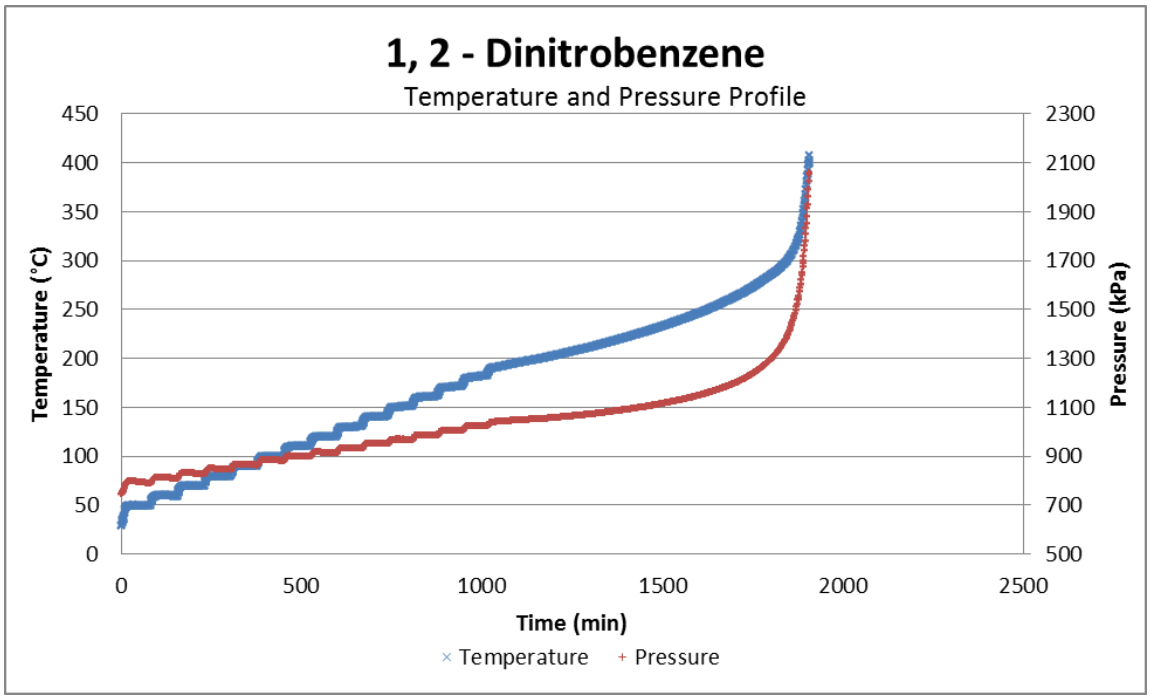

Fig. B.3 Temperature and Pressure Profiles - 1, 2 - Dinitrobenzene

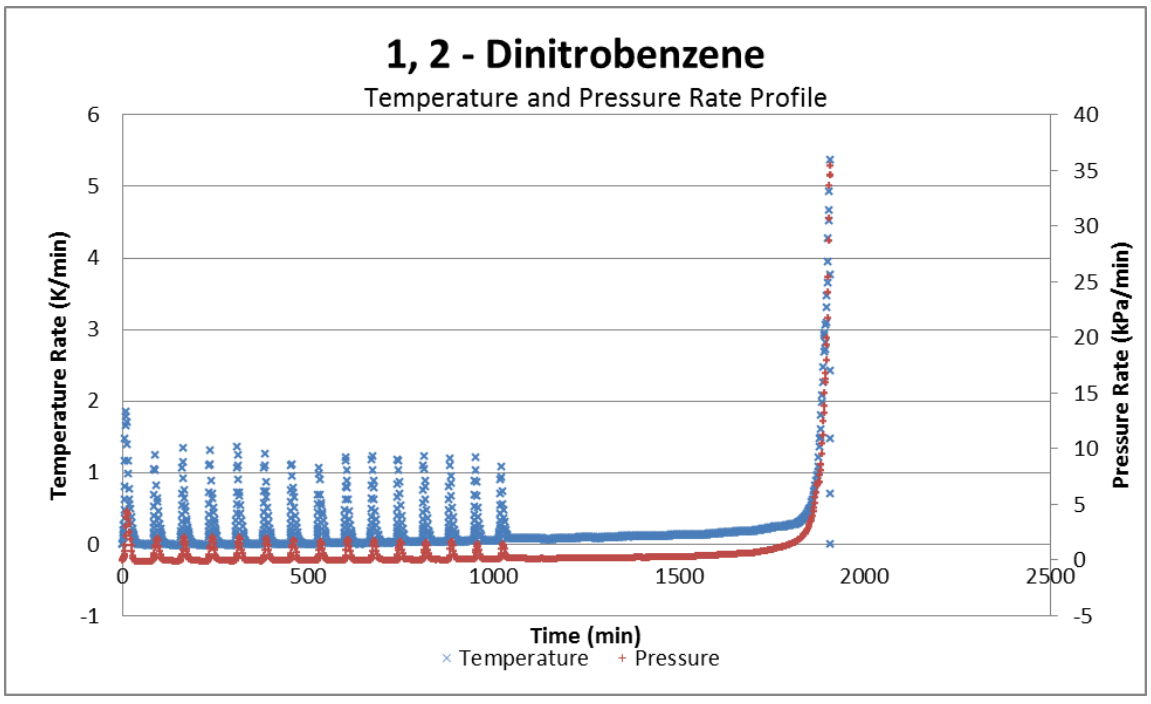

Fig. B.4 Temperature and Pressure Rate Profiles - 1, 2 - Dinitrobenzene

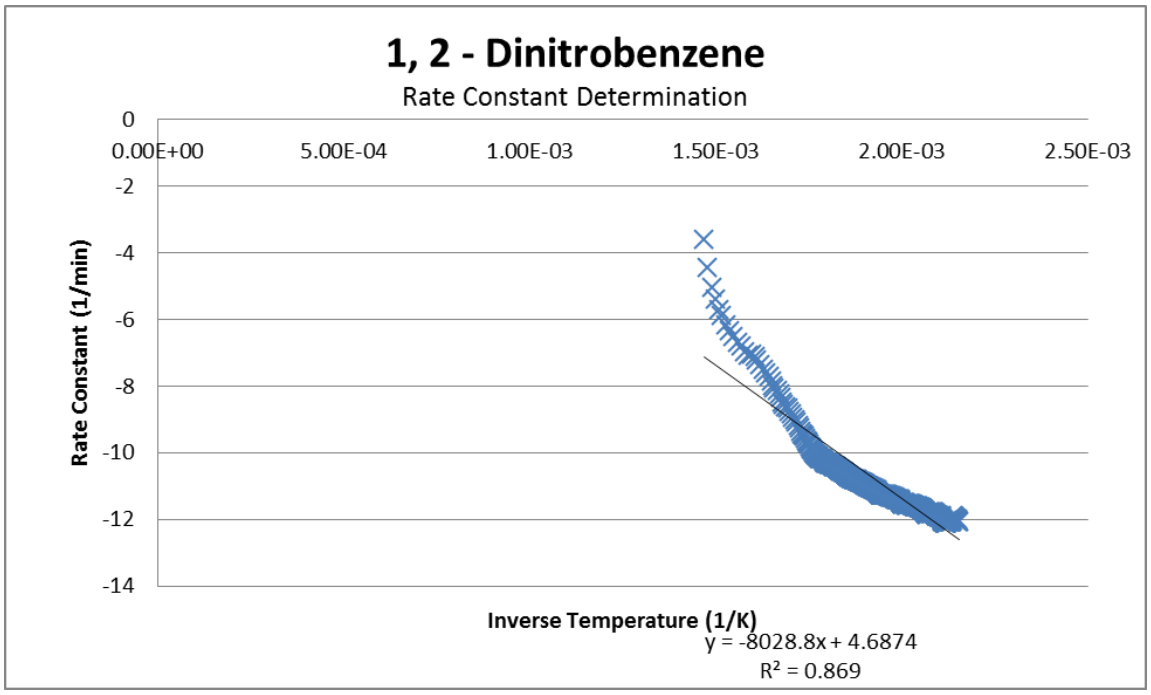

Fig. B.5 Rate Constant Determination - 1, 2 - Dinitrobenzene

B.2 2 - Butanone Peroxide

Table B.5
Material Properties - 2 - Butanone Peroxide

Property	Value
m_s (g)	8.13
ρ_s (g/mL)	1.053
C_s (J/(g*K))	2.3
MW (g/mol)	210.22

Table B.6
Cell Properties - 2 - Butanone Peroxide

Property	Value
m_{cell} (g)	57.61
V_{cell} (mL)	91.69
φ	3.588

Table B.7
IPD Properties - 2 - Butanone Peroxide

Property	Value
A (1/s)	3.047E+22
E_A (J/(mol*K))	1.901E+05
T_{onset} (°C)	80
T_{max} (°C)	160
ΔH (J/g)	6.602E+02
IPD (W/ml)	2.223E+06

Table B.8
Gas Properties - 2 - Butanone Peroxide

Property	Value
n_{max} (mol)	1.764E-02
dn/dt_{max} (mol/min)	5.301E-02
n_{maxn}	4.562E-01
dn/dt_{maxn} (1/min)	1.371E+00
GGP (1/min)	6.253E-01

Note – This compound exhibited an explosion event. This compound was run at atmospheric pressure and was not assumed to be pure (Lu et al., 2010).

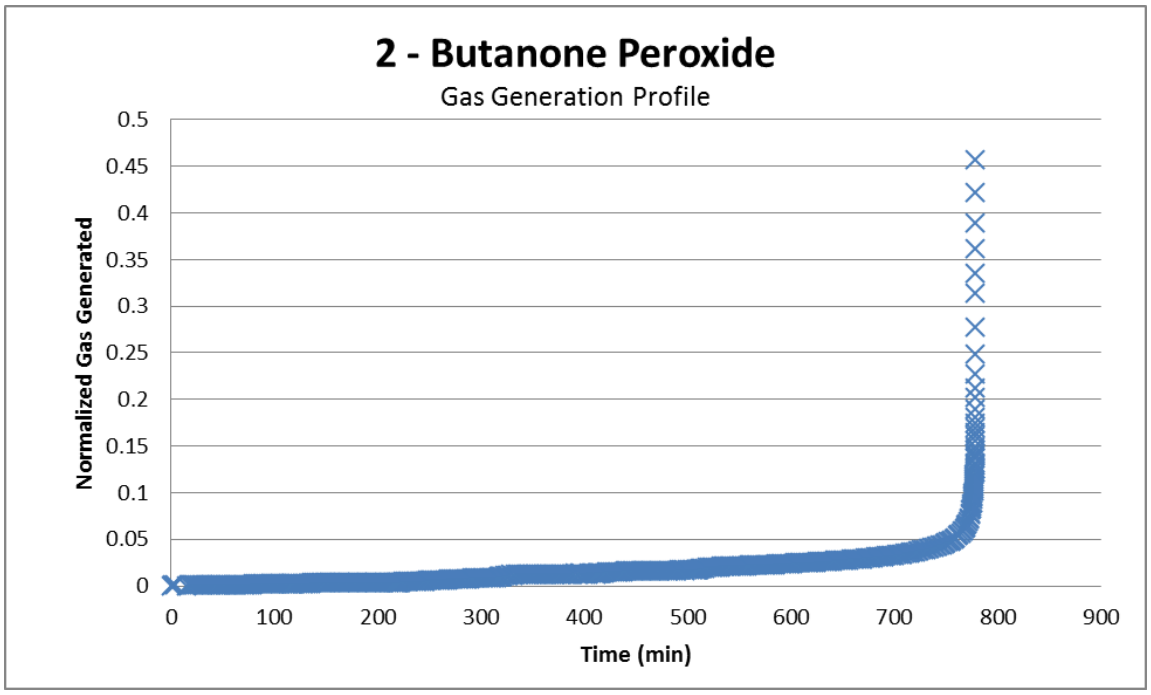

Fig. B.6 Normalized Gas Generation - 2 - Butanone Peroxide

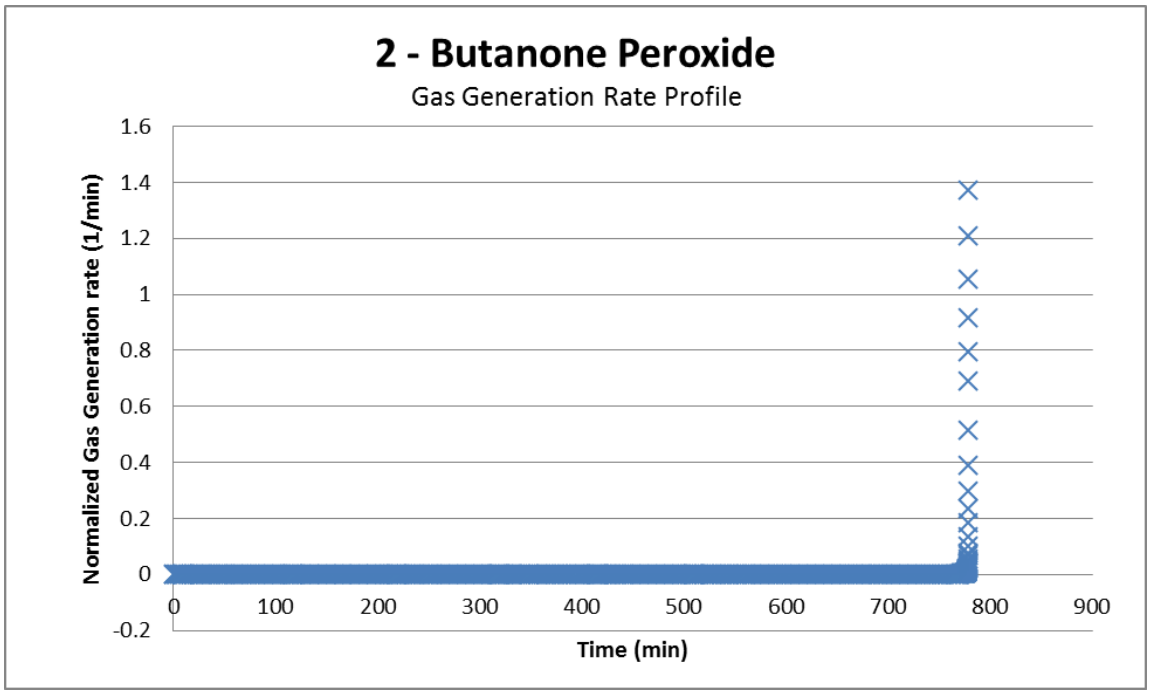

Fig. B.7 Normalized Gas Generation Rate - 2 - Butanone Peroxide

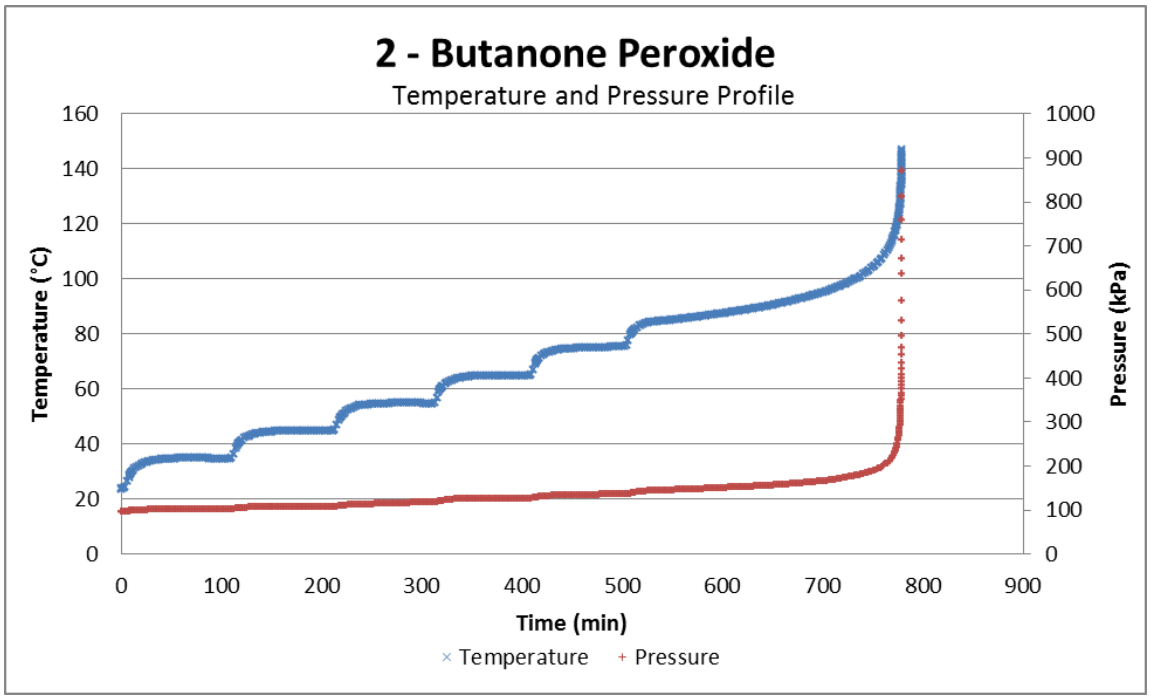

Fig. B.8 Temperature and Pressure Profiles - 2 - Butanone Peroxide

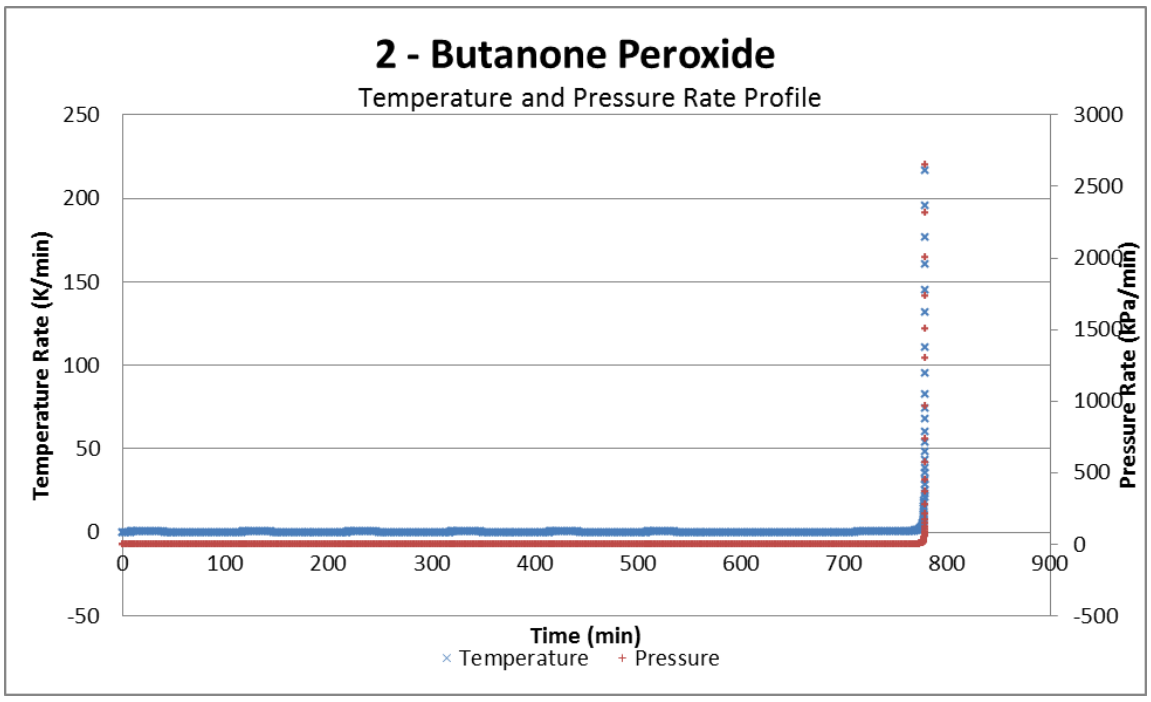

Fig. B.9 Temperature and Pressure Rate Profiles - 2 - Butanone Peroxide

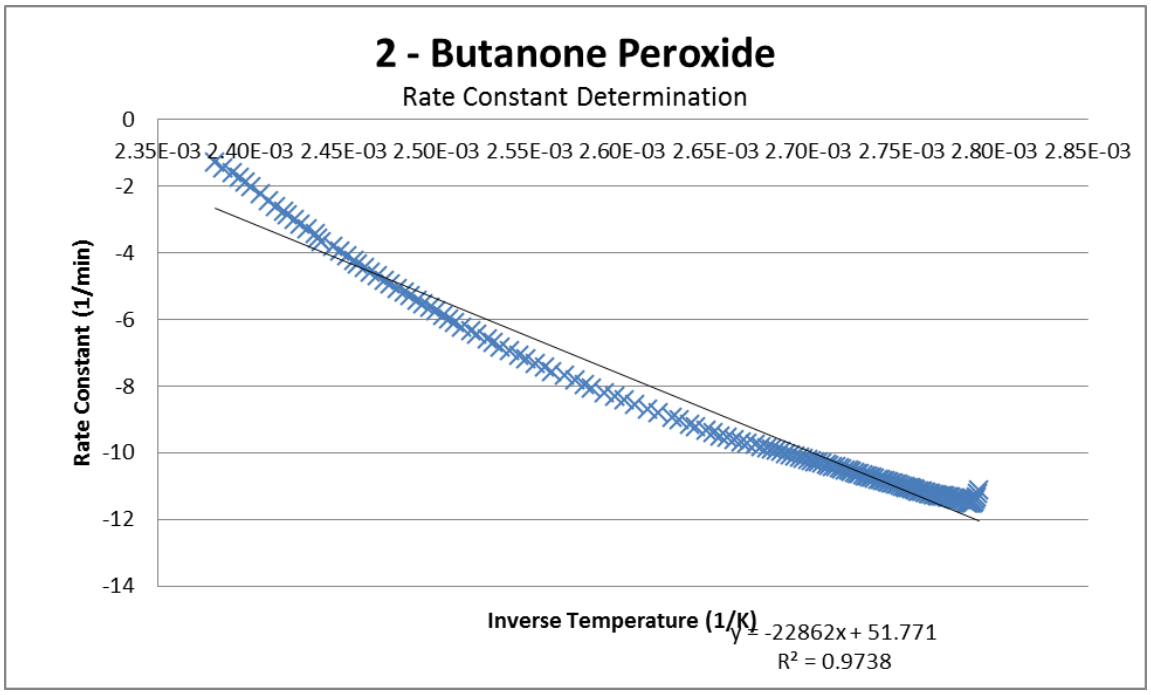

Fig. B.10 Rate Constant Determination - 2 - Butanone Peroxide

B.3 2, 4 - Dinitroaniline

Table B.9
Material Properties - 2, 4 - Dinitroaniline

Property	Value
m_s (g)	0.95
ρ_s (g/mL)	1.615
C_s (J/(g*K))	2
MW (g/mol)	183.12

Table B.10
Cell Properties - 2, 4 - Dinitroaniline

Property	Value
m_{cell} (g)	51.38
V_{cell} (mL)	97.13
φ	23.72

Table B.11
IPD Properties - 2, 4 - Dinitroaniline

Property	Value
A (1/s)	6.032E+05
E_A (J/(mol*K))	1.003E+05
T_{onset} (°C)	180
T_{max} (°C)	350
ΔH (J/g)	8063.
IPD (W/ml)	7.574E-01

Table B.12
Gas Properties - 2, 4 - Dinitroaniline

Property	Value
n_{max} (mol)	2.539E-02
dn/dt_{max} (mol/min)	4.878E-02
n_{maxn}	4.894E+00
dn/dt_{maxn} (1/min)	9.404E+00
GGP (1/min)	4.602E+01

Note – This compound exhibited an explosion event.

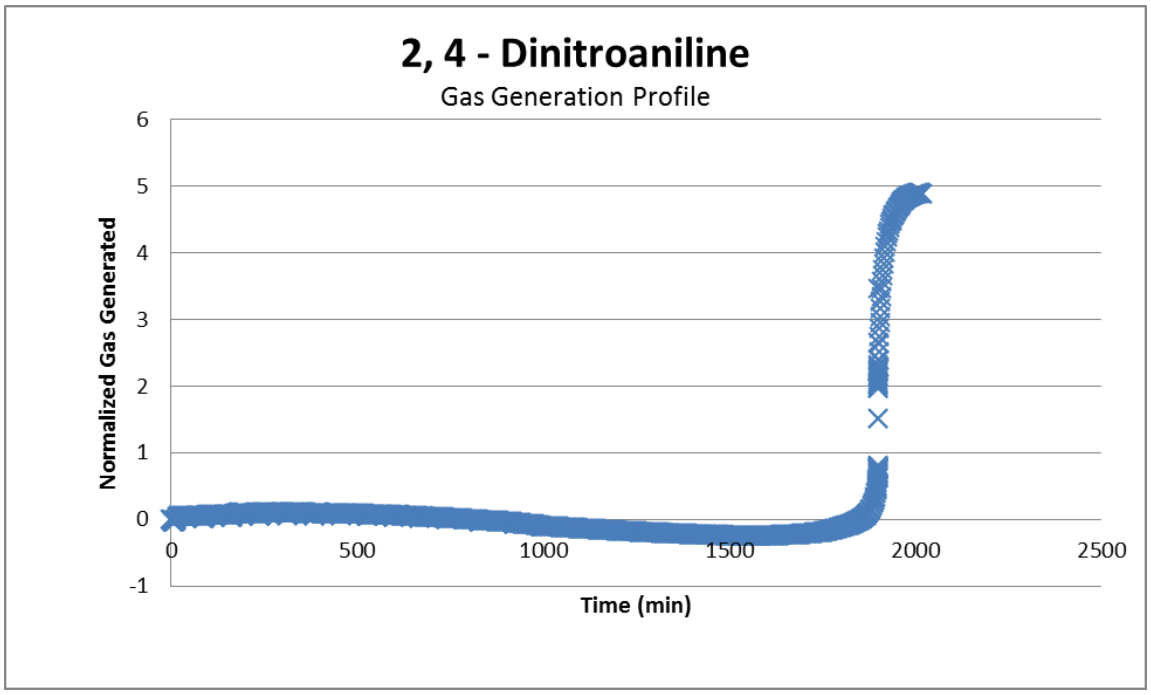

Fig. B.11 Normalized Gas Generation - 2, 4 - Dinitroaniline

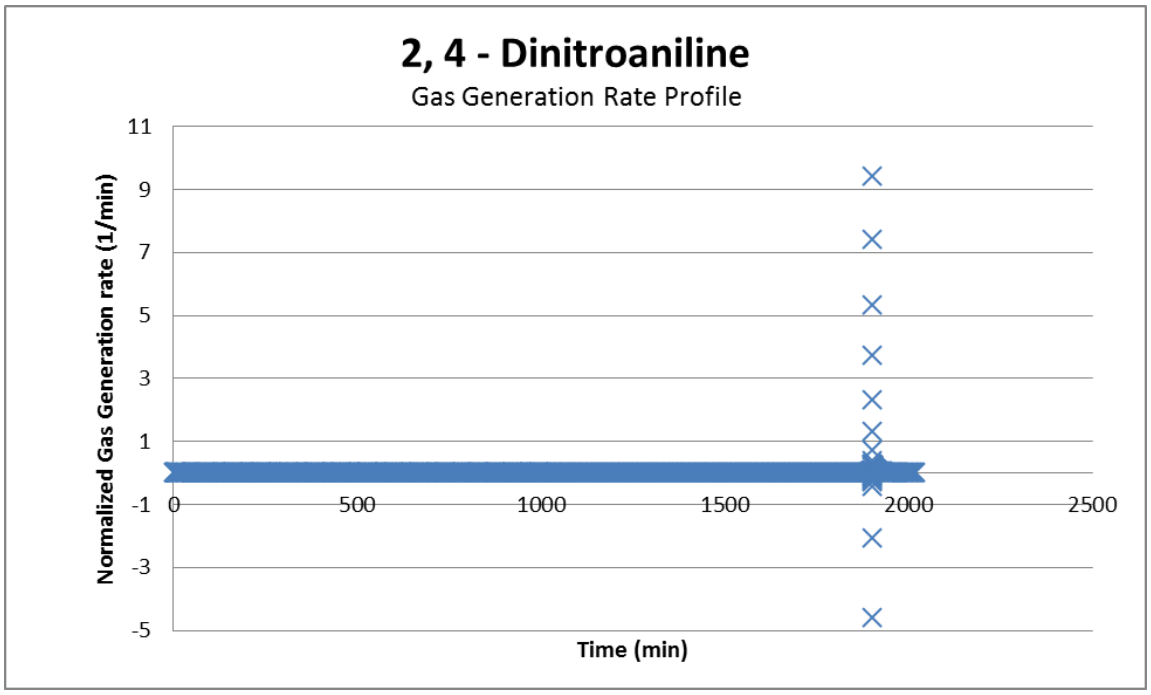

Fig. B.12 Normalized Gas Generation Rate - 2, 4 - Dinitroaniline

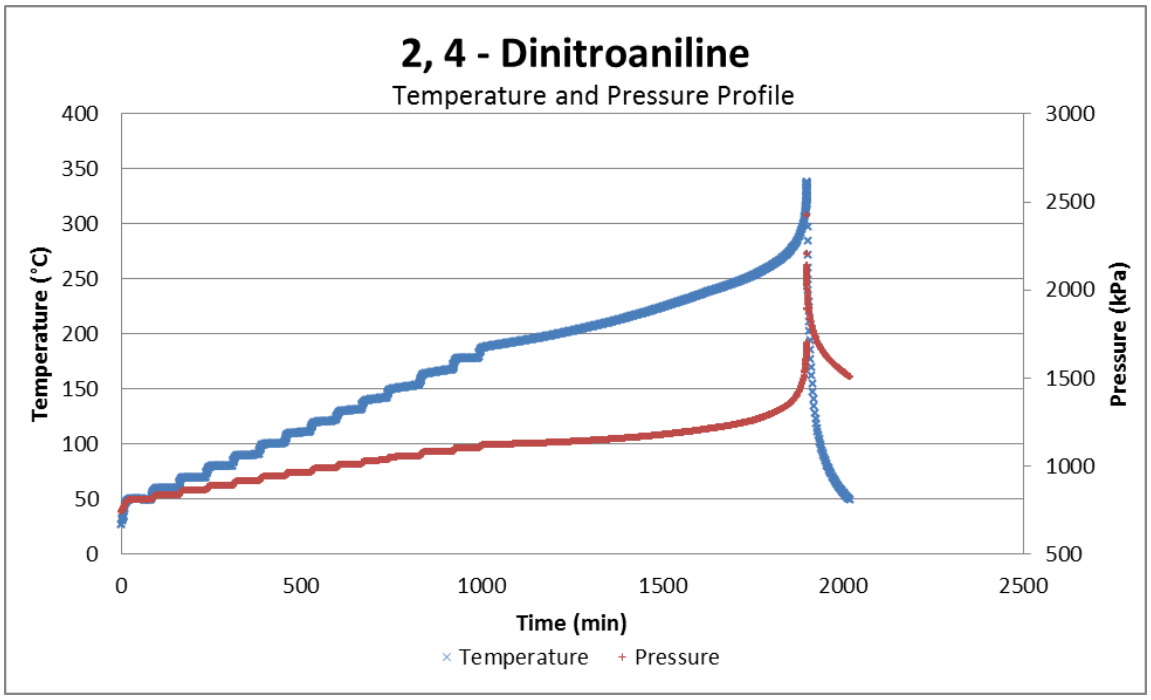

Fig. B.13 Temperature and Pressure Profiles - 2, 4 - Dinitroaniline

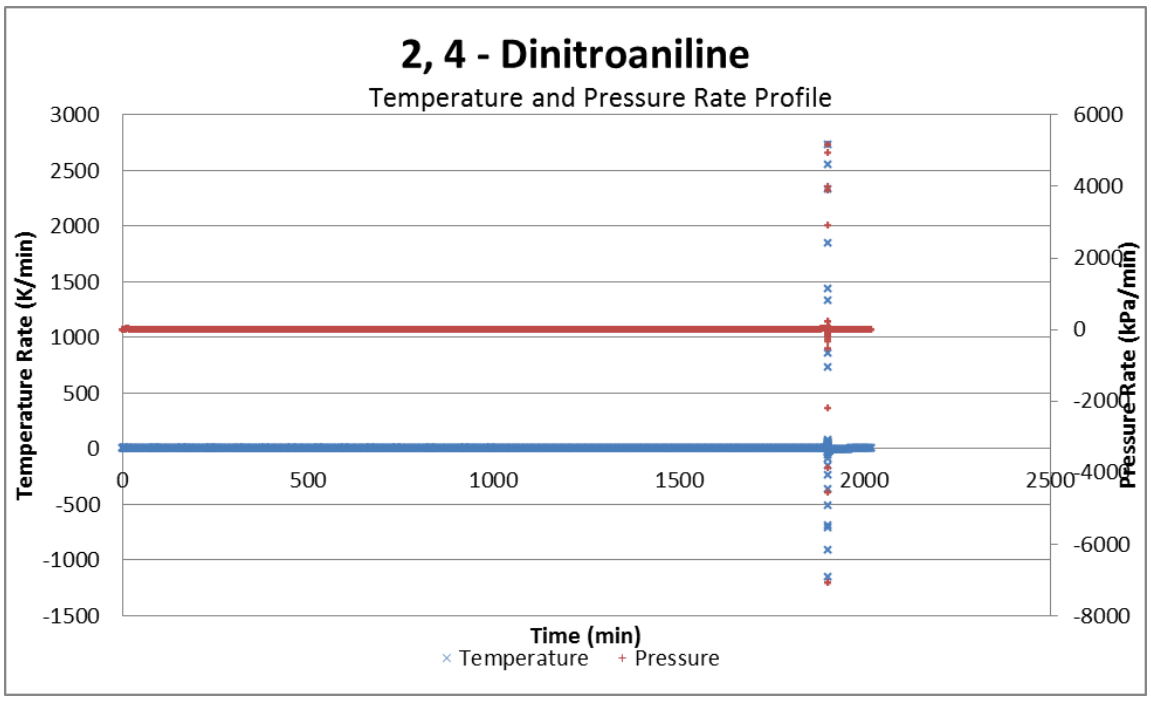

Fig. B.14 Temperature and Pressure Rate Profiles - 2, 4 - Dinitroaniline

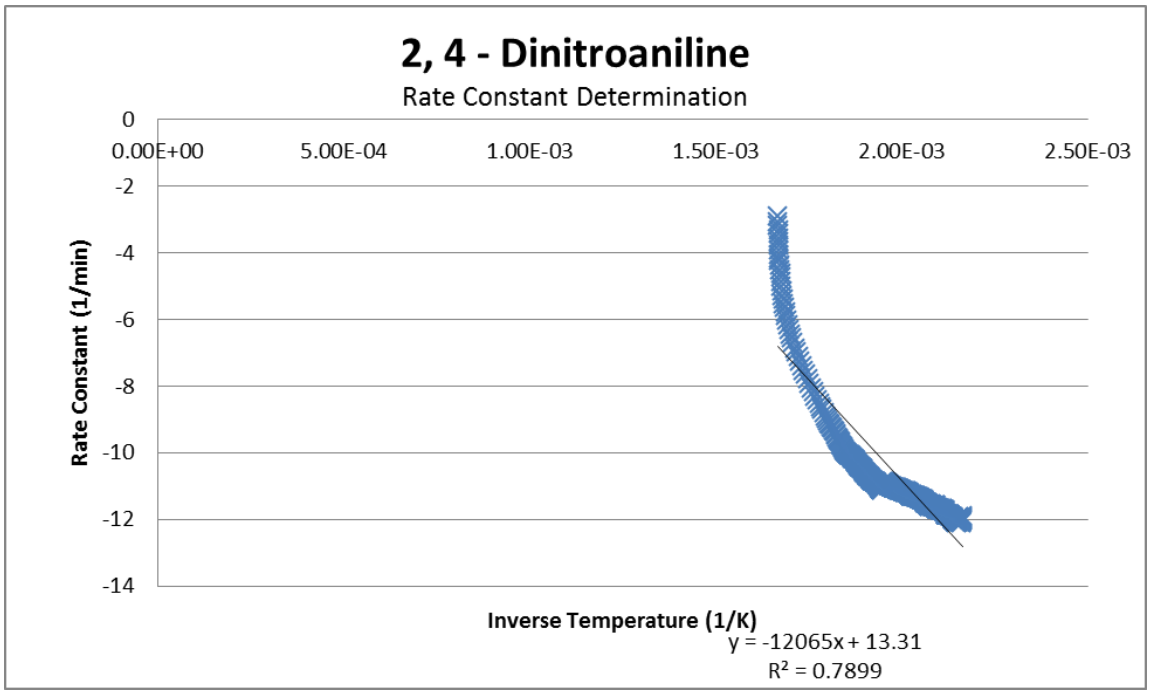

Fig. B.15 Rate Constant Determination - 2, 4 - Dinitroaniline

B.4 Acrylonitrile

Table B.13
Material Properties - Acrylonitrile

Property	Value
m_s (g)	4.00
ρ_s (g/mL)	0.806
C_s (J/(g*K))	2.09
MW (g/mol)	53.06

Table B.14
Cell Properties - Acrylonitrile

Property	Value
m_{cell} (g)	52.63
V_{cell} (mL)	92.61
φ	6.288

Table B.15
IPD Properties - Acrylonitrile

Property	Value
A (1/s)	1.785E+02
E_A (J/(mol*K))	5.365E+04
T_{onset} (°C)	100
T_{max} (°C)	205
ΔH (J/g)	1.380E+03
IPD (W/ml)	8.734E-01

Table B.16
Gas Properties - Acrylonitrile

Property	Value
n_{max} (mol)	3.926E-02
dn/dt_{max} (mol/min)	7.419E-04
n_{maxn}	5.208E-01
dn/dt_{maxn} (1/min)	9.841E-03
GGP (1/min)	5.125E-03

Note – This compound exhibited two exotherms with a sharp drop in pressure during the second. The second exotherm exceeded the temperature capabilities of the APTAC.

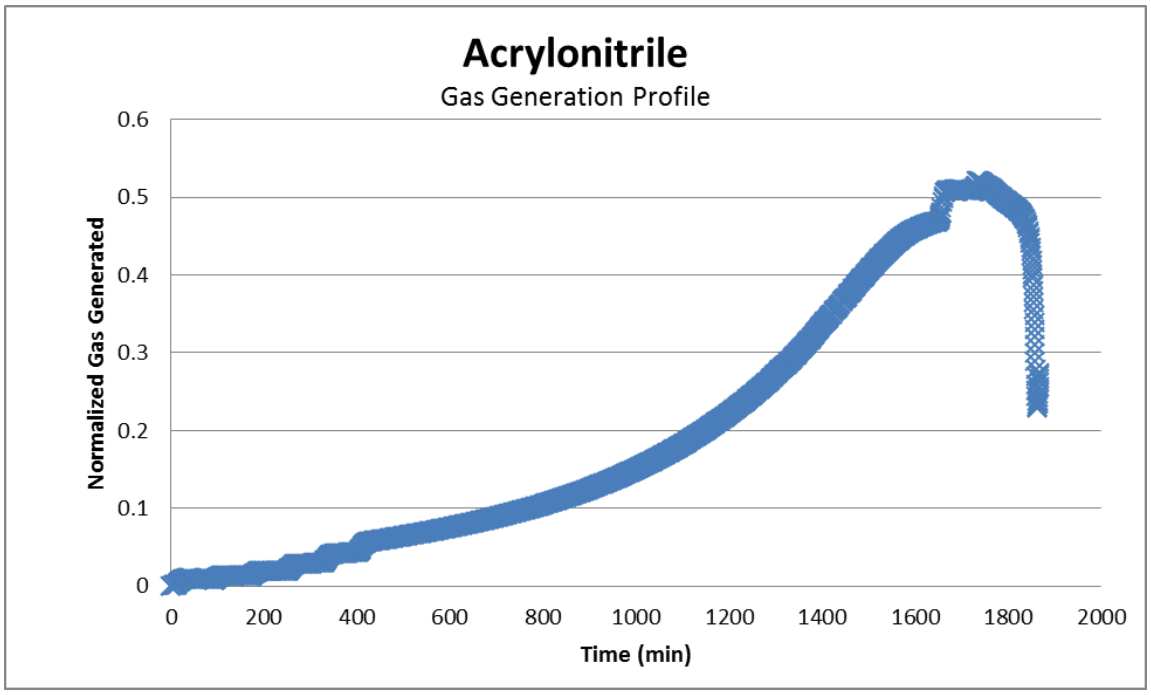

Fig. B.16 Normalized Gas Generation - Acrylonitrile

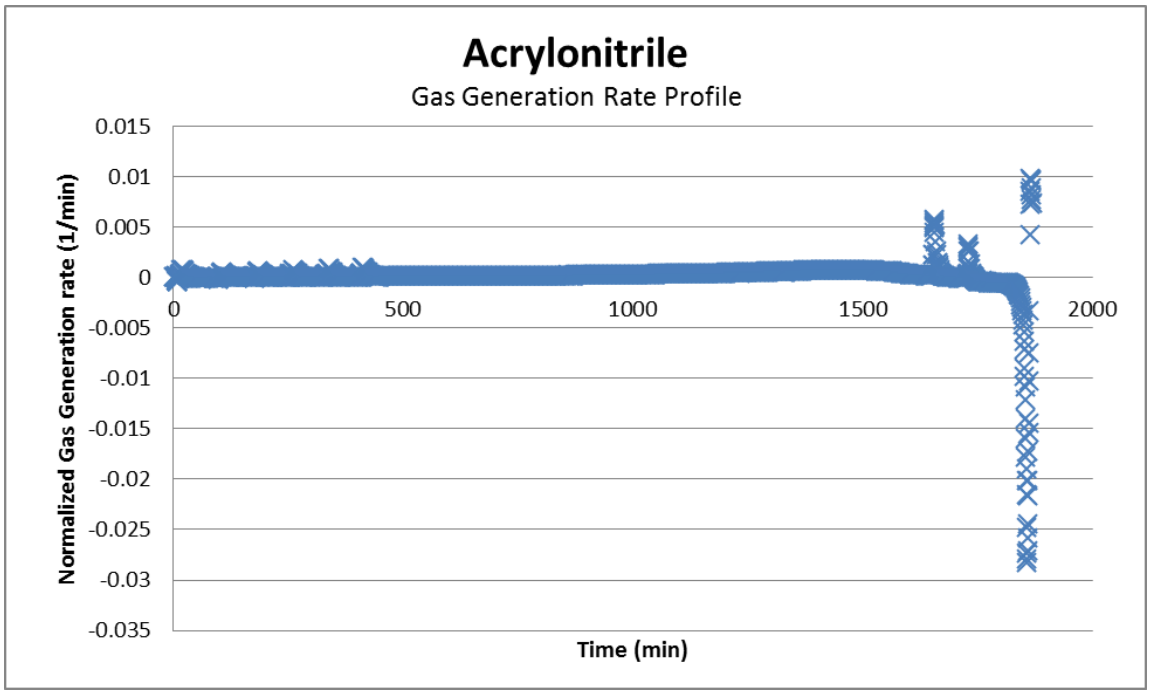

Fig. B.17 Normalized Gas Generation Rate - Acrylonitrile

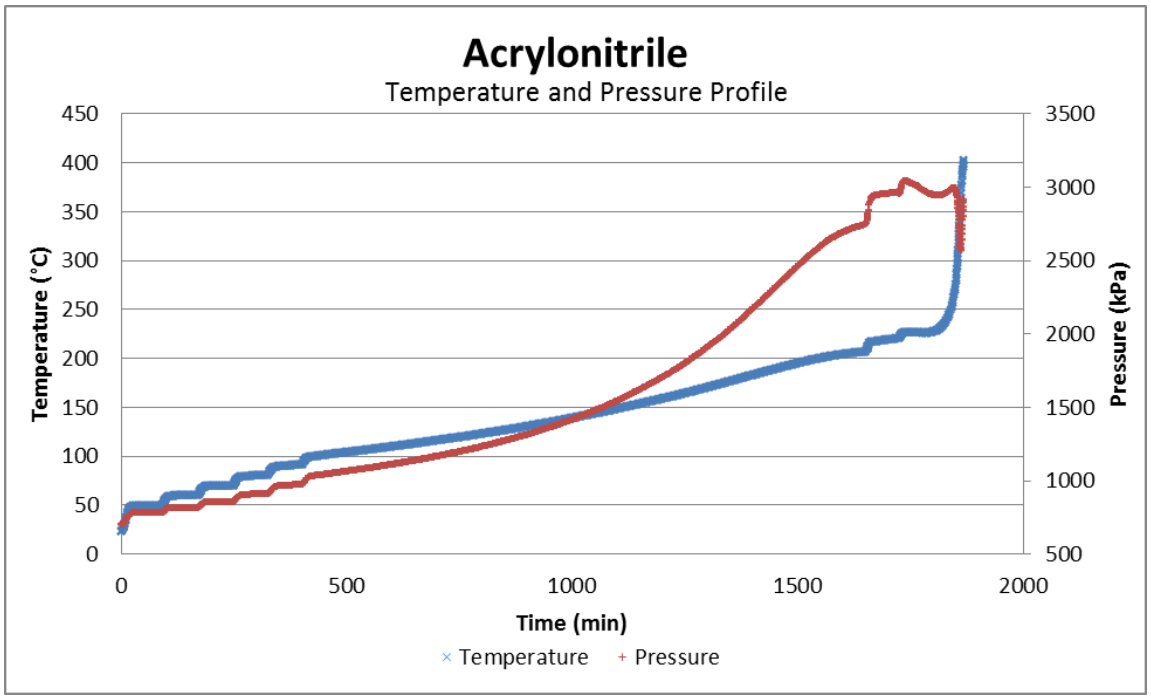

Fig. B.18 Temperature and Pressure Profiles - Acrylonitrile

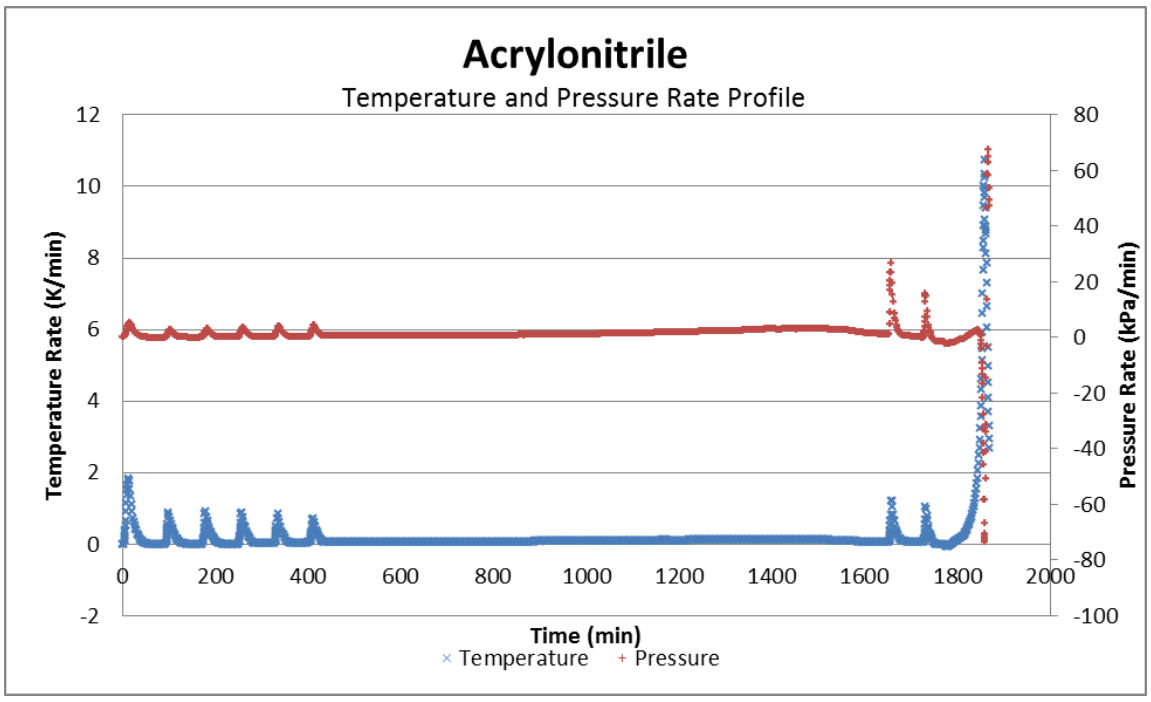

Fig. B.19 Temperature and Pressure Rate Profiles - Acrylonitrile

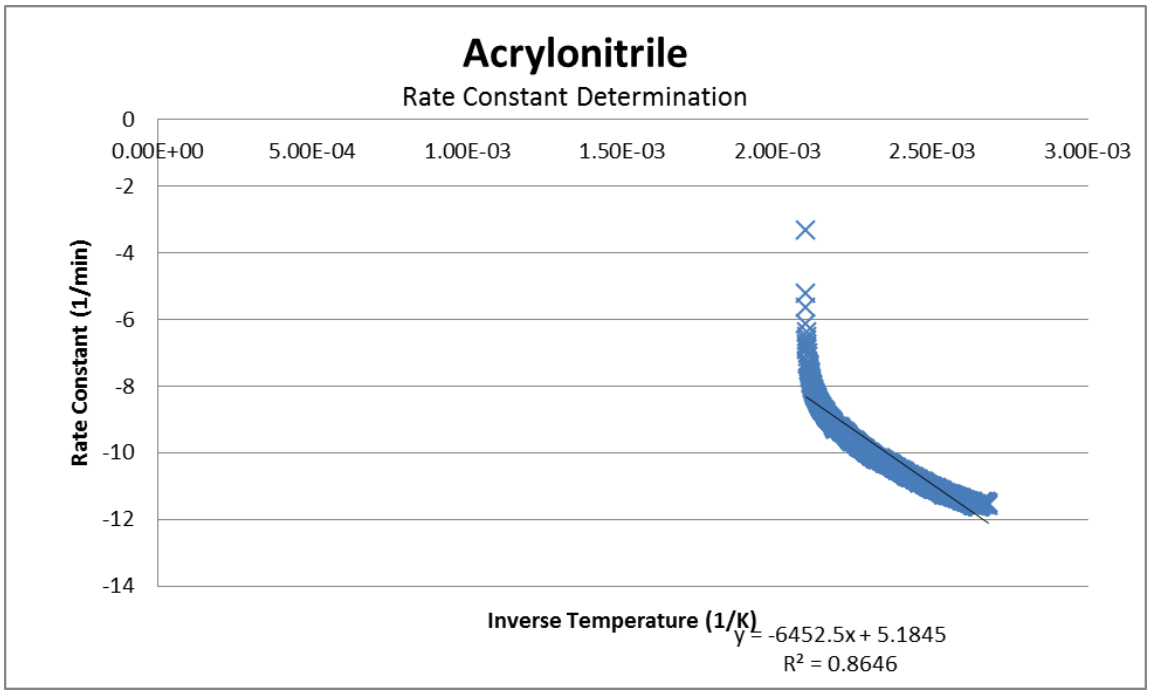

Fig. B.20 Rate Constant Determination - Acrylonitrile

B.5 Cumene

Table B.17
Material Properties - Cumene

Property	Value
m_s (g)	1.95
ρ_s (g/mL)	0.862
C_s (J/(g*K))	1.670
MW (g/mol)	120.19

Table B.18
Cell Properties - Cumene

Property	Value
m_{cell} (g)	50.77
V_{cell} (mL)	97.38
φ	14.09

Table B.19
IPD Properties - Cumene

Property	Value
A (1/s)	4.374E+02
E_A (J/(mol*K))	5.839E+04
T_{onset} (°C)	130
T_{max} (°C)	220
ΔH (J/g)	2.119E+03
IPD (W/ml)	1.181E+00

Table B.20
Gas Properties - Cumene

Property	Value
n_{max} (mol)	0.000E+00
dn/dt_{max} (mol/min)	5.134E-06
n_{maxn}	0.000E+00
dn/dt_{maxn} (1/min)	3.164E-04
GGP (1/min)	0.000E+00

Note – This compound showed a large pressure drop likely due to the endothermic reaction incorporating oxygen.

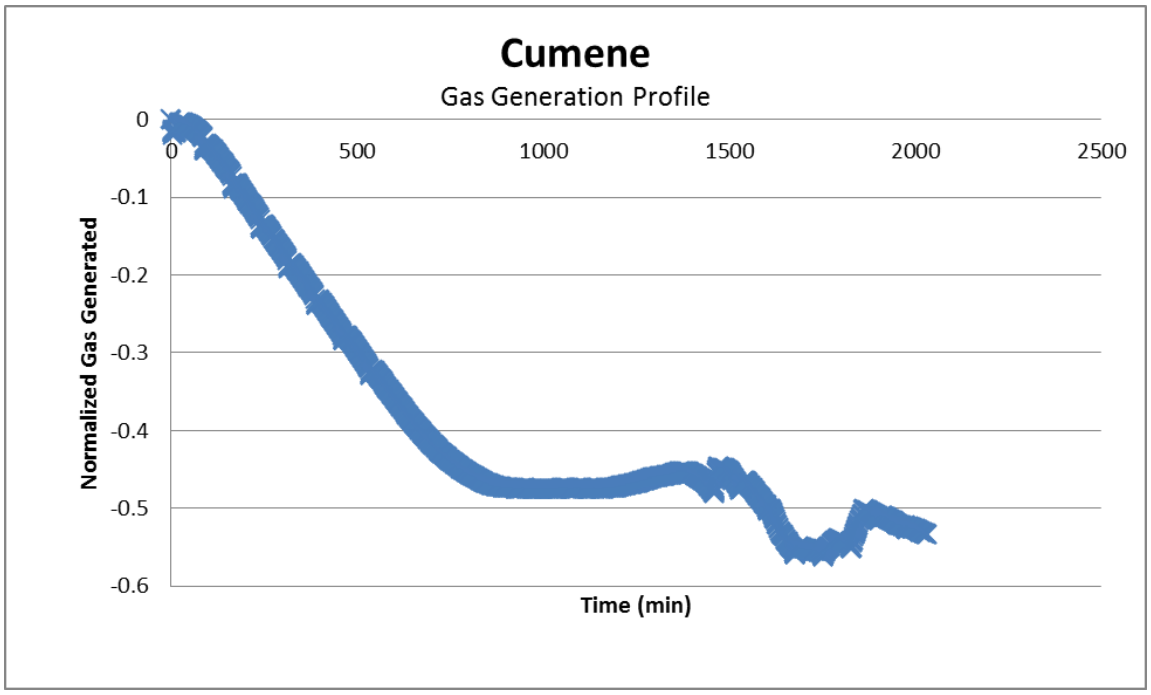

Fig. B.21 Normalized Gas Generation - Cumene

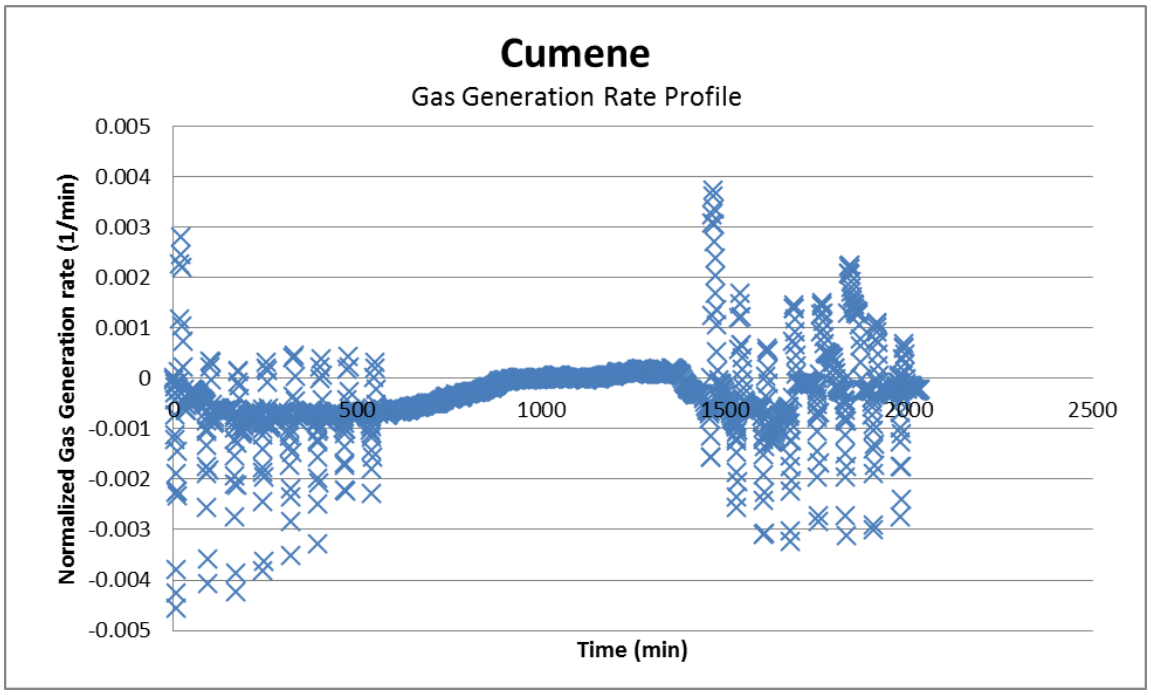

Fig. B.22 Normalized Gas Generation Rate - Cumene

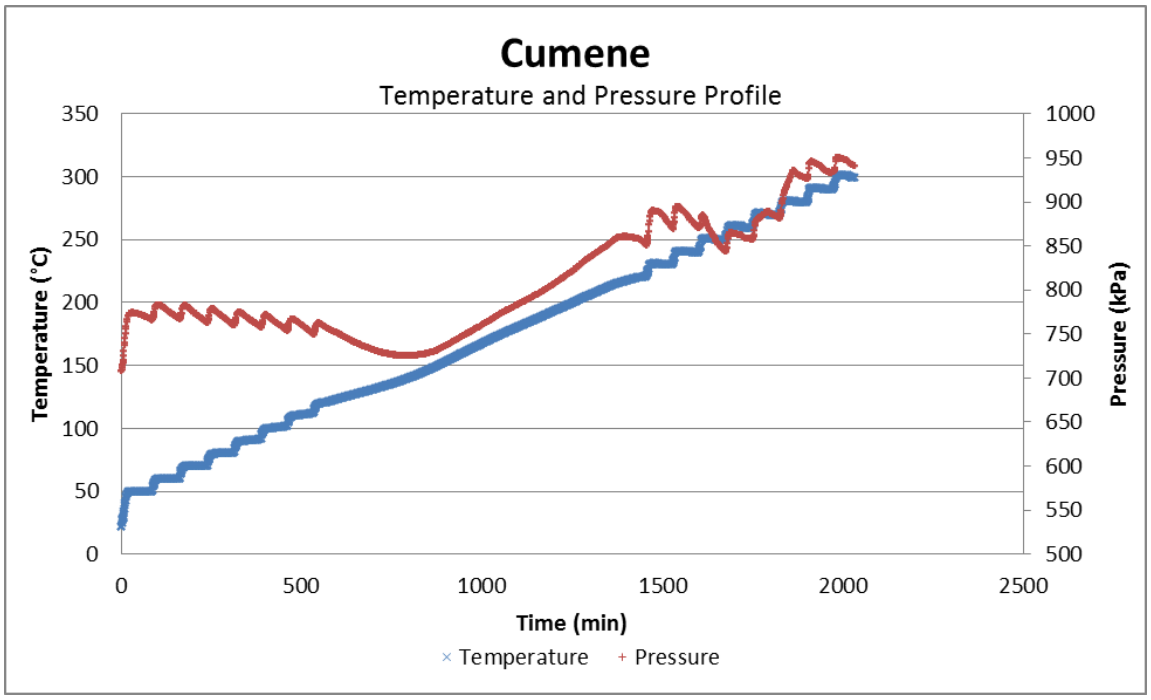

Fig. B.23 Temperature and Pressure Profiles - Cumene

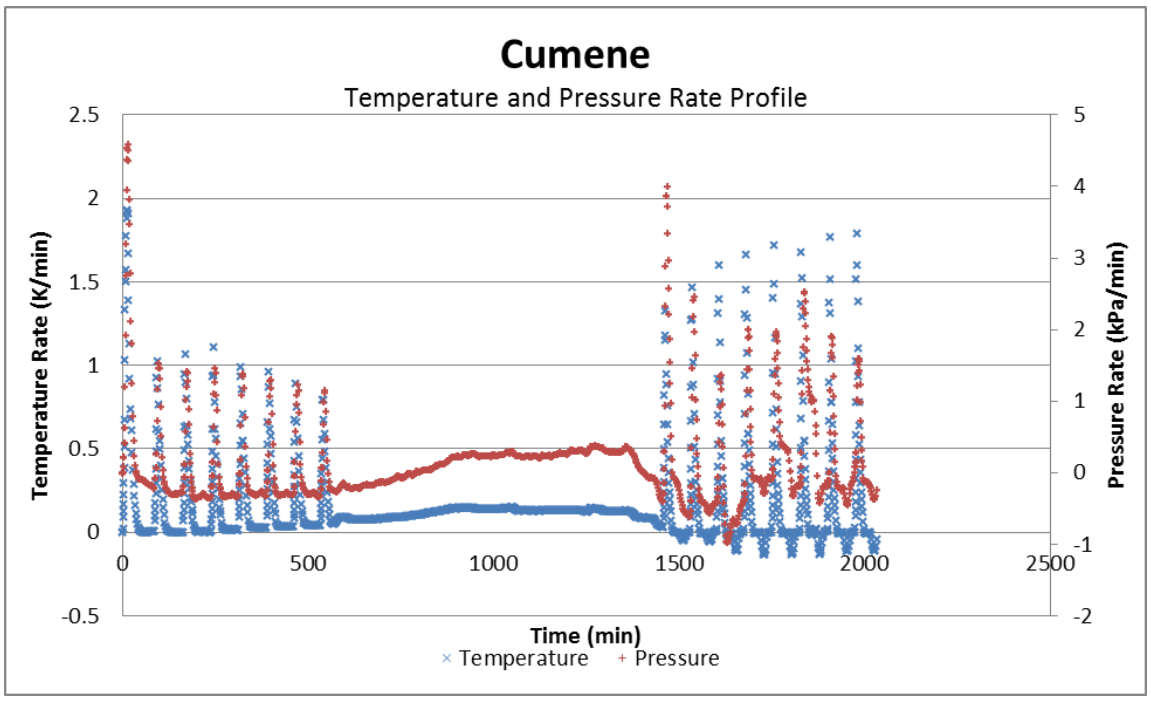

Fig. B.24 Temperature and Pressure Rate Profiles - Cumene

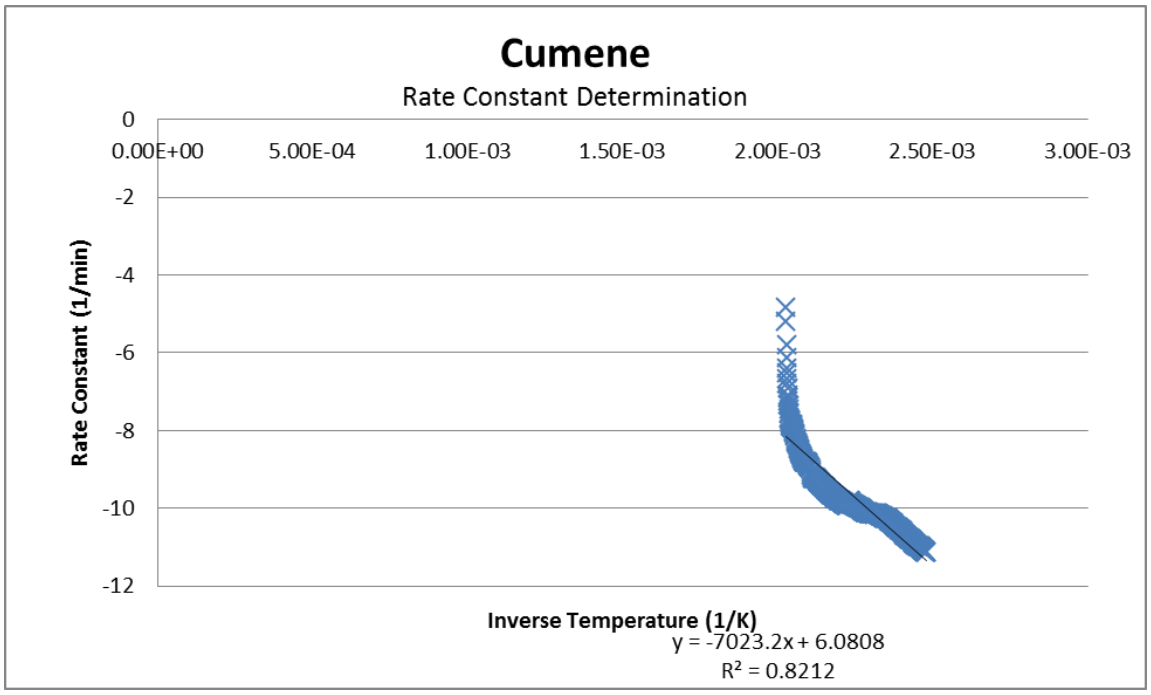

Fig. B.25 Rate Constant Determination - Cumene

B.6 Cumene Hydroperoxide

Table B.21
Material Properties - Cumene Hydroperoxide

Property	Value
m_s (g)	0.99
ρ_s (g/mL)	1.02
C_s (J/(g*K))	1.884
MW (g/mol)	152.19

Table B.22
Cell Properties - Cumene Hydroperoxide

Property	Value
m_{cell} (g)	51.9
V_{cell} (mL)	97.00
φ	24.37

Table B.23
IPD Properties - Cumene Hydroperoxide

Property	Value
A (1/s)	6.675E+08
E_A (J/(mol*K))	1.006E+05
T_{onset} (°C)	120
T_{max} (°C)	240
ΔH (J/g)	5.510E+03
IPD (W/ml)	3.409E+02

Table B.24
Gas Properties - Cumene Hydroperoxide

Property	Value
n_{max} (mol)	7.562E-03
dn/dt_{max} (mol/min)	2.314E-03
n_{maxn}	1.162E+00
dn/dt_{maxn} (1/min)	3.558E-01
GGP (1/min)	4.136E-01

Note – This compound exhibited an explosion event.

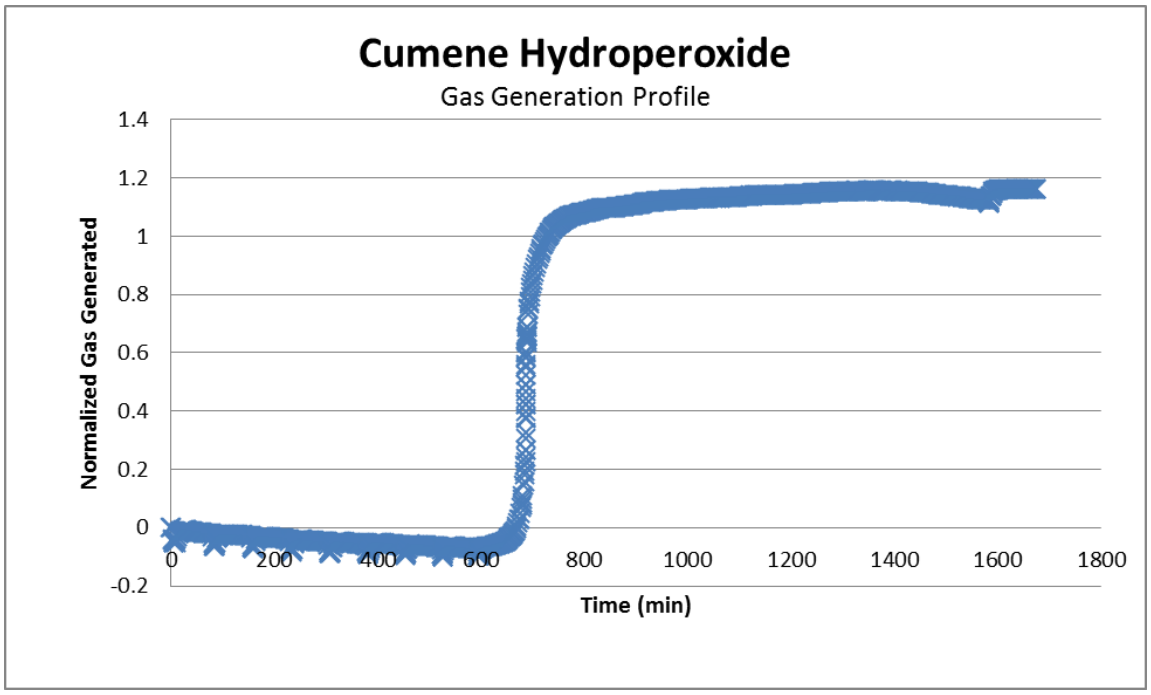

Fig. B.26 Normalized Gas Generation - Cumene Hydroperoxide

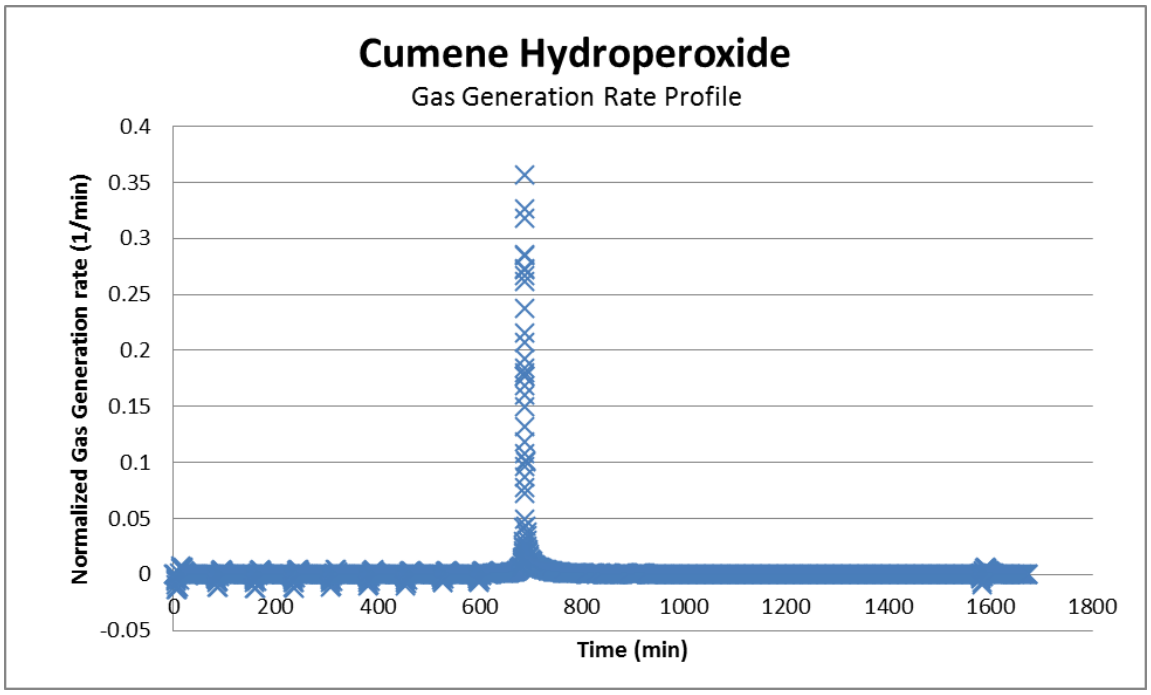

Fig. B.27 Normalized Gas Generation Rate - Cumene Hydroperoxide

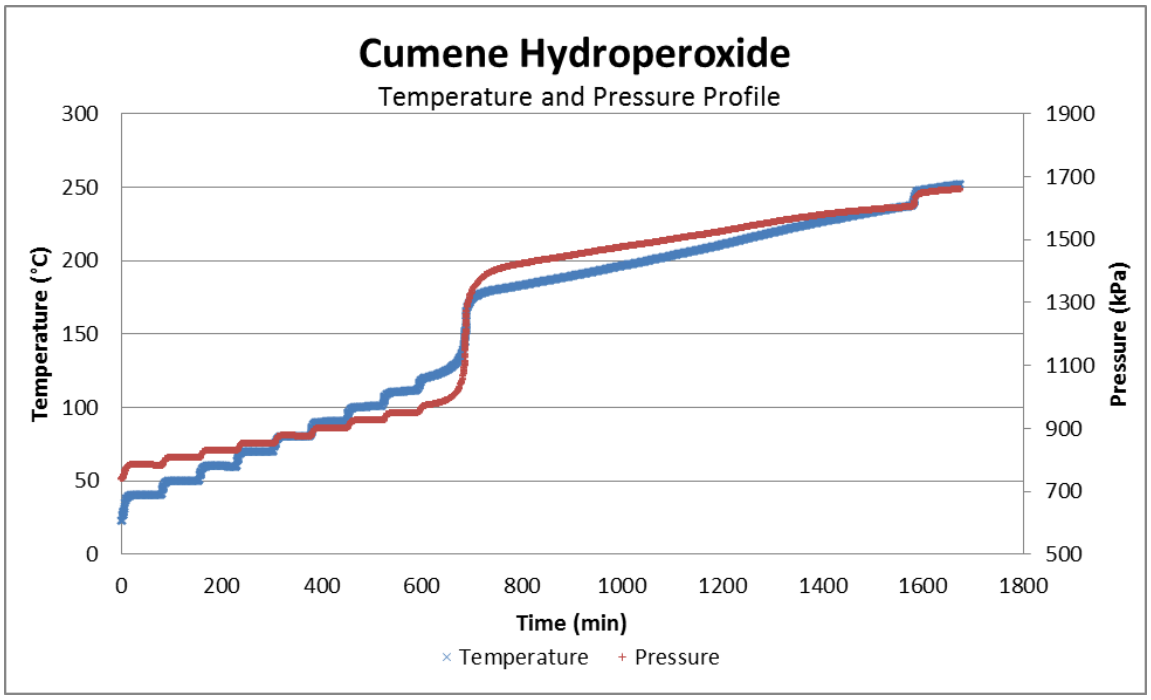

Fig. B.28 Temperature and Pressure Profiles - Cumene Hydroperoxide

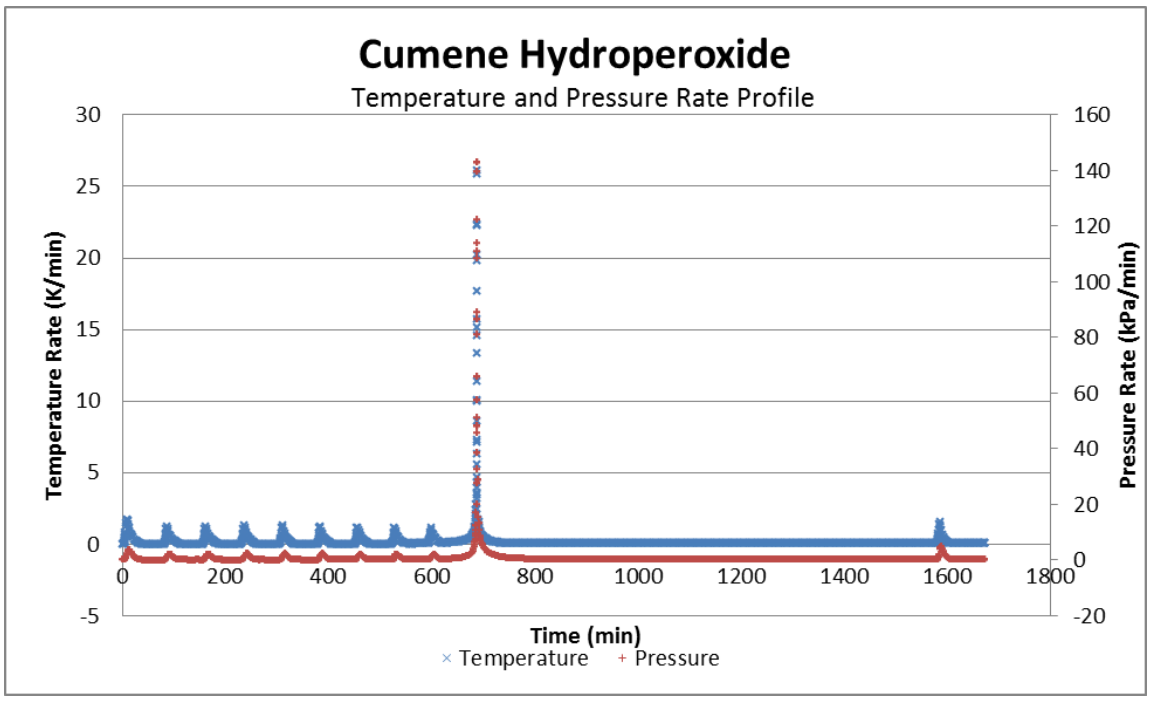

Fig. B.29 Temperature and Pressure Rate Profiles - Cumene Hydroperoxide

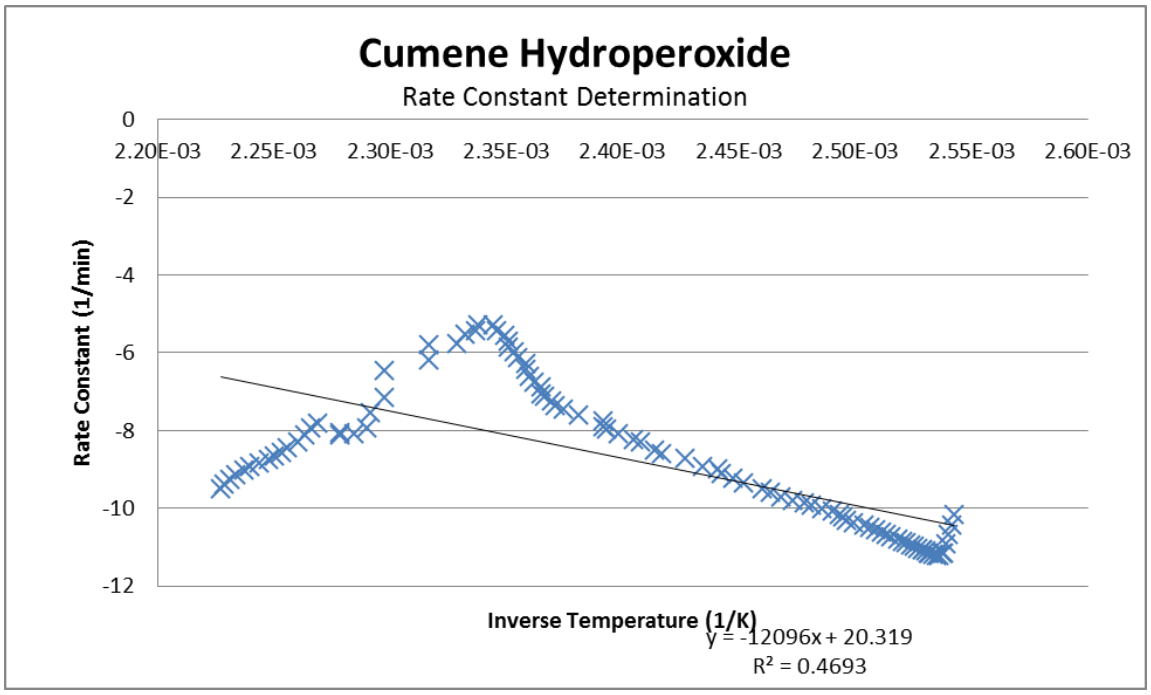

Fig. B.30 Rate Constant Determination - Cumene Hydroperoxide

B.7 Ethylene Oxide

Table B.25
Material Properties - Ethylene Oxide

Property	Value
m_s (g)	14.0
ρ_s (g/mL)	N/A
C_s (J/(g*K))	1.093
MW (g/mol)	44.05

Table B.26
Cell Properties - Ethylene Oxide

Property	Value
m_{cell} (g)	31.61
V_{cell} (mL)	130.00
φ	2.073

Table B.27
IPD Properties - Ethylene Oxide

Property	Value
A (1/s)	8.846E+03
E_A (J/(mol*K))	8.598E+04
T_{onset} (°C)	180
T_{max} (°C)	600
ΔH (J/g)	9.526E+02
IPD (W/ml)	2.362E-03

Table B.28
Gas Properties - Ethylene Oxide

Property	Value
n_{max} (mol)	4.157E-01
dn/dt_{max} (mol/min)	4.462E-01
n_{maxn}	1.308E+00
dn/dt_{maxn} (1/min)	1.404E+00
GGP (1/min)	1.836E+00

Note – This compound exhibited an explosion event, was run at atmospheric initial pressure, under nitrogen (Dinh, 2008). A titanium bomb was used.

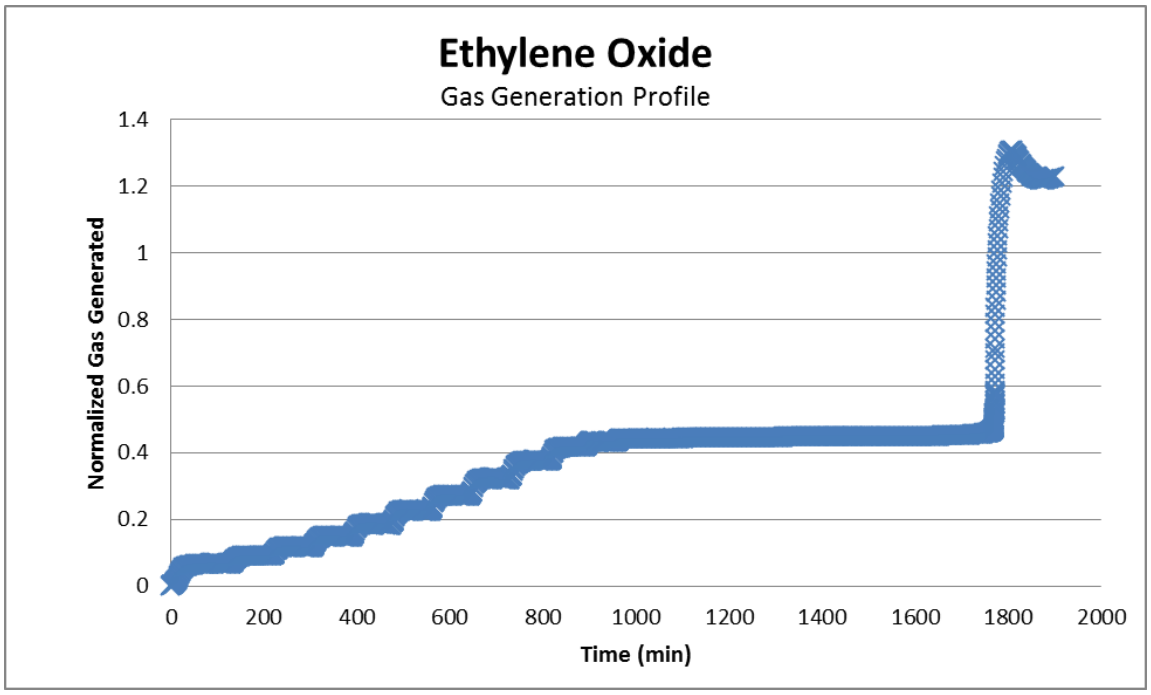

Fig. B.31 Normalized Gas Generation - Ethylene Oxide

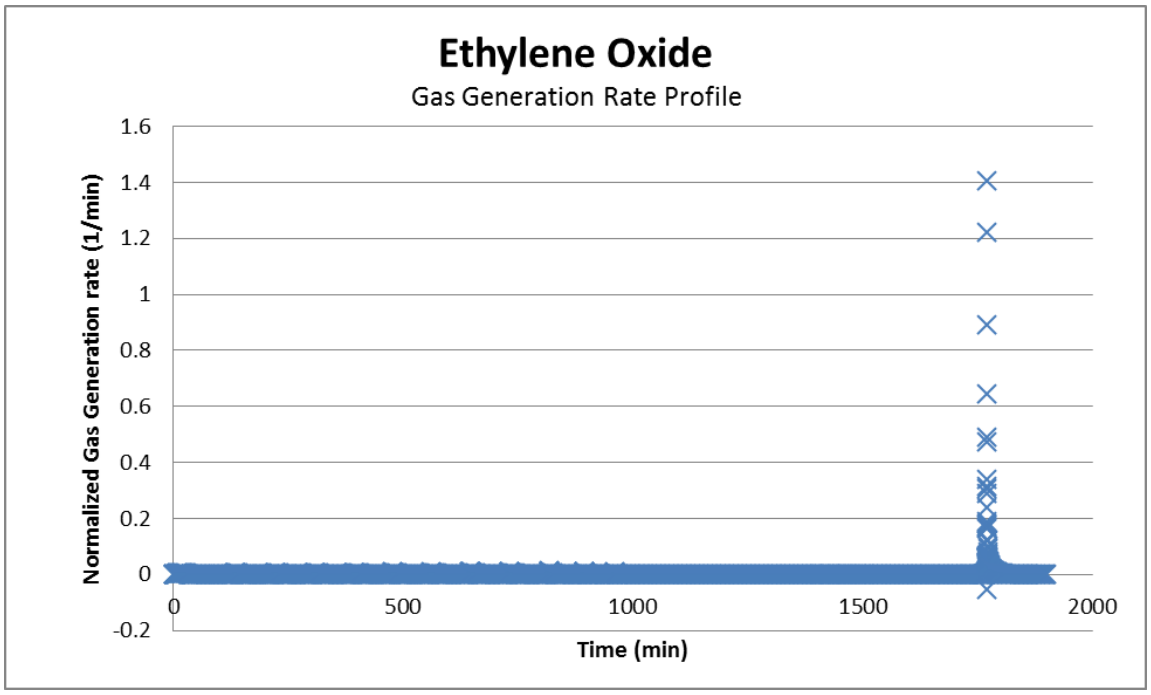

Fig. B.32 Normalized Gas Generation Rate - Ethylene Oxide

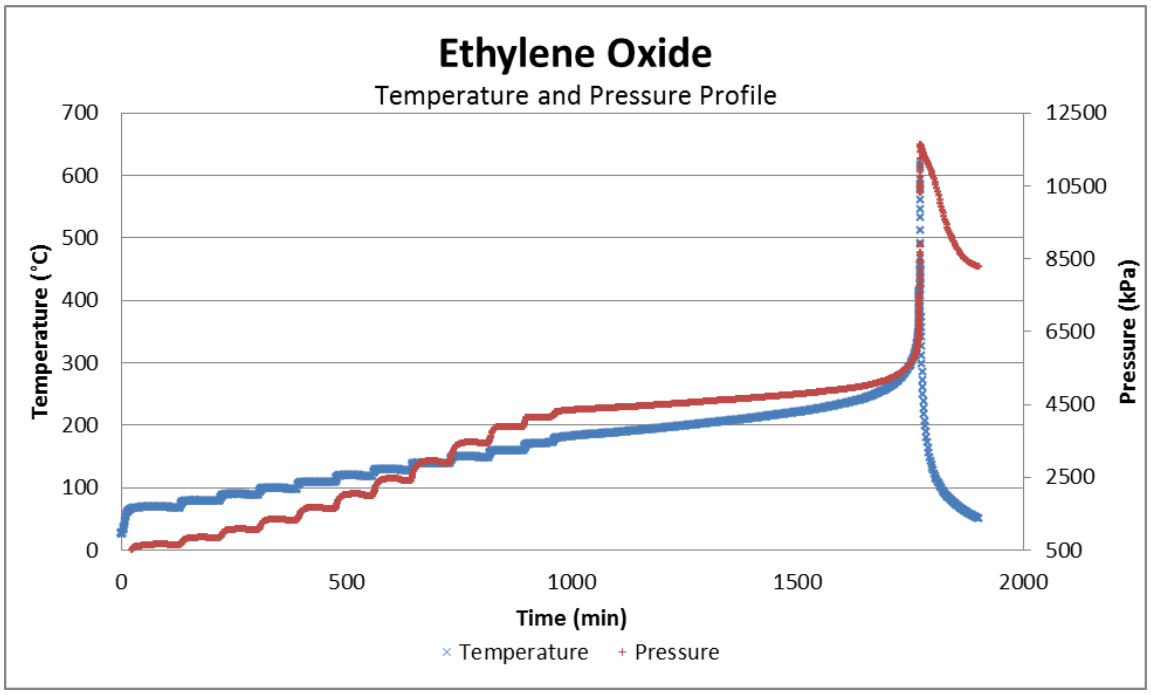

Fig. B.33 Temperature and Pressure Profiles - Ethylene Oxide

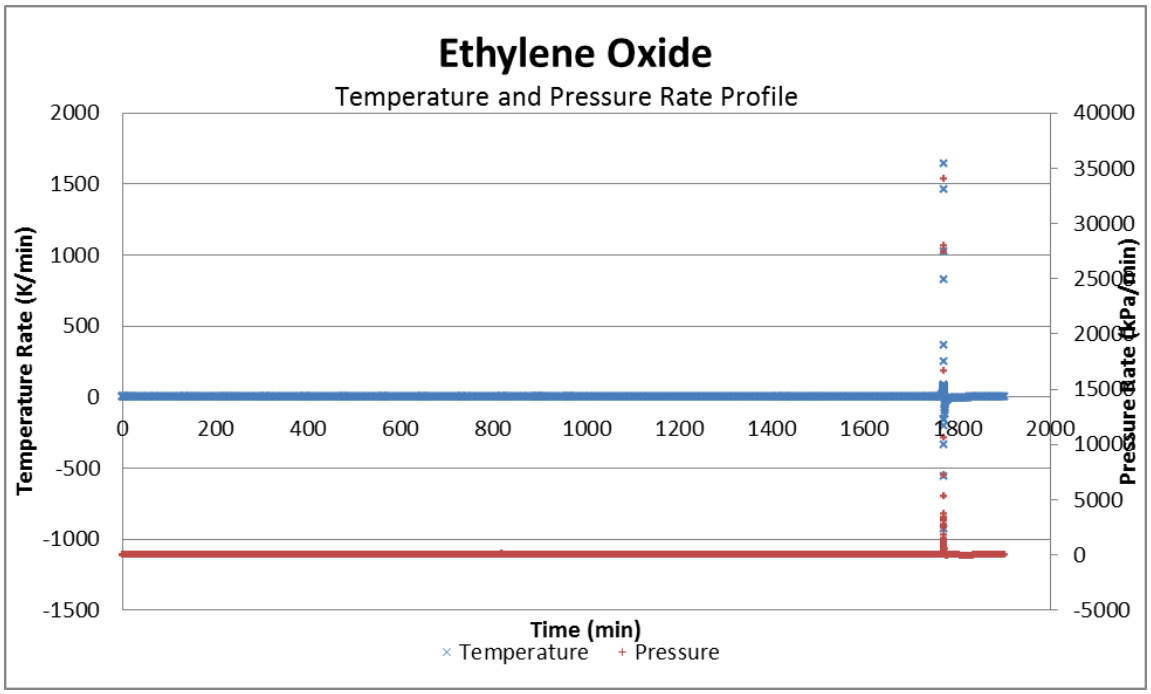

Fig. B.34 Temperature and Pressure Rate Profiles - Ethylene Oxide

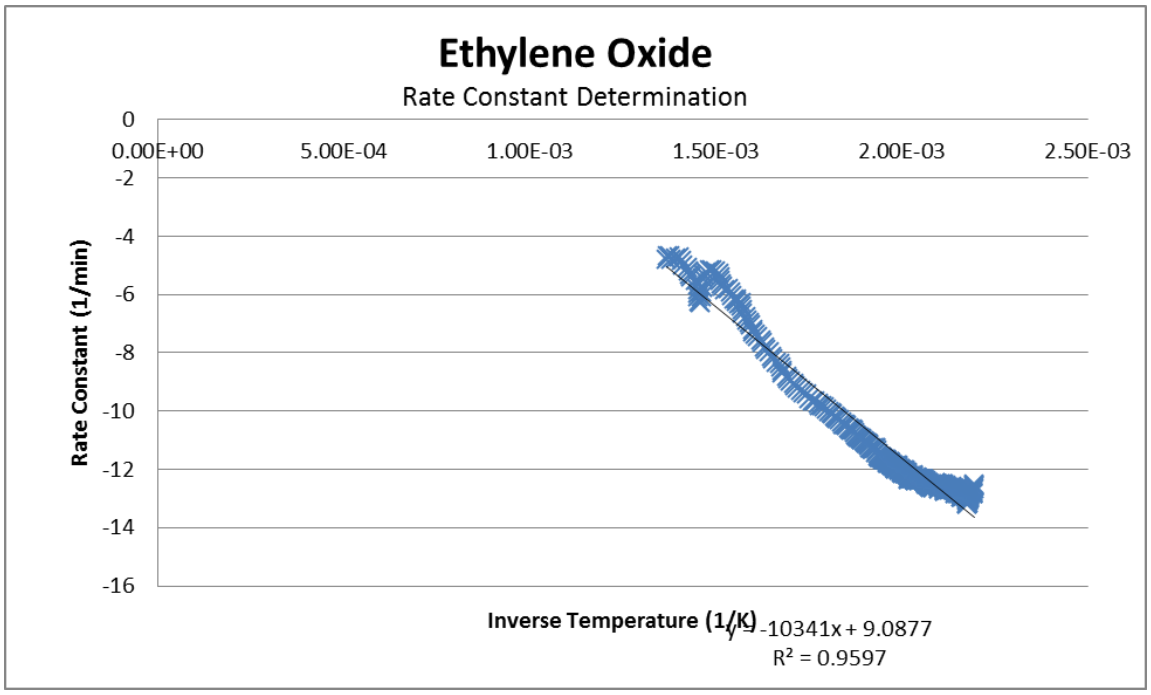

Fig. B.35 Rate Constant Determination - Ethylene Oxide

B.8 Hydrogen Peroxide - 12.5%

Table B.29
Material Properties - Hydrogen Peroxide - 12.5%

Property	Value
m_s (g)	2.52
ρ_s (g/mL)	1.13
C_s (J/(g*K))	2.619
MW (g/mol)	34.015

Table B.30
Cell Properties - Hydrogen Peroxide - 12.5%

Property	Value
m_{cell} (g)	58.81
V_{cell} (mL)	100.00
φ	16.02

Table B.31
IPD Properties - Hydrogen Peroxide - 12.5%

Property	Value
A (1/s)	8.609E+14
E_A (J/(mol*K))	1.580E+05
T_{onset} (°C)	140
T_{max} (°C)	250
ΔH (J/g)	4.614E+03
IPD (W/ml)	7.472E+02

Table B.32
Gas Properties - Hydrogen Peroxide - 12.5%

Property	Value
n_{max} (mol)	1.671E-01
dn/dt_{max} (mol/min)	6.029E-02
n_{maxn}	2.256E+00
dn/dt_{maxn} (1/min)	8.138E-01
GGP (1/min)	1.836E+00

Note – This compound exhibited an explosion event and was run under atmospheric pressure (Saenz et al., 2009). It was not assumed to be pure.

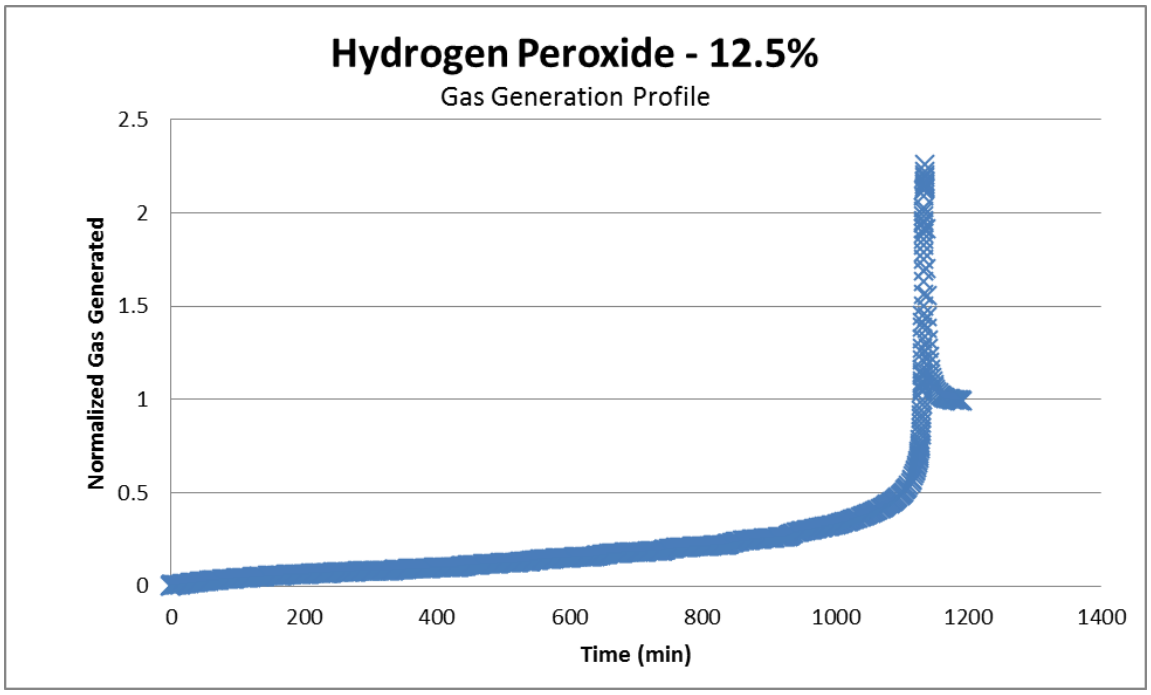

Fig. B.36 Normalized Gas Generation - Hydrogen Peroxide - 12.5%

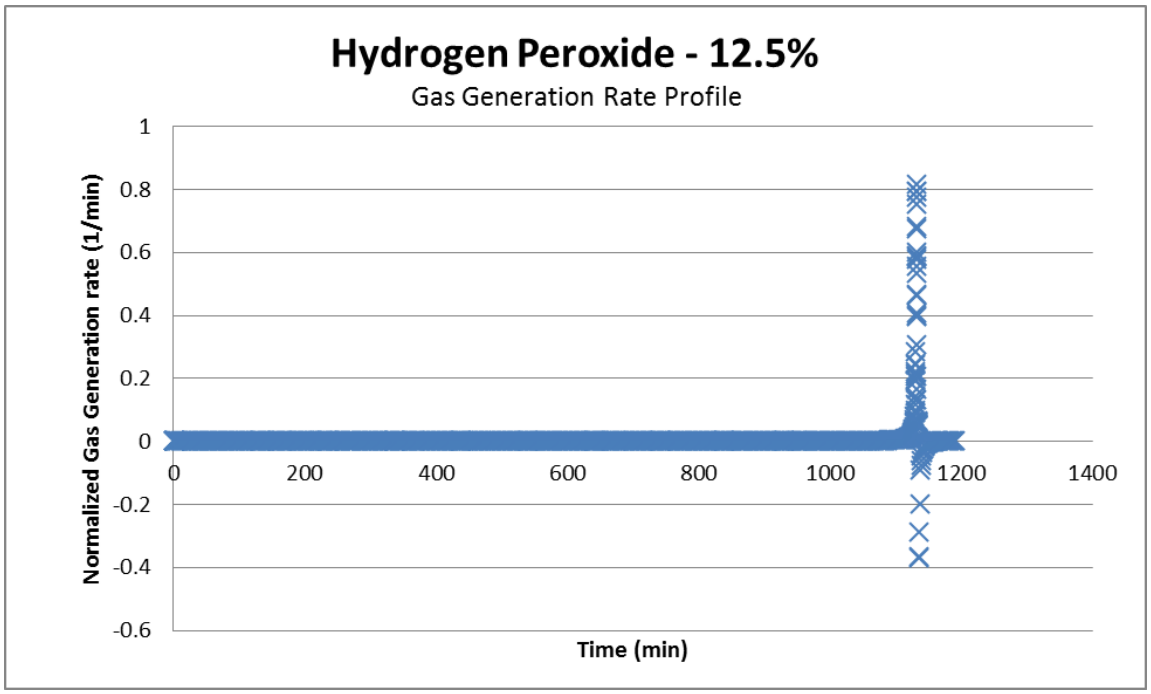

Fig. B.37 Normalized Gas Generation Rate - Hydrogen Peroxide - 12.5%

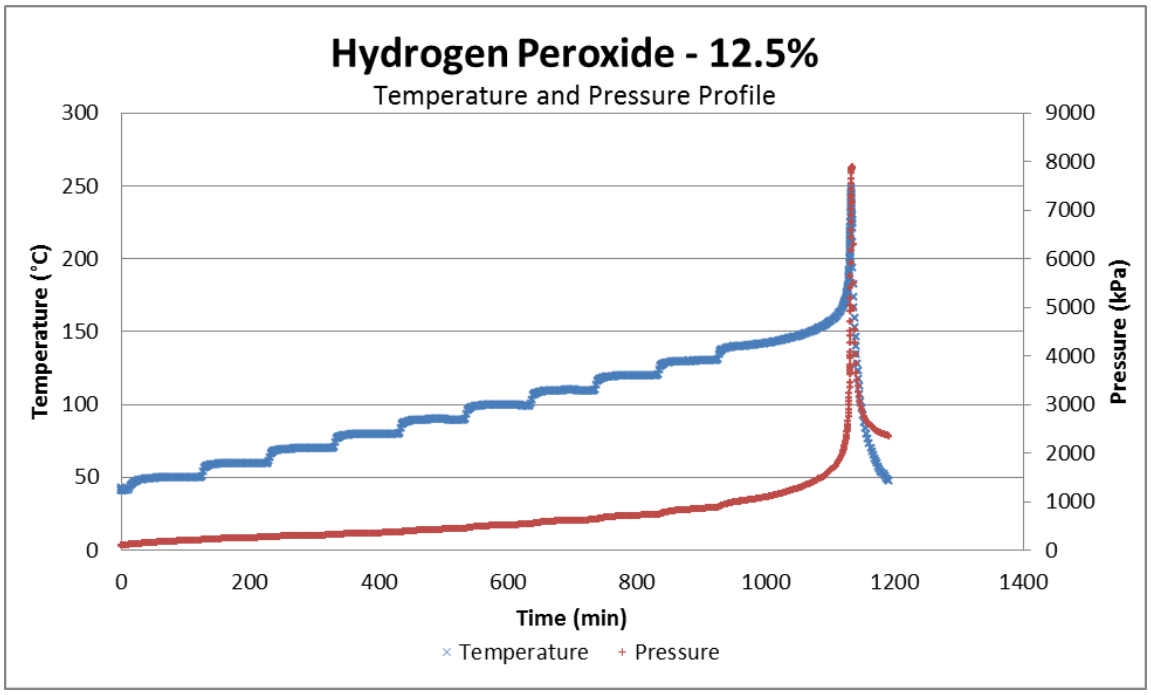

Fig. B.38 Temperature and Pressure Profiles - Hydrogen Peroxide - 12.5%

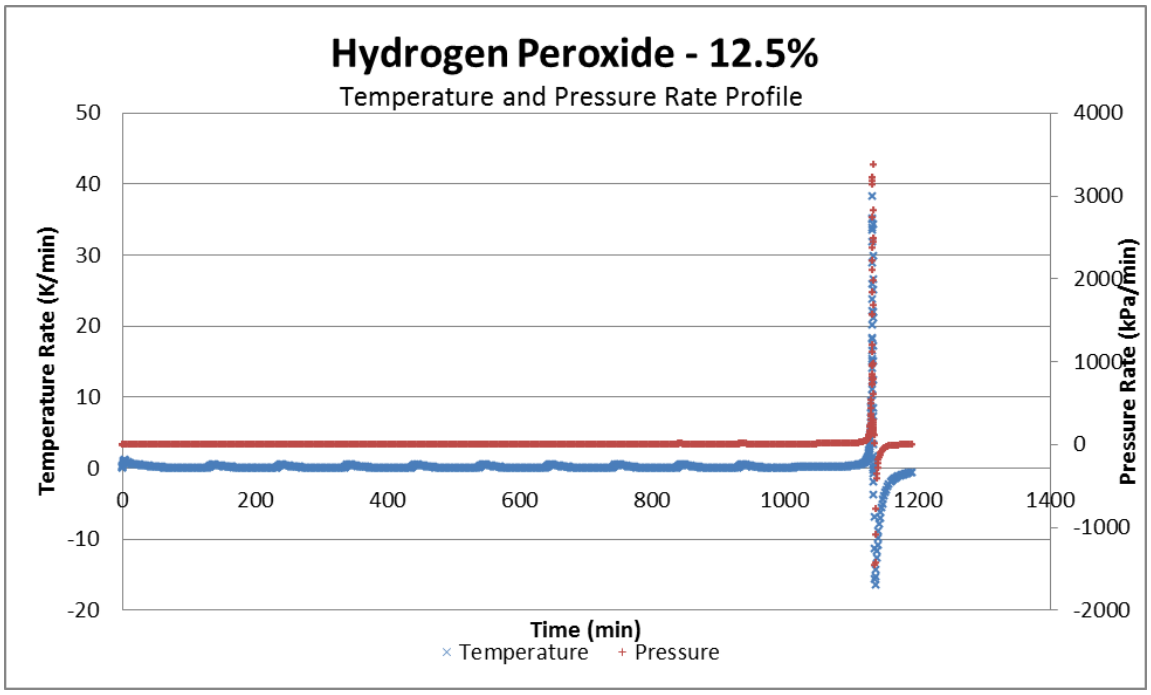

Fig. B.39 Temperature and Pressure Rate Profiles - Hydrogen Peroxide - 12.5%

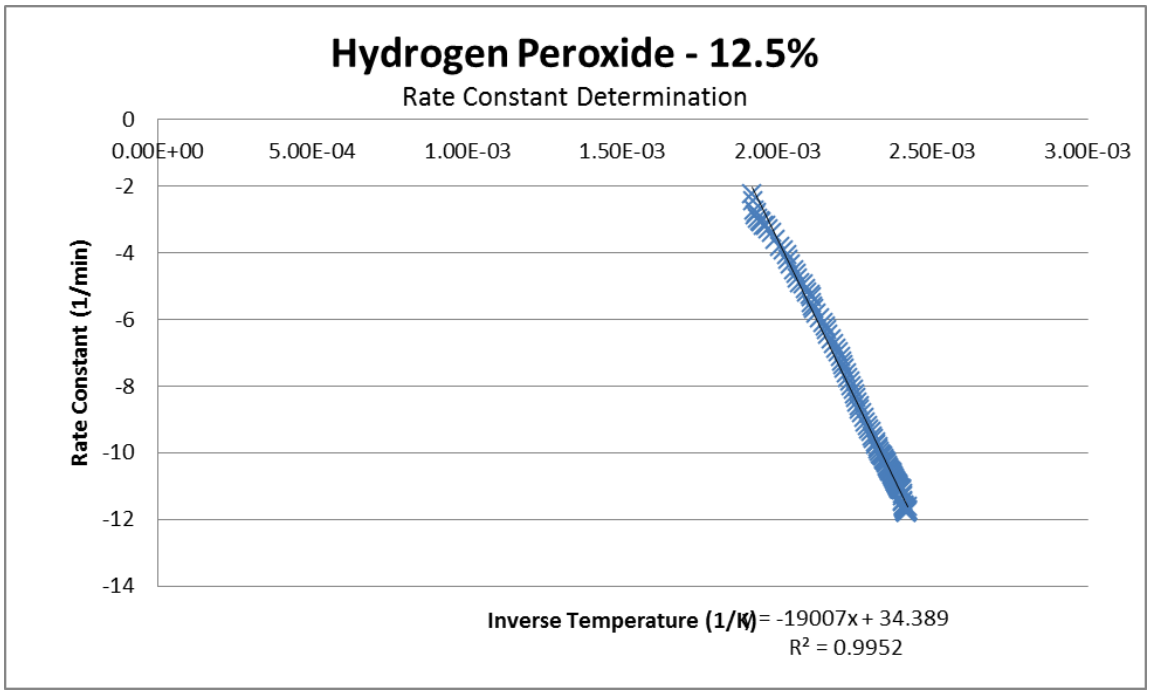

Fig. B.40 Rate Constant Determination - Hydrogen Peroxide - 12.5%

B.9 Hydroxylamine Chloride

Table B.33
Material Properties - Hydroxylamine Chloride

Property	Value
m_s (g)	1.00
ρ_s (g/mL)	1.67
C_s (J/(g*K))	0.6687
MW (g/mol)	69.49

Table B.34
Cell Properties - Hydroxylamine Chloride

Property	Value
m_{cell} (g)	53.04
V_{cell} (mL)	92.96
φ	67.62

Table B.35
IPD Properties - Hydroxylamine Chloride

Property	Value
A (1/s)	7.991E+25
E_A (J/(mol*K))	2.490E+05
T_{onset} (°C)	150
T_{max} (°C)	194
ΔH (J/g)	1.990E+03
IPD (W/ml)	3.633E+04

Table B.36
Gas Properties - Hydroxylamine Chloride

Property	Value
n_{max} (mol)	1.189E-02
dn/dt_{max} (mol/min)	8.283E-04
n_{maxn}	8.266E-01
dn/dt_{maxn} (1/min)	5.756E-02
GGP (1/min)	4.757E-02

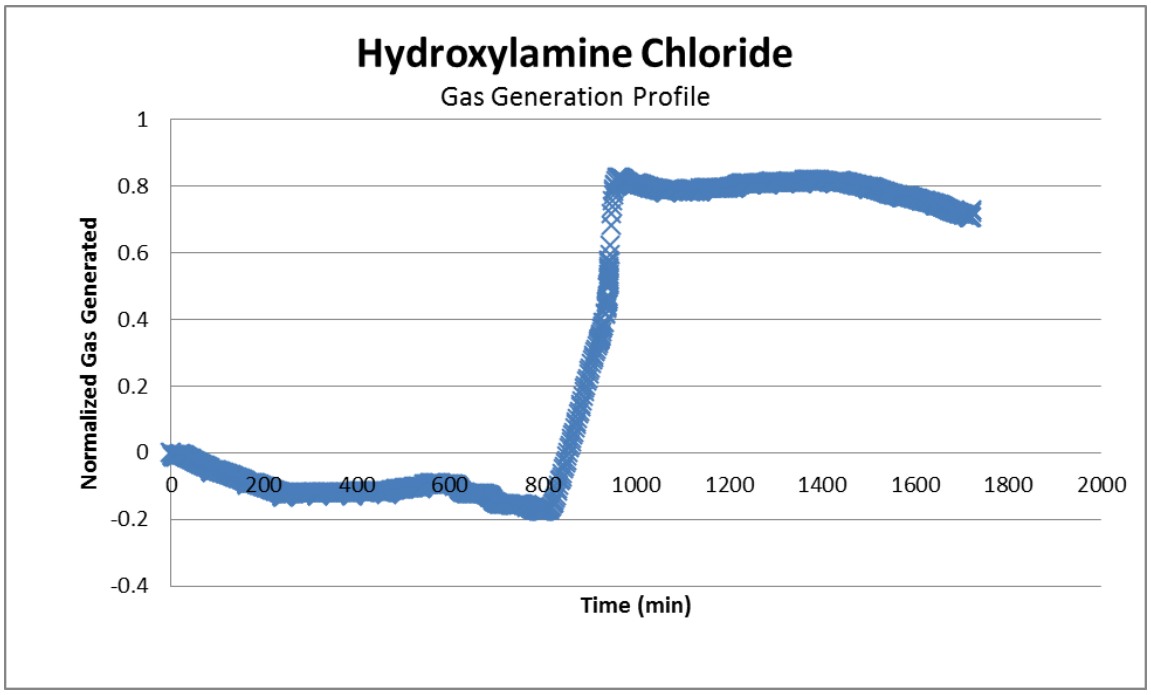

Fig. B.41 Normalized Gas Generation - Hydroxylamine Chloride

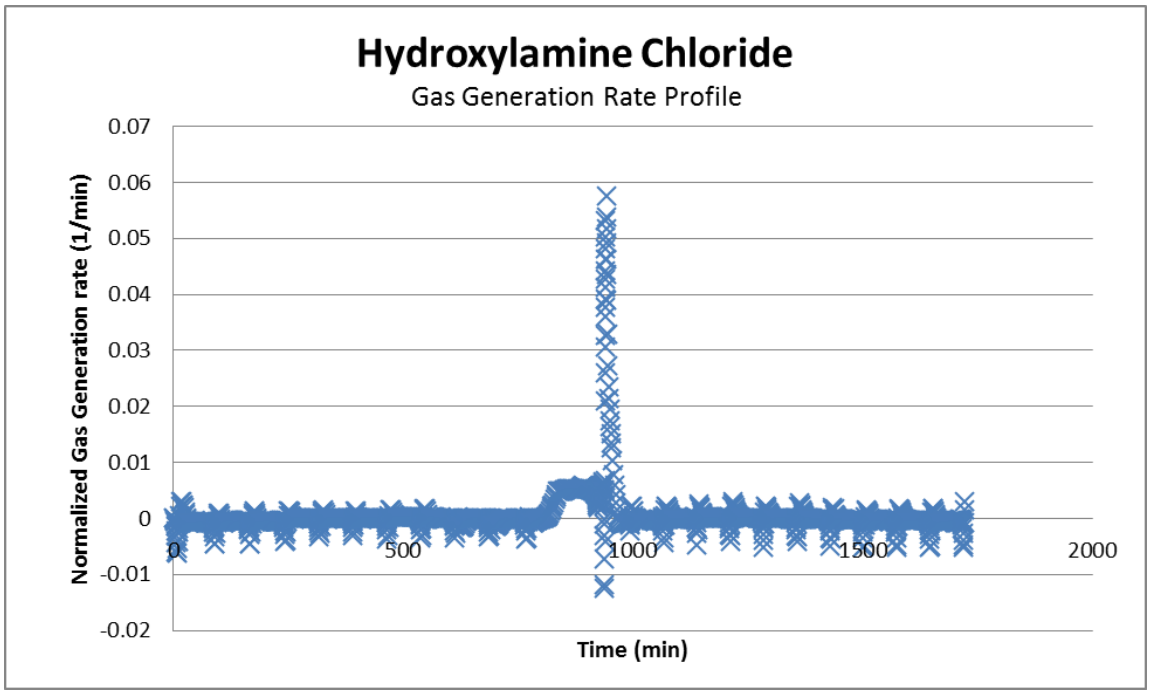

Fig. B.42 Normalized Gas Generation Rate - Hydroxylamine Chloride

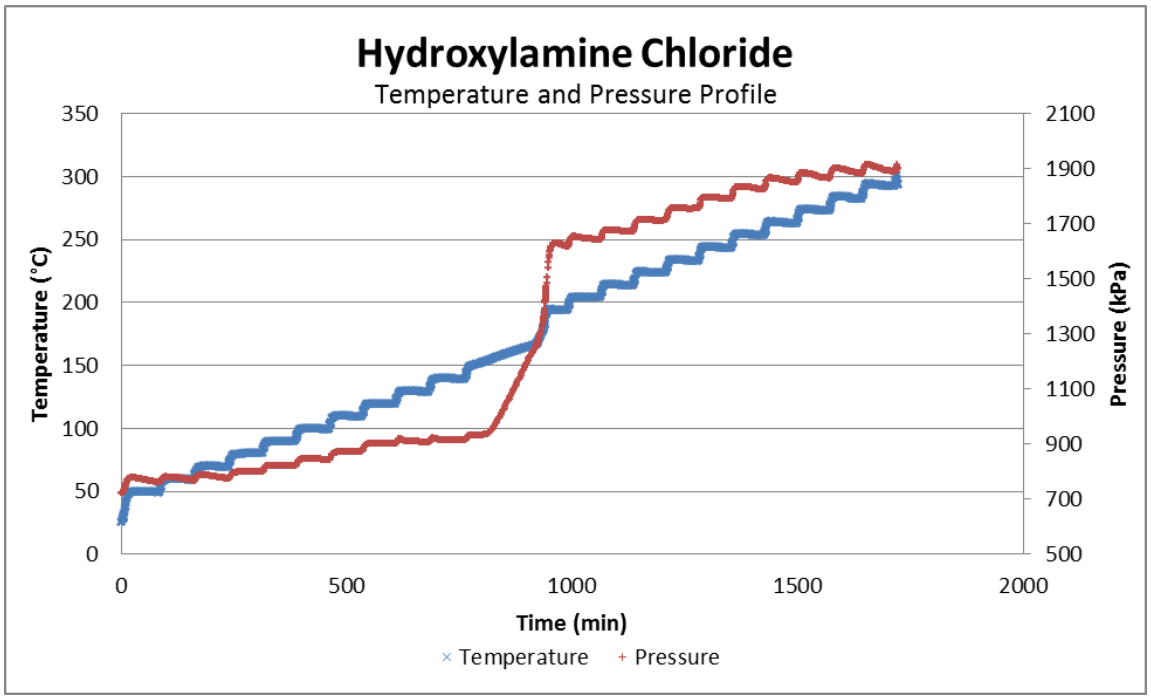

Fig. B.43 Temperature and Pressure Profiles - Hydroxylamine Chloride

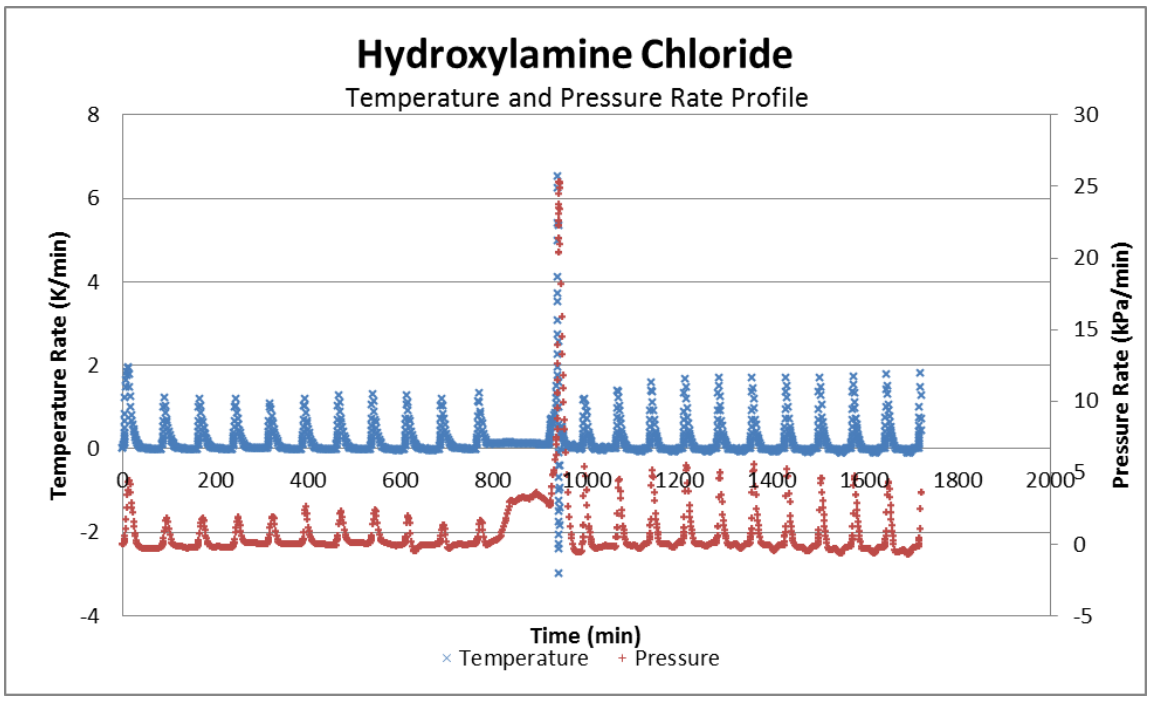

Fig. B.44 Temperature and Pressure Rate Profiles - Hydroxylamine Chloride

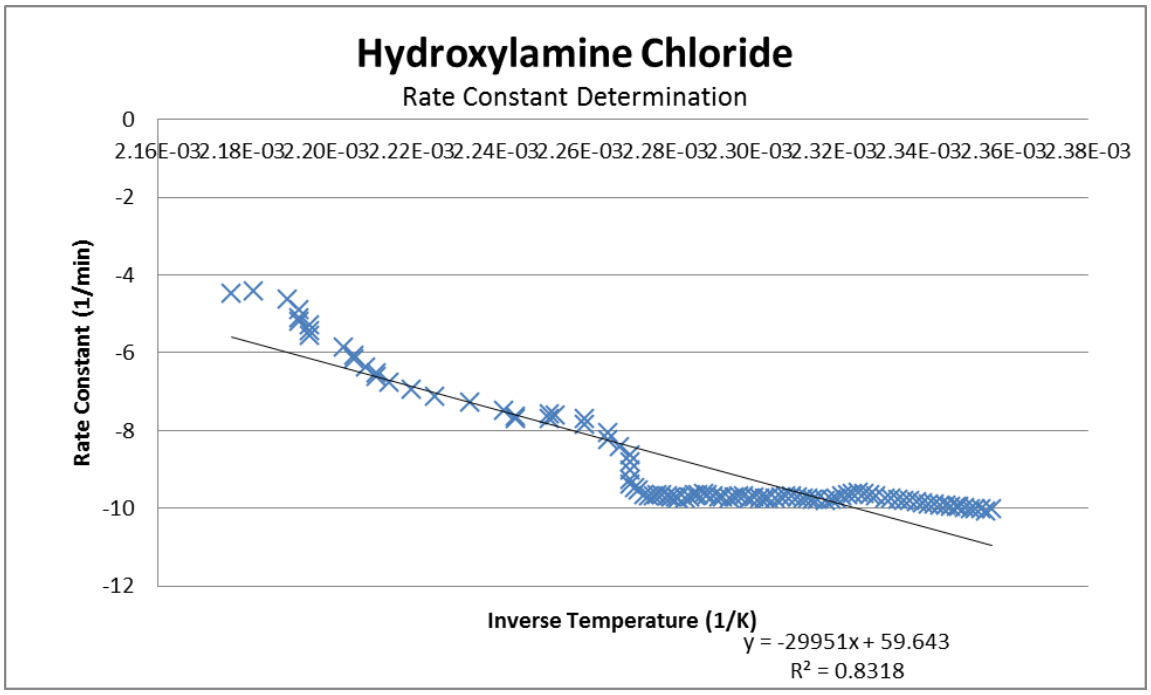

Fig. B.45 Rate Constant Determination - Hydroxylamine Chloride

B.10 Isoprene

Table B.37
Material Properties - Isoprene

Property	Value
m_s (g)	5.13
ρ_s (g/mL)	0.681
C_s (J/(g*K))	2.139
MW (g/mol)	68.12

Table B.38
Cell Properties - Isoprene

Property	Value
m_{cell} (g)	52.41
V_{cell} (mL)	96.61
φ	5.011

Table B.39
IPD Properties - Isoprene

Property	Value
A (1/s)	2.892E+00
E_A (J/(mol*K))	4.041E+04
T_{onset} (°C)	90
T_{max} (°C)	317
ΔH (J/g)	2.434E+03
IPD (W/ml)	4.420E-01

Table B.40
Gas Properties - Isoprene

Property	Value
n_{max} (mol)	3.004E-02
dn/dt_{max} (mol/min)	8.909E-05
n_{maxn}	3.989E-01
dn/dt_{maxn} (1/min)	1.183E-03
GGP (1/min)	4.719E-04

Note – The exotherm for this compound exceeded the temperature range for the APTAC. The compound also exhibited a sharp drop in pressure during the exotherm.

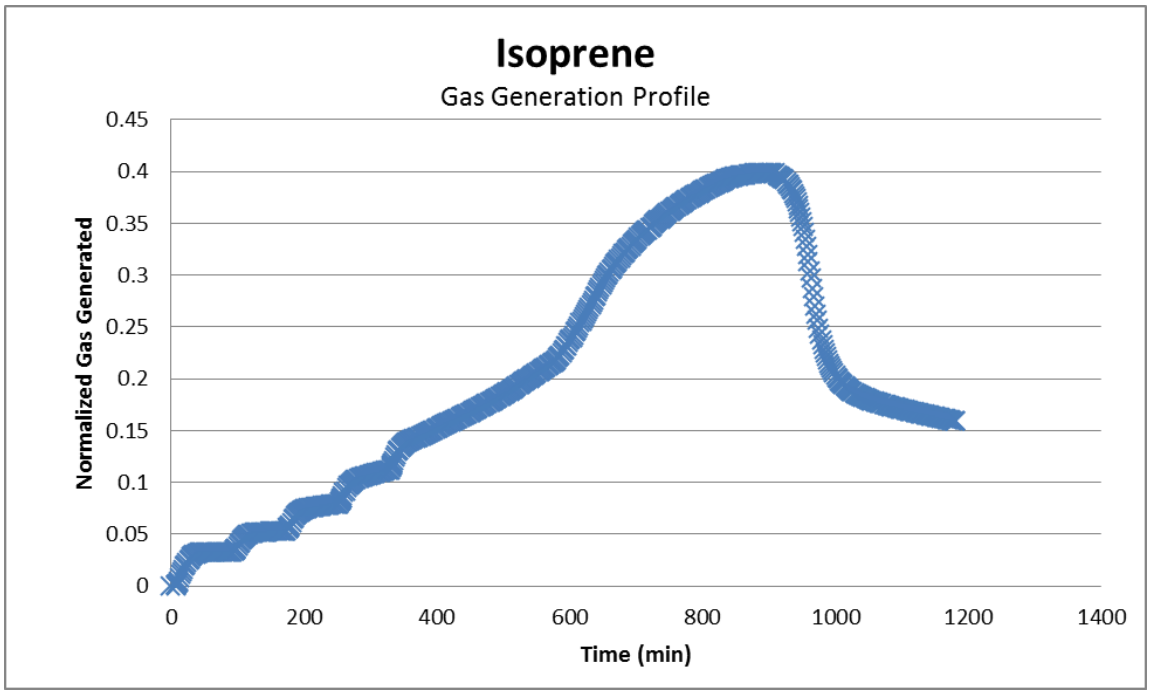

Fig. B.46 Normalized Gas Generation - Isoprene

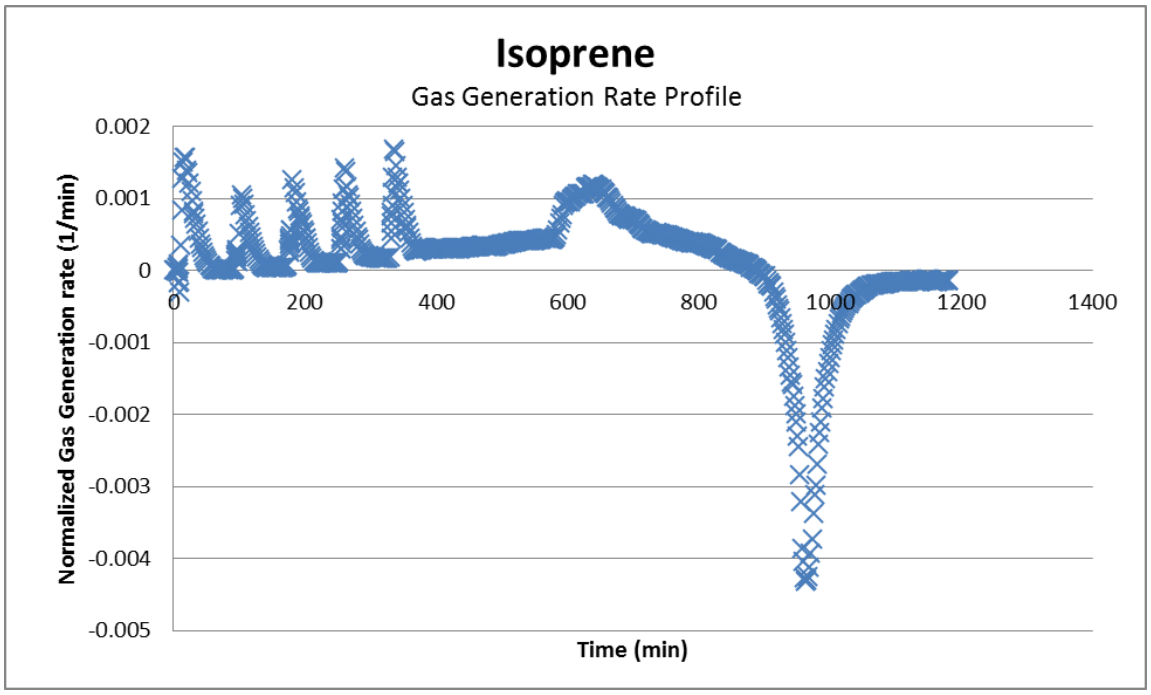

Fig. B.47 Normalized Gas Generation Rate - Isoprene

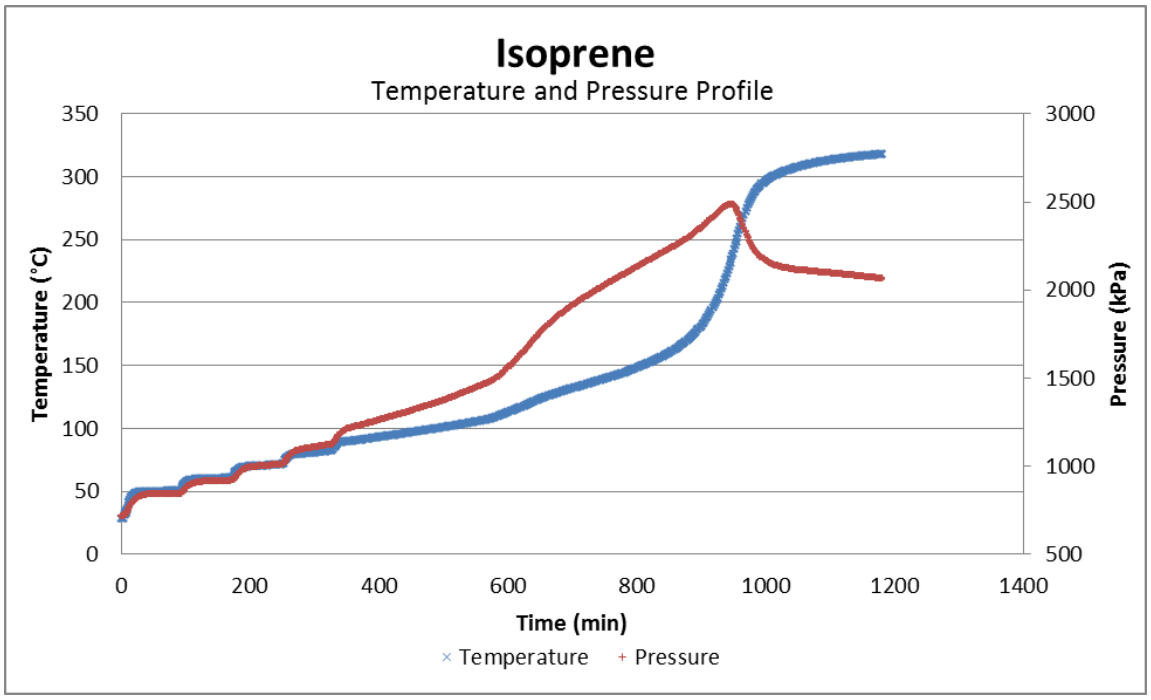

Fig. B.48 Temperature and Pressure Profiles - Isoprene

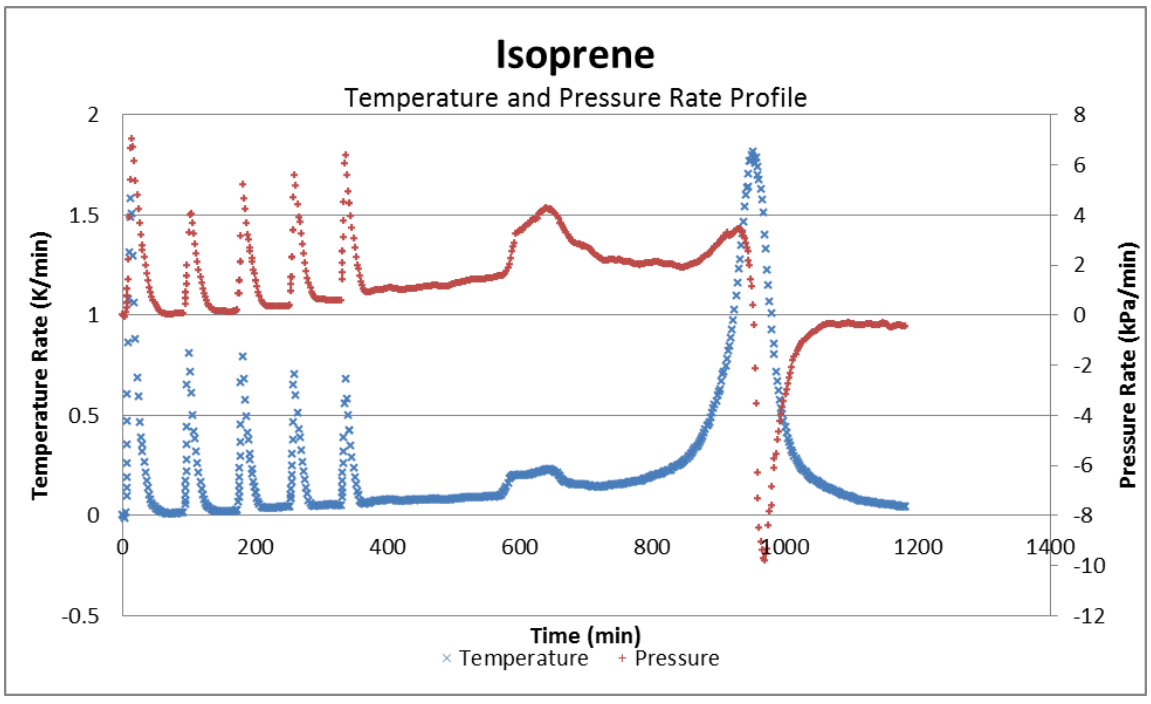

Fig. B.49 Temperature and Pressure Rate Profiles - Isoprene

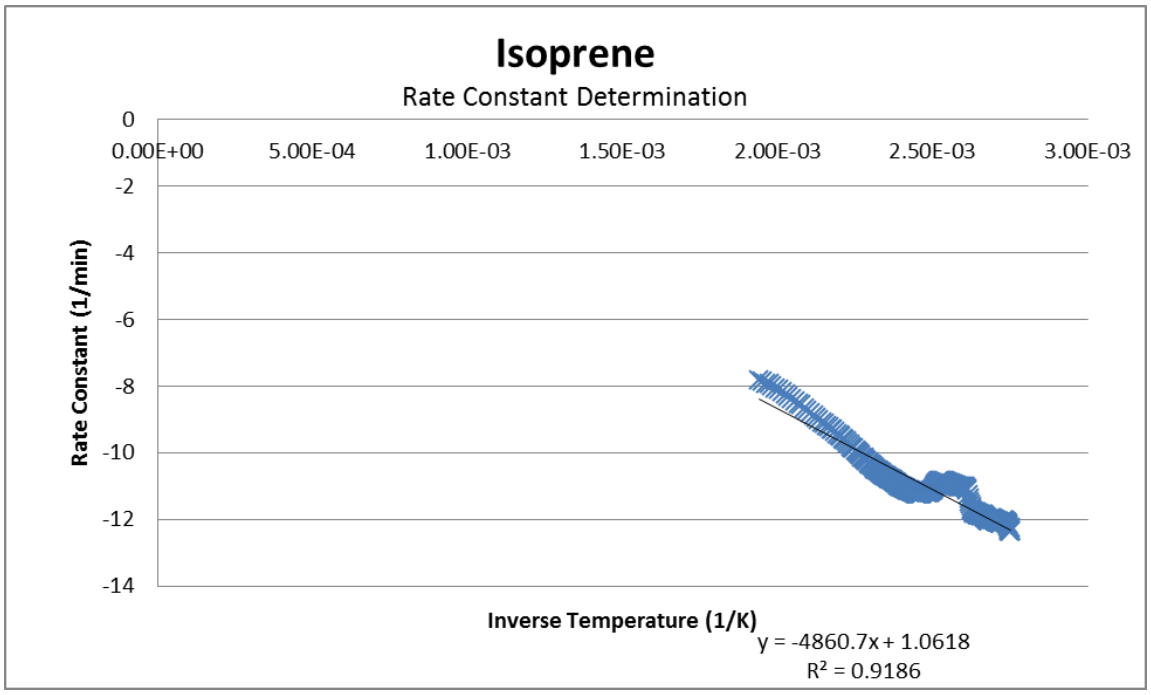

Fig. B.50 Rate Constant Determination - Isoprene

B.11 Isopropyl Alcohol

Table B.41
Material Properties - Isopropyl Alcohol

Property	Value
m_s (g)	8.1
ρ_s (g/mL)	0.785
C_s (J/(g*K))	2.562
MW (g/mol)	60.1

Table B.42
Cell Properties - Isopropyl Alcohol

Property	Value
m_{cell} (g)	58.83
V_{cell} (mL)	92.67
φ	3.381

Table B.43
IPD Properties - Isopropyl Alcohol

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	N/A
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.44
Gas Properties - Isopropyl Alcohol

Property	Value
n_{max} (mol)	1.097E-01
dn/dt_{max} (mol/min)	8.348E-04
n_{maxn}	8.137E-01
dn/dt_{maxn} (1/min)	6.194E-03
GGP (1/min)	5.040E-03

Note – This compound was run at atmospheric pressure and did not exhibit a decomposition reaction. An IPD cannot be calculated. (Carreto-Vasquez et al., 2010).

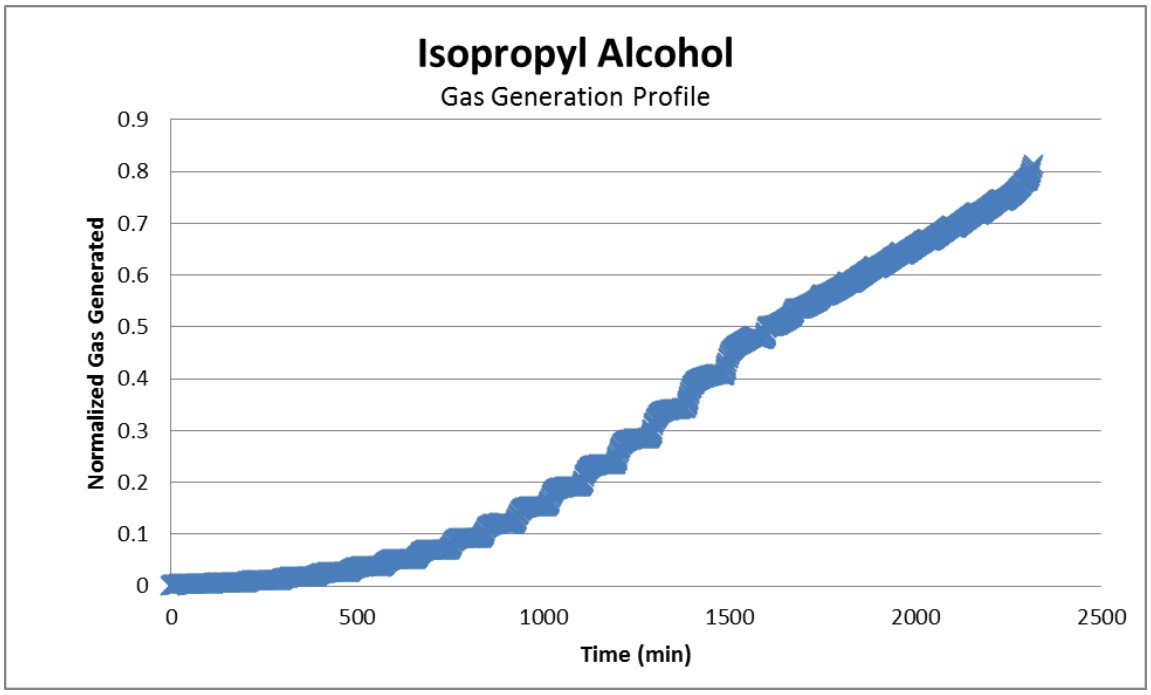

Fig. B.51 Normalized Gas Generation - Isopropyl Alcohol

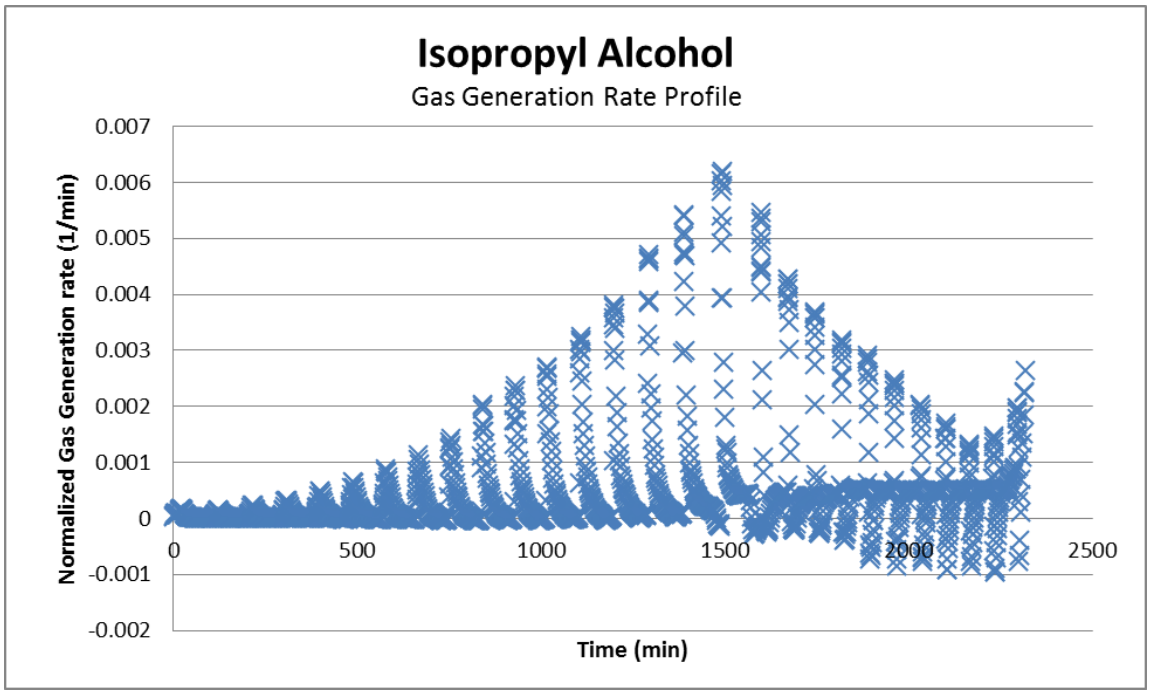

Fig. B.52 Normalized Gas Generation Rate - Isopropyl Alcohol

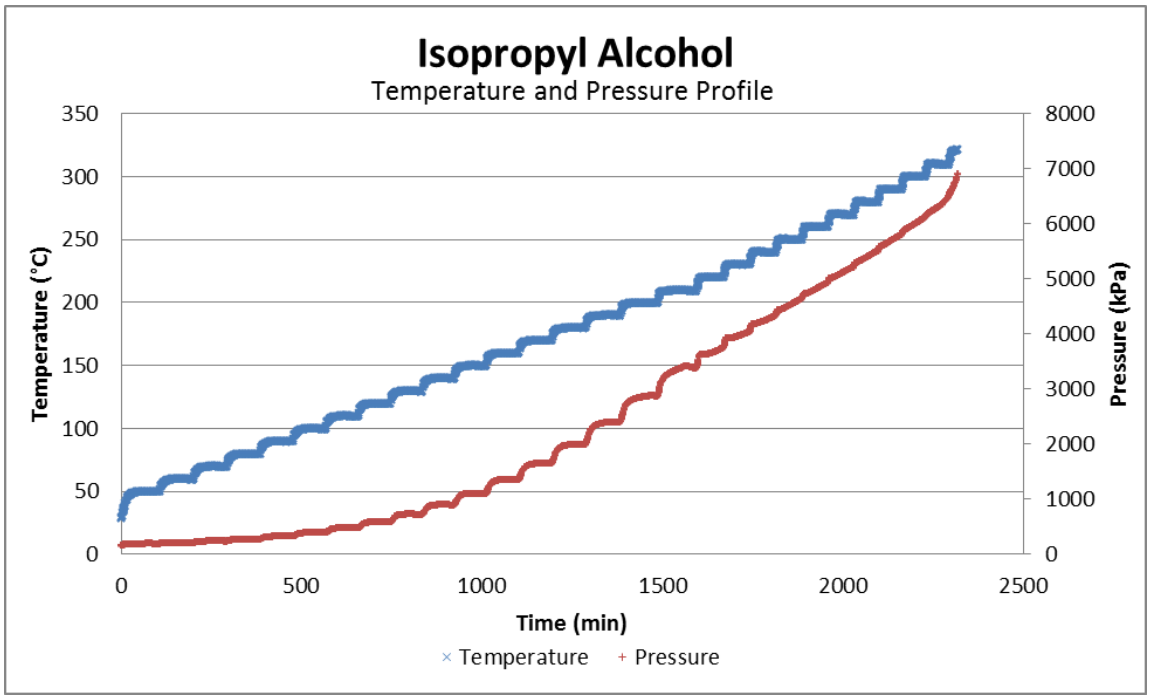

Fig. B.53 Temperature and Pressure Profiles - Isopropyl Alcohol

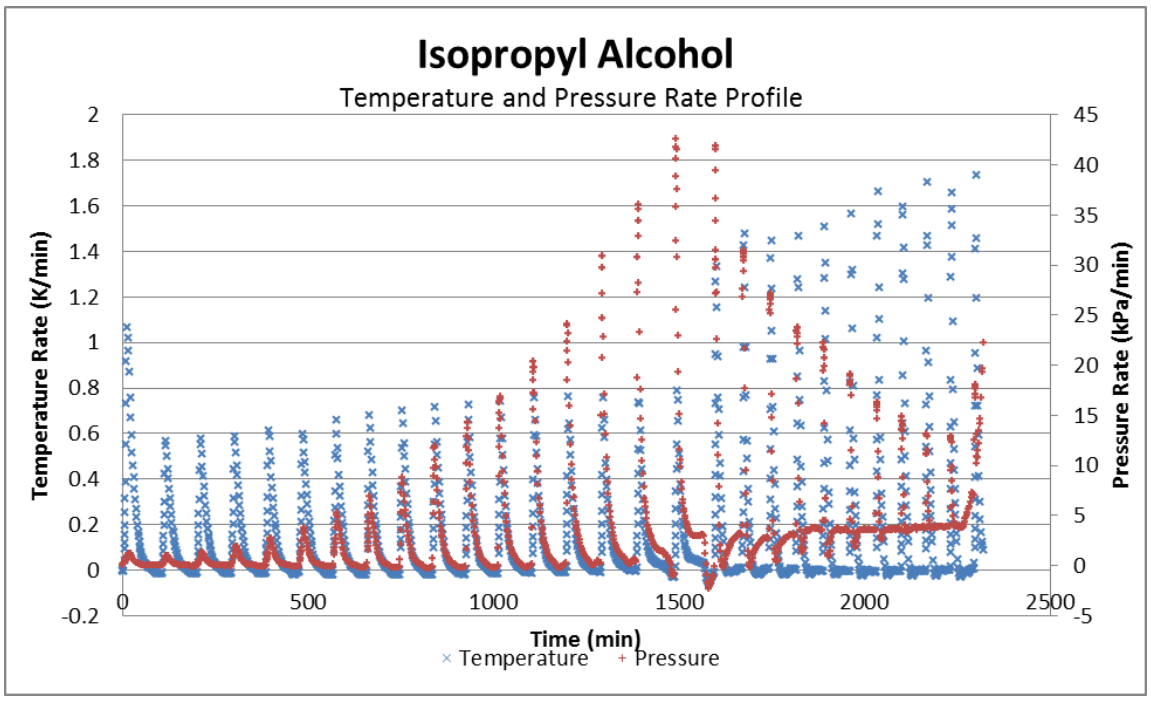

Fig. B.54 Temperature and Pressure Rate Profiles - Isopropyl Alcohol

B.12 Maleic Anhydride

Table B.45
Material Properties - Maleic Anhydride

Property	Value
m_s (g)	7.39
ρ_s (g/mL)	0.936
C_s (J/(g*K))	1.530
MW (g/mol)	98.06

Table B.46
Cell Properties - Maleic Anhydride

Property	Value
m_{cell} (g)	53.24
V_{cell} (mL)	93.04
φ	4.956

Table B.47
IPD Properties - Maleic Anhydride

Property	Value
A (1/s)	2.074E+16
E_A (J/(mol*K))	2.055E+05
T_{onset} (°C)	220
T_{max} (°C)	338
ΔH (J/g)	8.946E+02
IPD (W/ml)	5.319E-02

Table B.48
Gas Properties - Maleic Anhydride

Property	Value
n_{max} (mol)	5.977E-02
dn/dt_{max} (mol/min)	1.616E-02
n_{maxn}	7.931E-01
dn/dt_{maxn} (1/min)	2.144E-01
GGP (1/min)	1.700E-01

Note – This compound's exotherm exceeded the temperature limit of the APTAC.

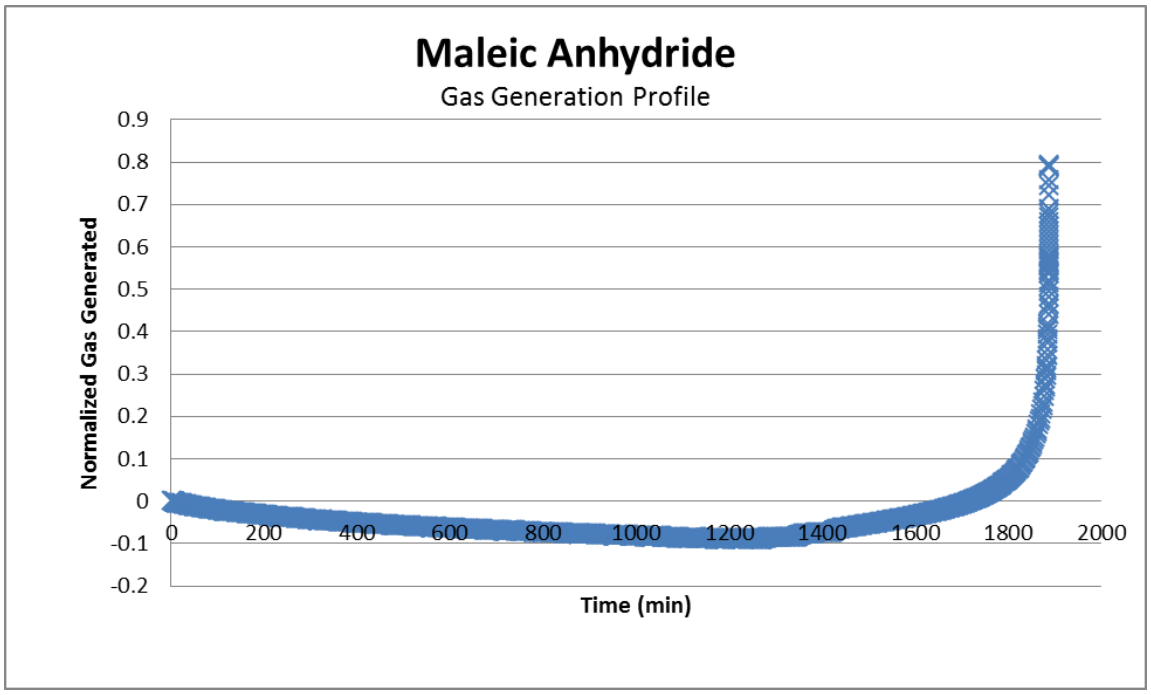

Fig. B.55 Normalized Gas Generation - Maleic Anhydride

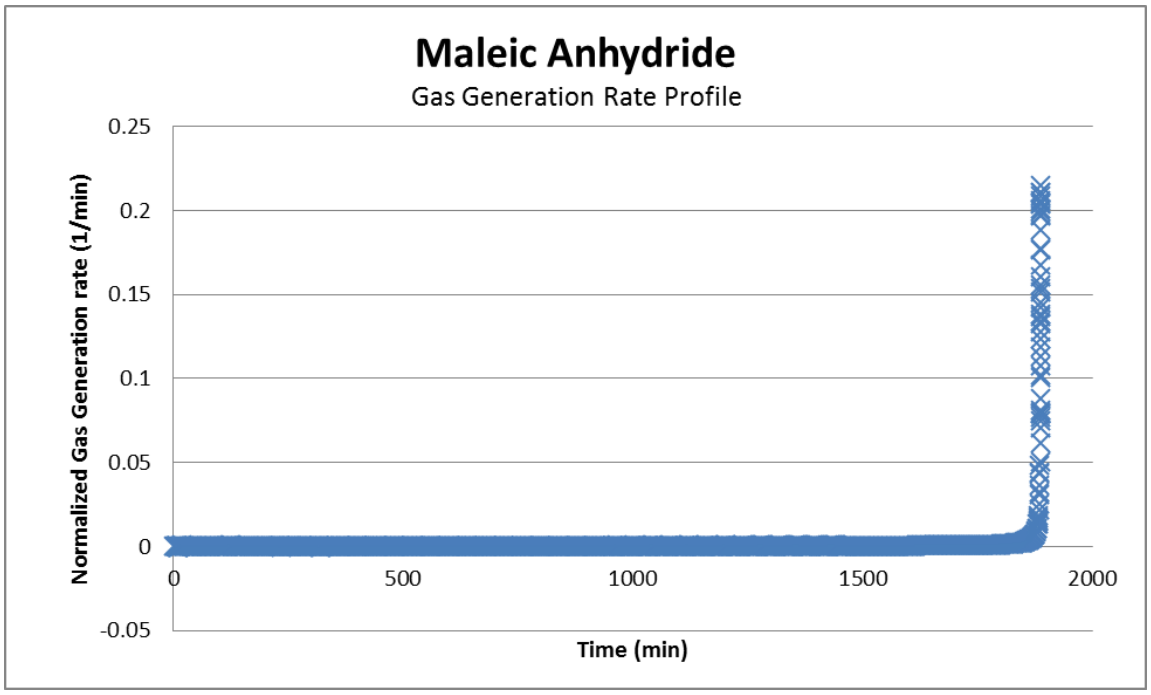

Fig. B.56 Normalized Gas Generation Rate - Maleic Anhydride

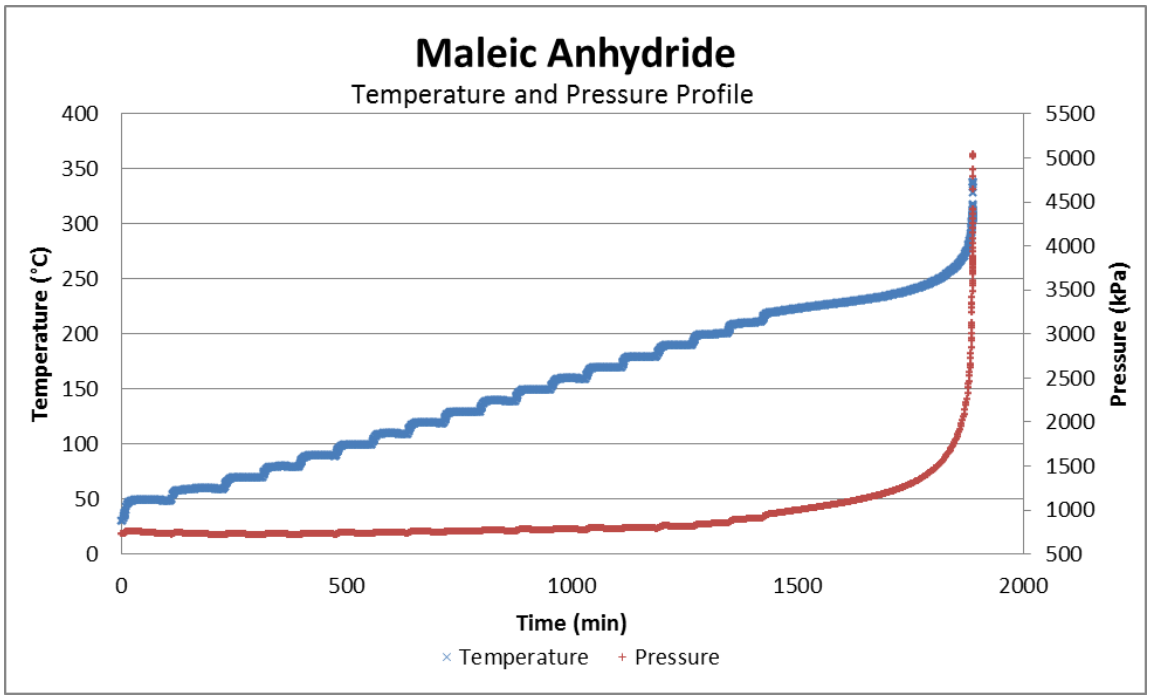

Fig. B.57 Temperature and Pressure Profiles - Maleic Anhydride

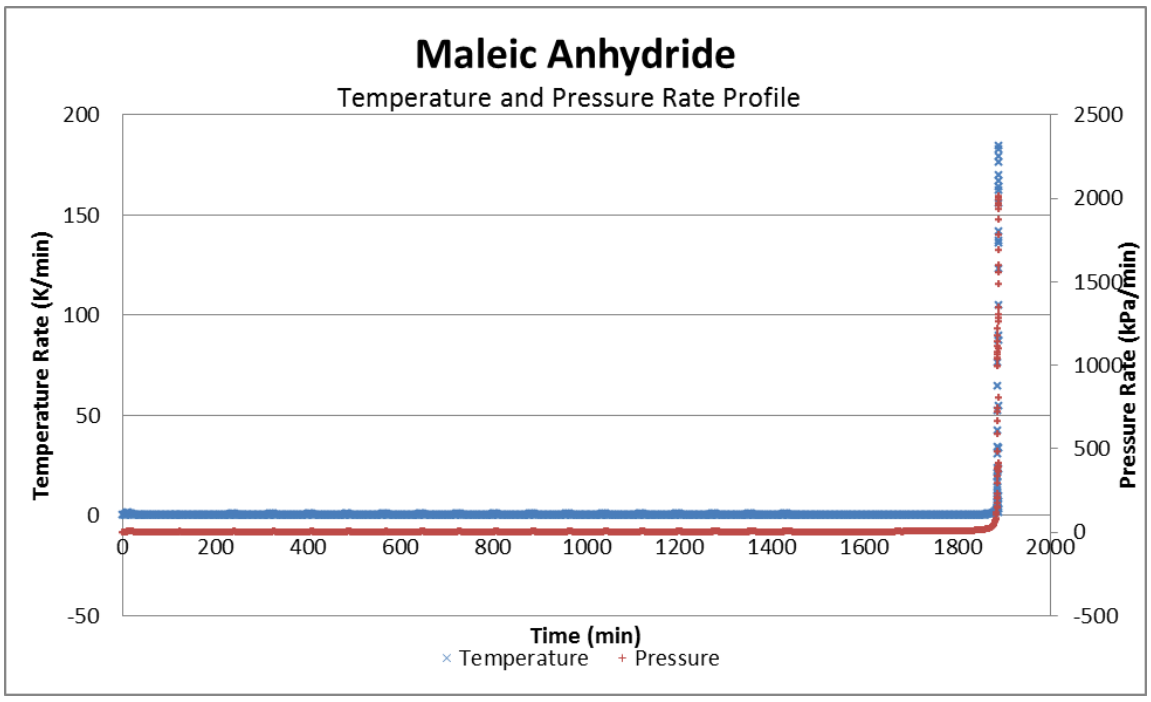

Fig. B.58 Temperature and Pressure Rate Profiles - Maleic Anhydride

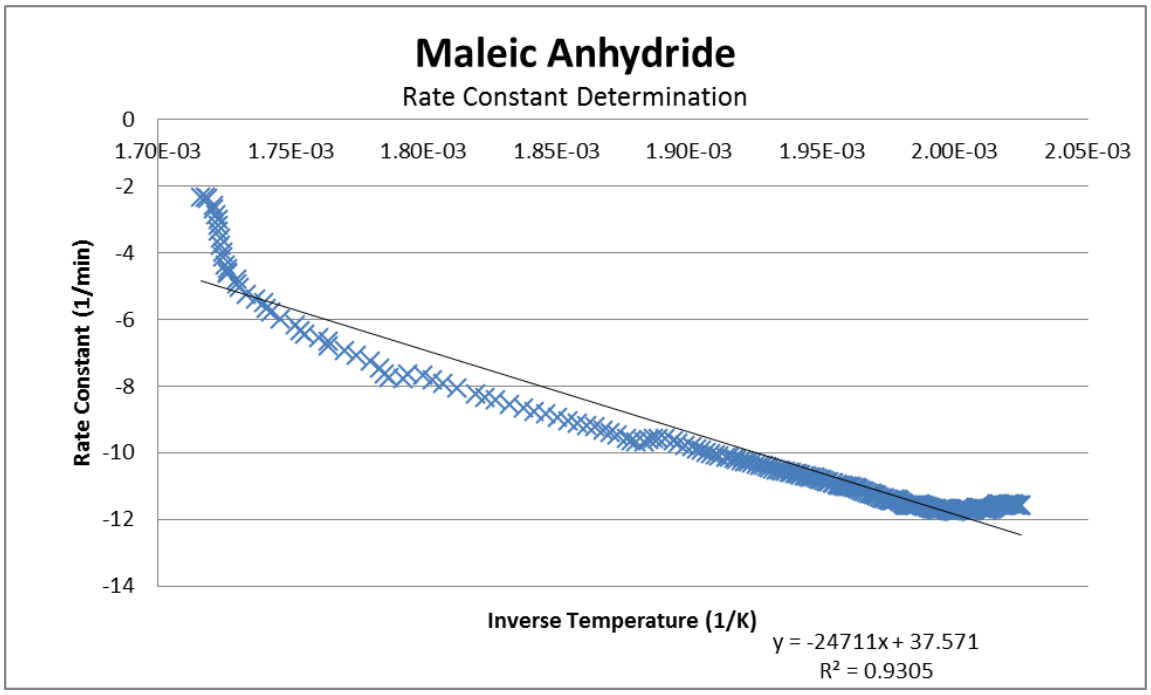

Fig. B.59 Rate Constant Determination - Maleic Anhydride

B.13 Manganese Carbonate

Table B.49
Material Properties - Manganese Carbonate

Property	Value
m_s (g)	8.39
ρ_s (g/mL)	3.12
C_s (J/(g*K))	0.709
MW (g/mol)	114.95

Table B.50
Cell Properties - Manganese Carbonate

Property	Value
m_{cell} (g)	56.18
V_{cell} (mL)	92.34
φ	8.933

Table B.51
IPD Properties - Manganese Carbonate

Property	Value
A (1/s)	1.335E-02
E_A (J/(mol*K))	2.769E+04
T_{onset} (°C)	140
T_{max} (°C)	315
ΔH (J/g)	1.108E+03
IPD (W/ml)	7.929E-02

Table B.52
Gas Properties - Manganese Carbonate

Property	Value
n_{max} (mol)	9.259E-03
dn/dt_{max} (mol/min)	2.108E-05
n_{maxn}	1.269E-01
dn/dt_{maxn} (1/min)	2.888E-04
GGP (1/min)	3.664E-05

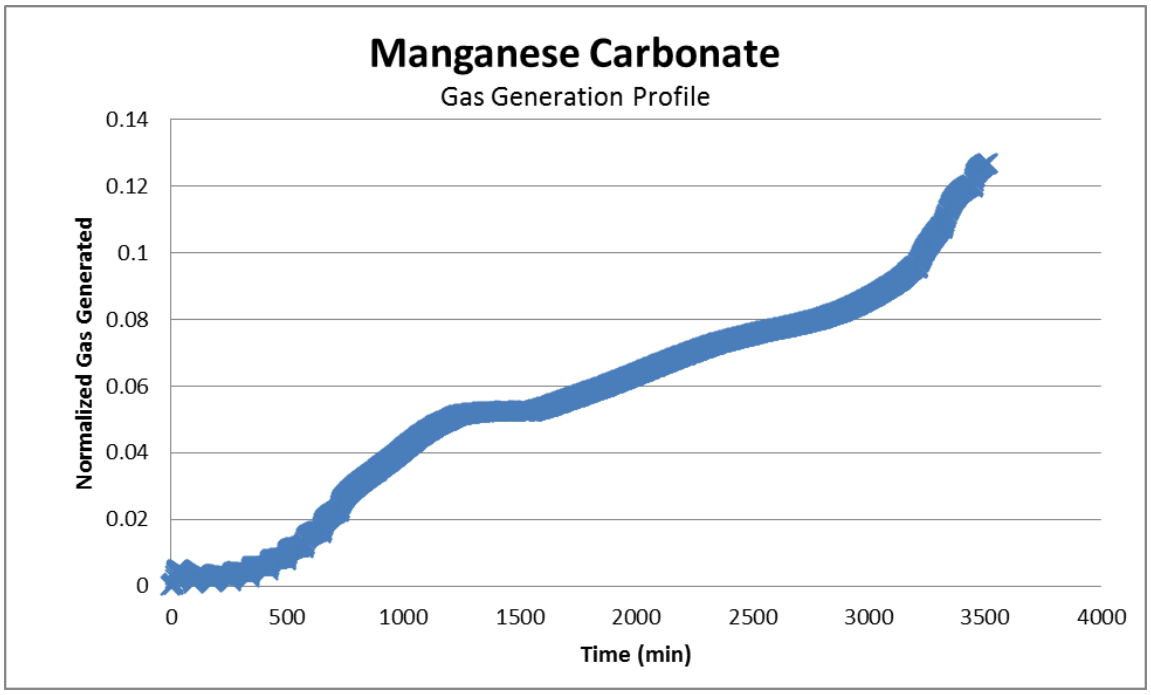

Fig. B.60 Normalized Gas Generation - Manganese Carbonate

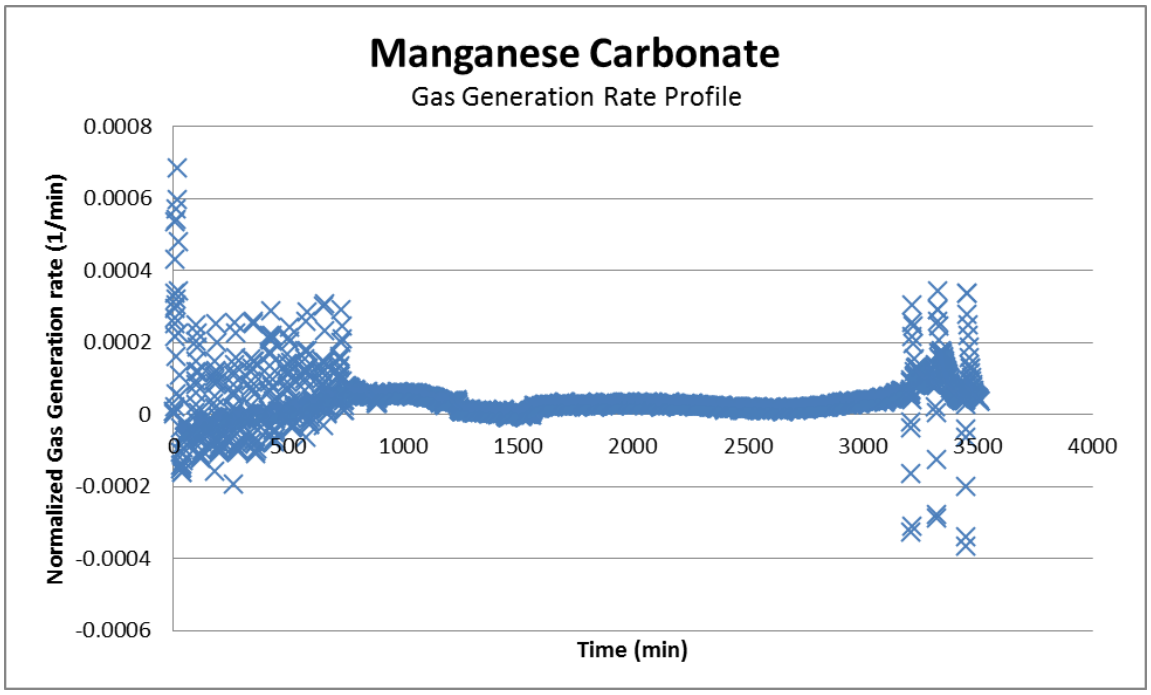

Fig. B.61 Normalized Gas Generation Rate - Manganese Carbonate

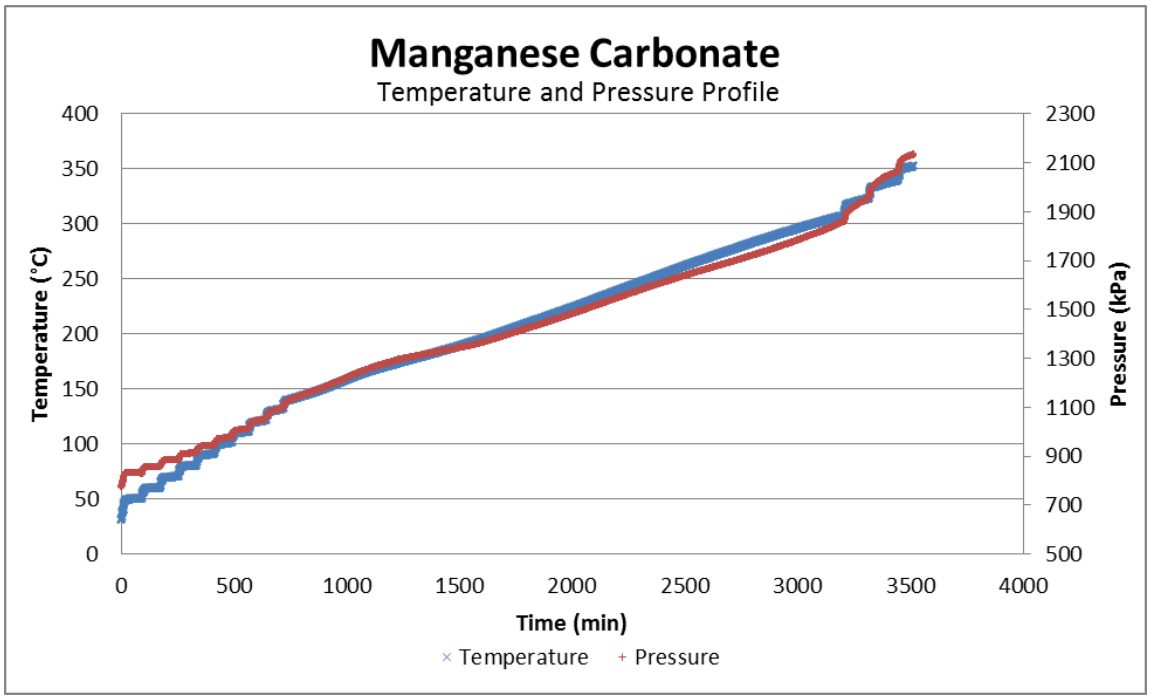

Fig. B.62 Temperature and Pressure Profiles - Manganese Carbonate

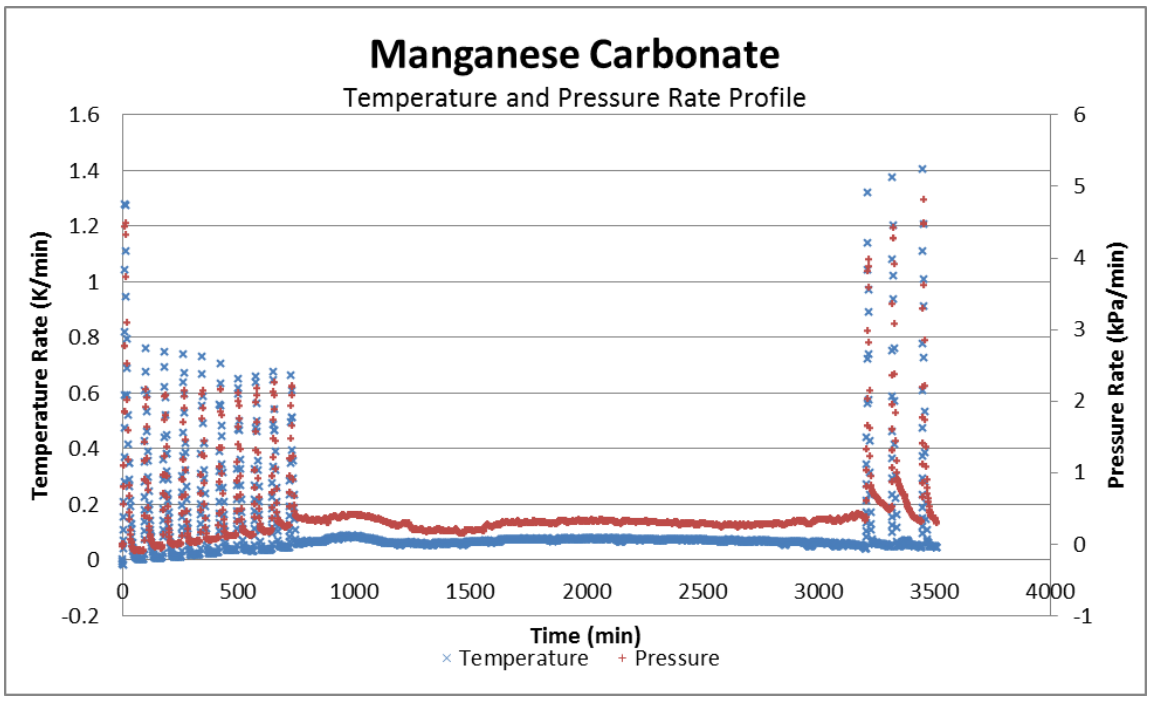

Fig. B.63 Temperature and Pressure Rate Profiles - Manganese Carbonate

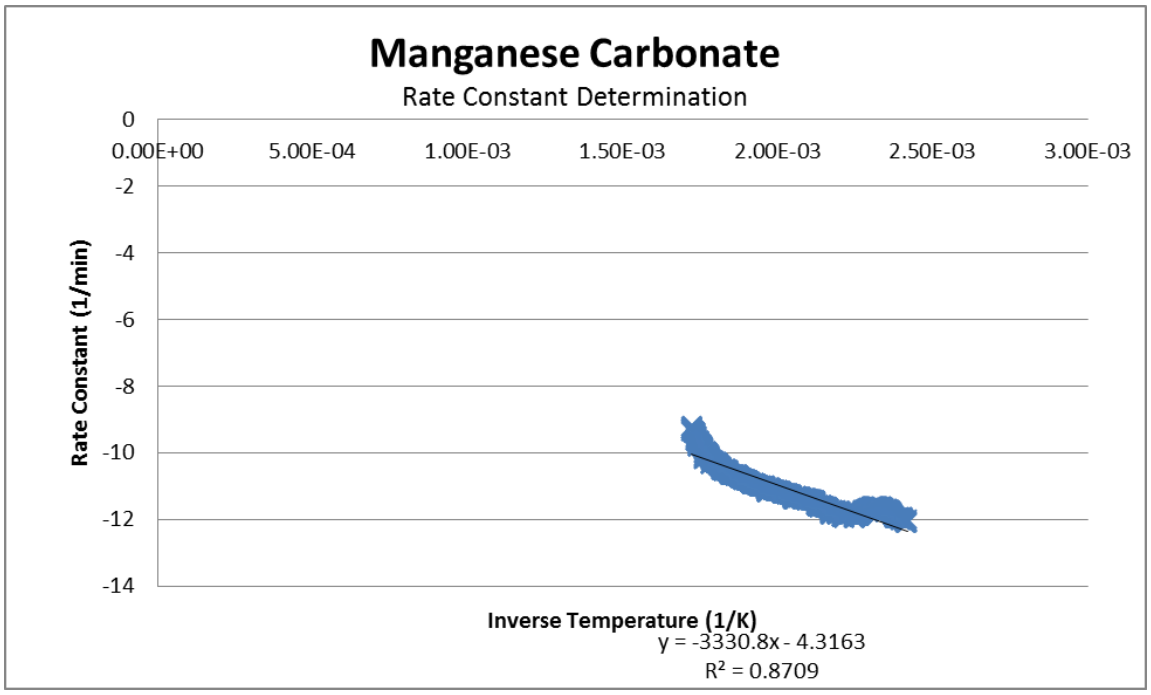

Fig. B.64 Rate Constant Determination - Manganese Carbonate

B.14 Methyl Methacrylate

Table B.53
Material Properties - Methyl Methacrylate

Property	Value
m_s (g)	7.54
ρ_s (g/mL)	0.936
C_s (J/(g*K))	1.910
MW (g/mol)	100.12

Table B.54
Cell Properties - Methyl Methacrylate

Property	Value
m_{cell} (g)	52.89
V_{cell} (mL)	92.22
φ	4.085

Table B.55
IPD Properties - Methyl Methacrylate

Property	Value
A (1/s)	6.339E+09
E_A (J/(mol*K))	1.030E+05
T_{onset} (°C)	100
T_{max} (°C)	200
ΔH (J/g)	7.802E+02
IPD (W/ml)	2.426E+02

Table B.56
Gas Properties - Methyl Methacrylate

Property	Value
n_{max} (mol)	4.700E-02
dn/dt_{max} (mol/min)	1.018E-03
n_{maxn}	6.241E-01
dn/dt_{maxn} (1/min)	1.352E-02
GGP (1/min)	8.435E-03

Note – This compound exhibited two exotherms. The second of which exceeded the temperature limit of the APTAC.

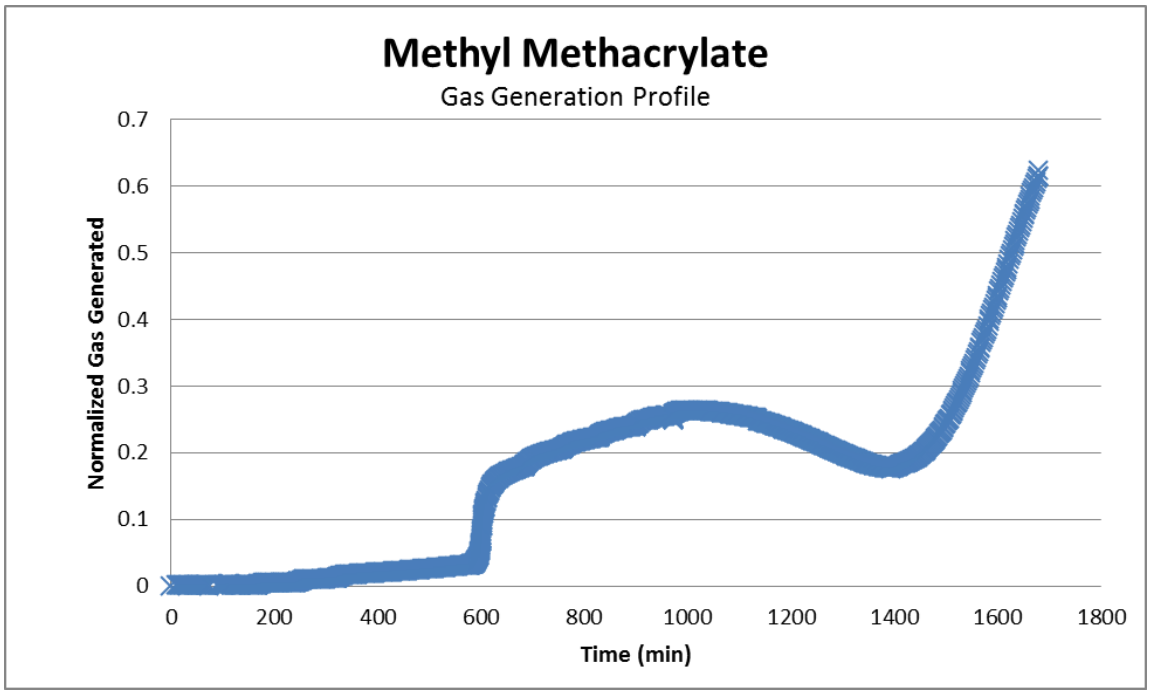

Fig. B.65 Normalized Gas Generation - Methyl Methacrylate

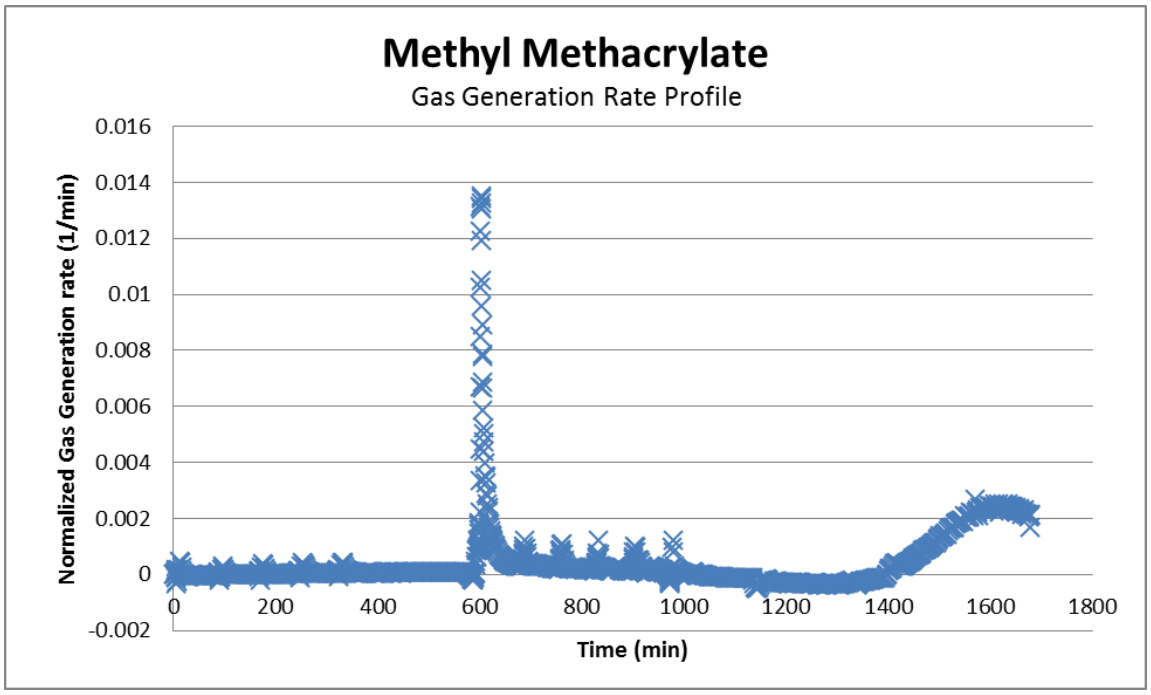

Fig. B.66 Normalized Gas Generation Rate - Methyl Methacrylate

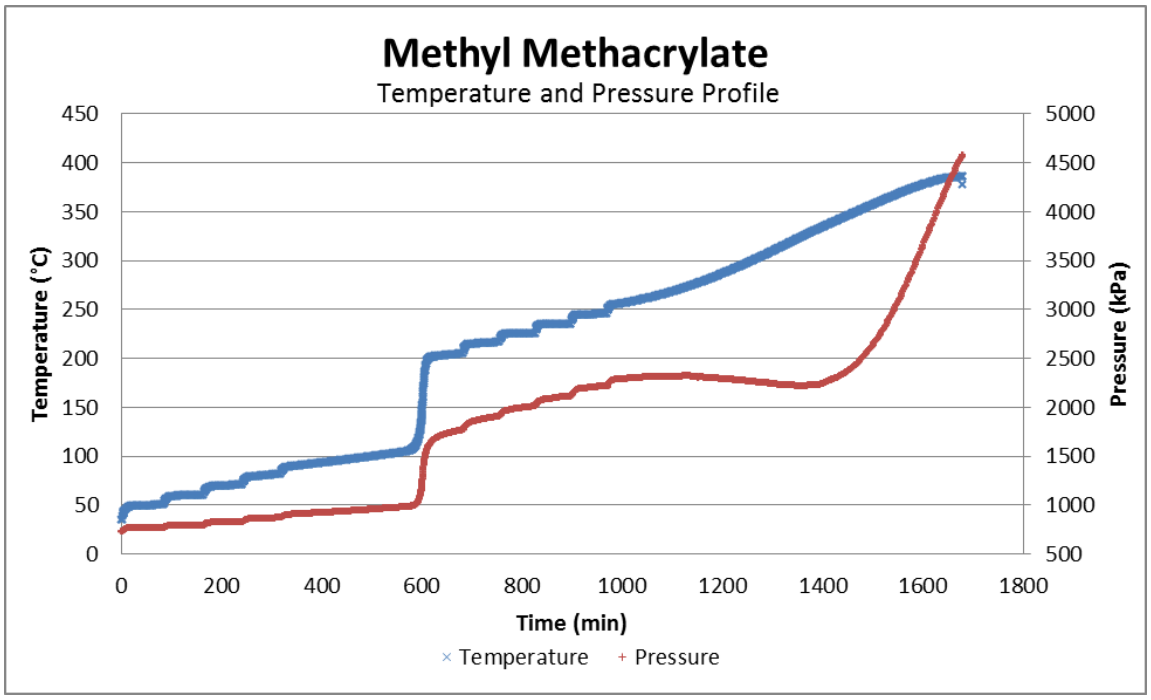

Fig. B.67 Temperature and Pressure Profiles - Methyl Methacrylate

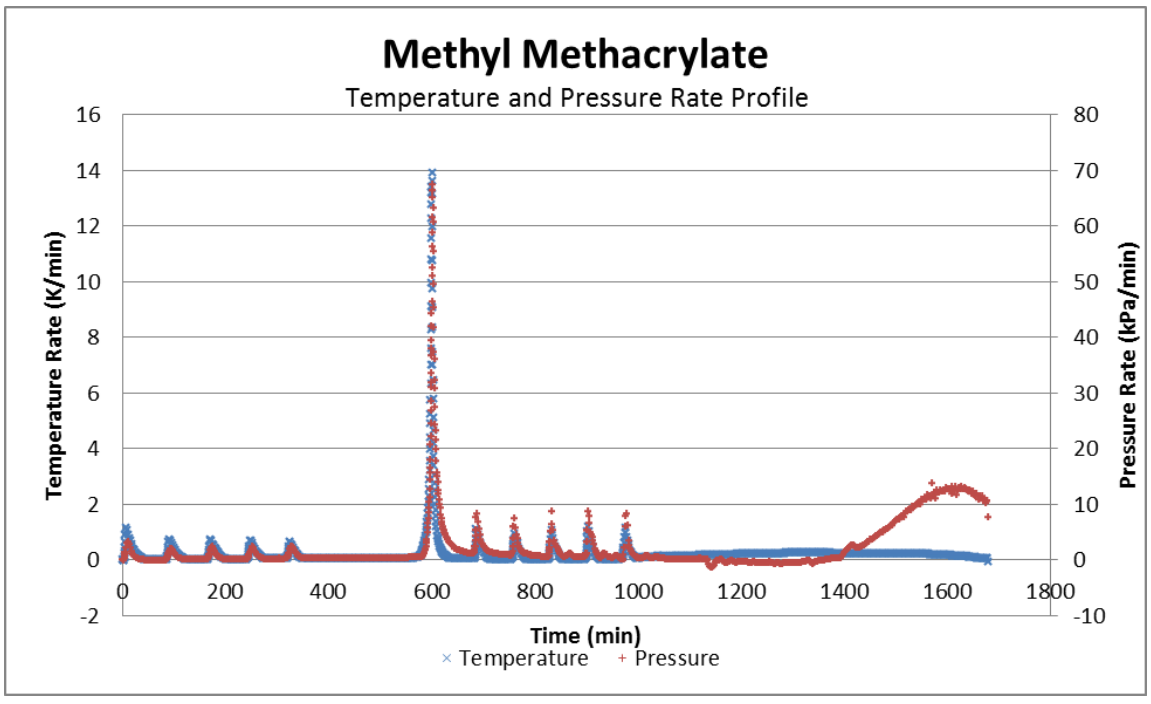

Fig. B.68 Temperature and Pressure Rate Profiles - Methyl Methacrylate

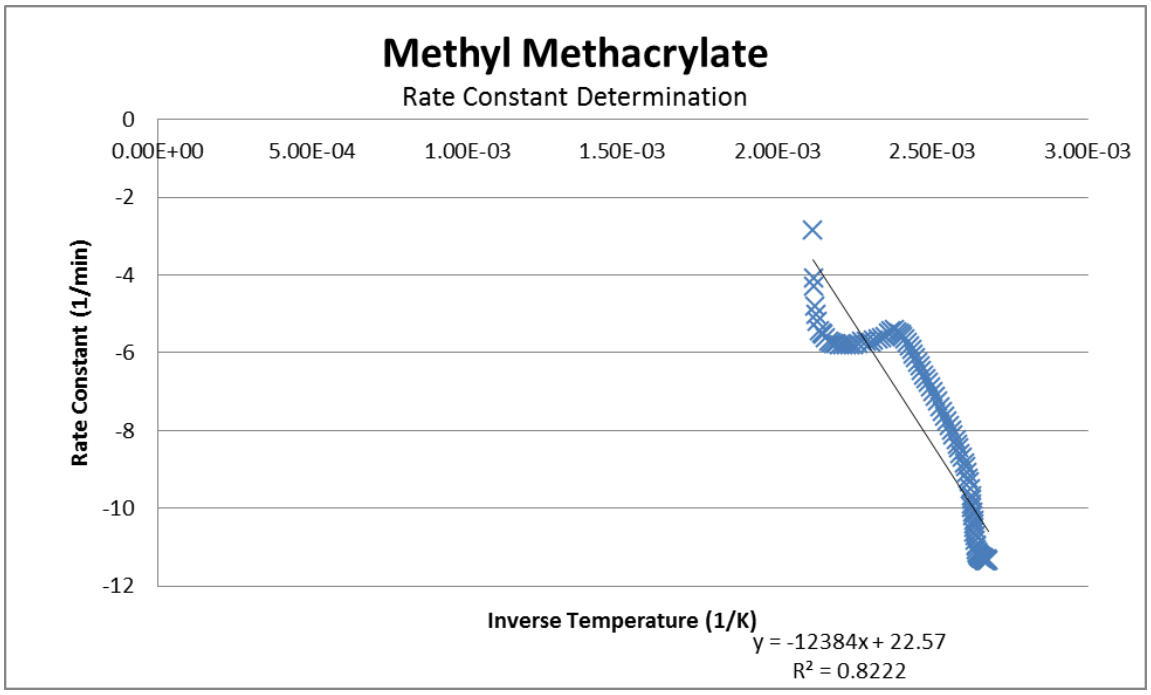

Fig. B.69 Rate Constant Determination - Methyl Methacrylate

B.15 Nitrobenzene

Table B.57
Material Properties - Nitrobenzene

Property	Value
m_s (g)	0.76
ρ_s (g/mL)	1.199
C_s (J/(g*K))	1.4
MW (g/mol)	123.11

Table B.58
Cell Properties - Nitrobenzene

Property	Value
m_{cell} (g)	52.08
V_{cell} (mL)	97.41
φ	42.12

Table B.59
IPD Properties - Nitrobenzene

Property	Value
A (1/s)	1.163E+04
E_A (J/(mol*K))	7.856E+04
T_{onset} (°C)	190
T_{max} (°C)	265
ΔH (J/g)	4.422E+03
IPD (W/ml)	8.838E-01

Table B.60
Gas Properties - Nitrobenzene

Property	Value
n_{max} (mol)	4.039E-03
dn/dt_{max} (mol/min)	1.196E-05
n_{maxn}	6.543E-01
dn/dt_{maxn} (1/min)	1.938E-03
GGP (1/min)	1.268E-03

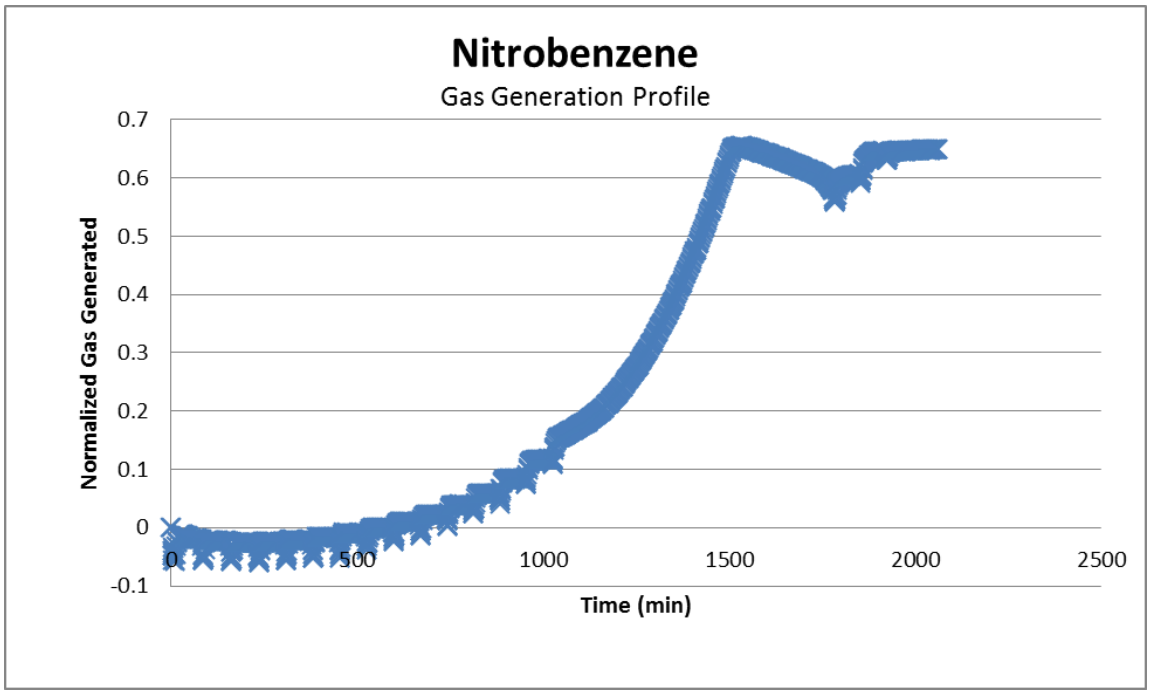

Fig. B.70 Normalized Gas Generation - Nitrobenzene

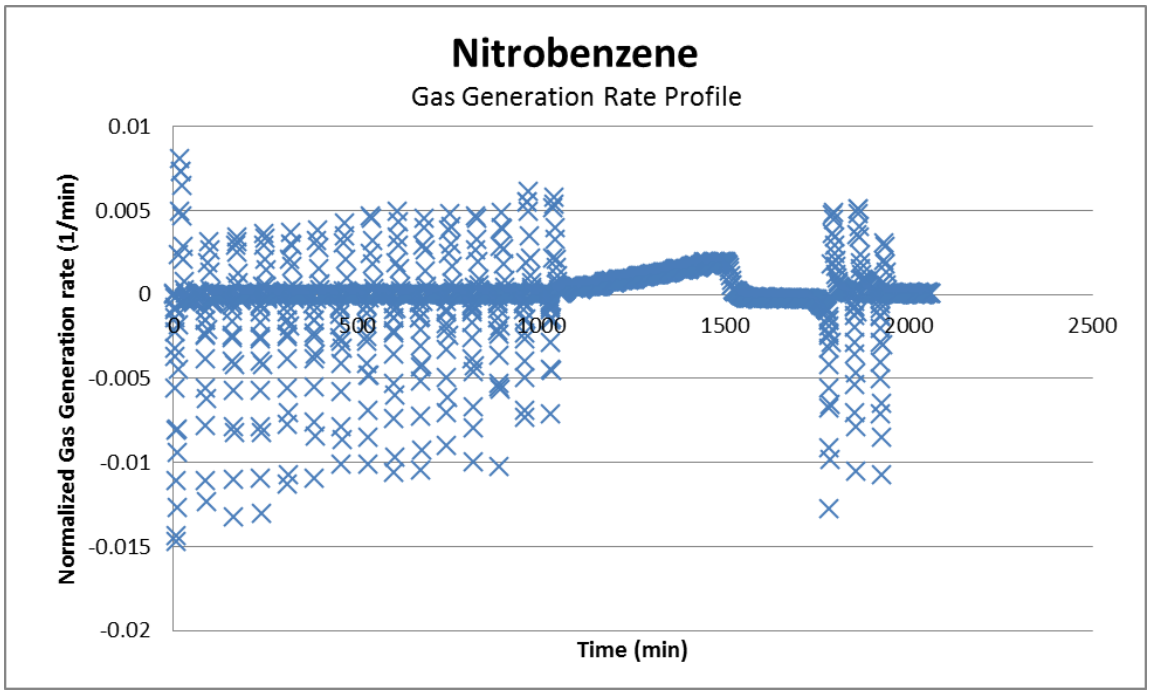

Fig. B.72 Normalized Gas Generation Rate - Nitrobenzene

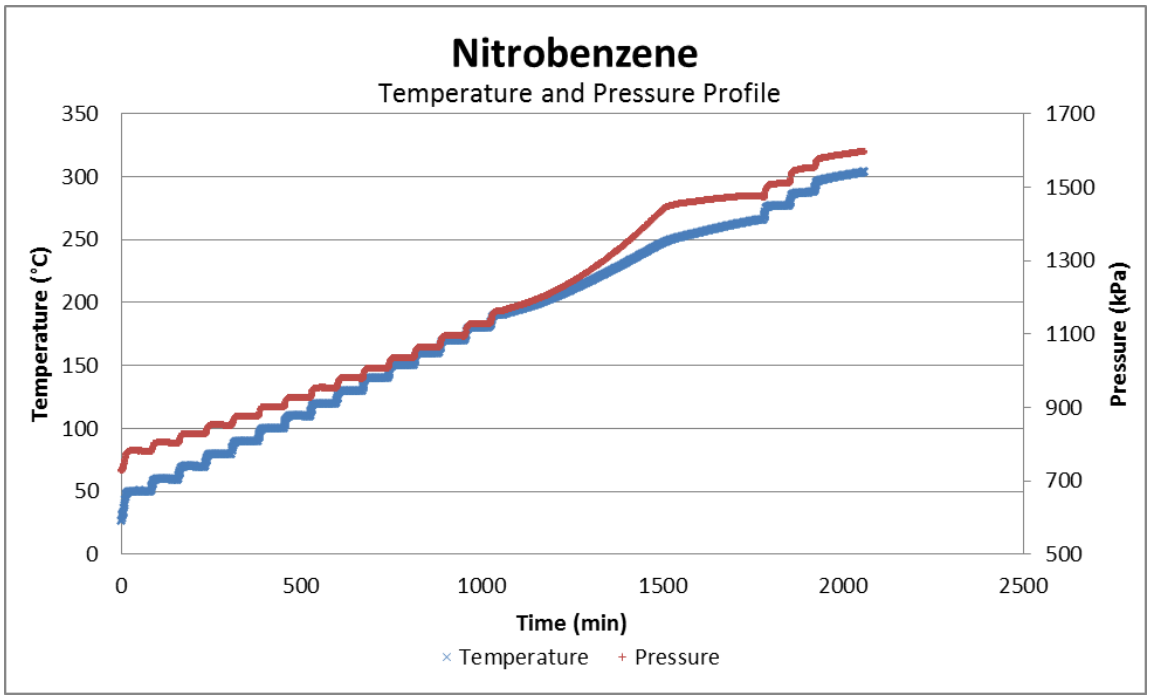

Fig. B.71 Temperature and Pressure Profiles - Nitrobenzene

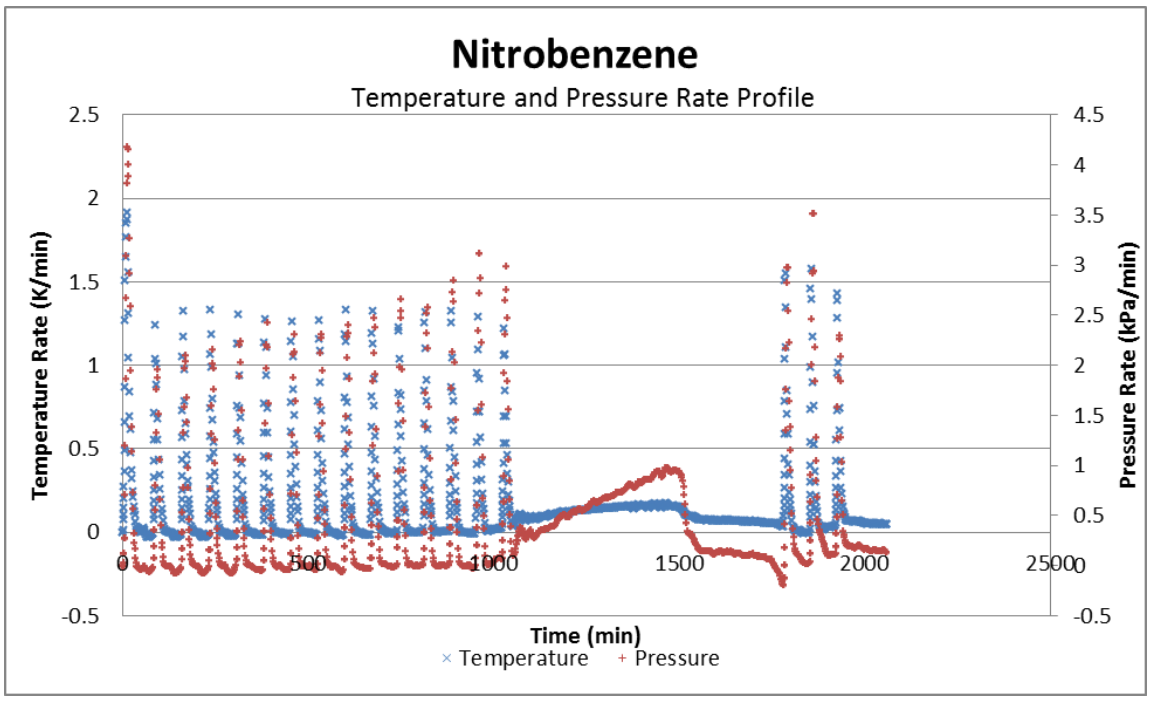

Fig. B.73 Temperature and Pressure Rate Profiles - Nitrobenzene

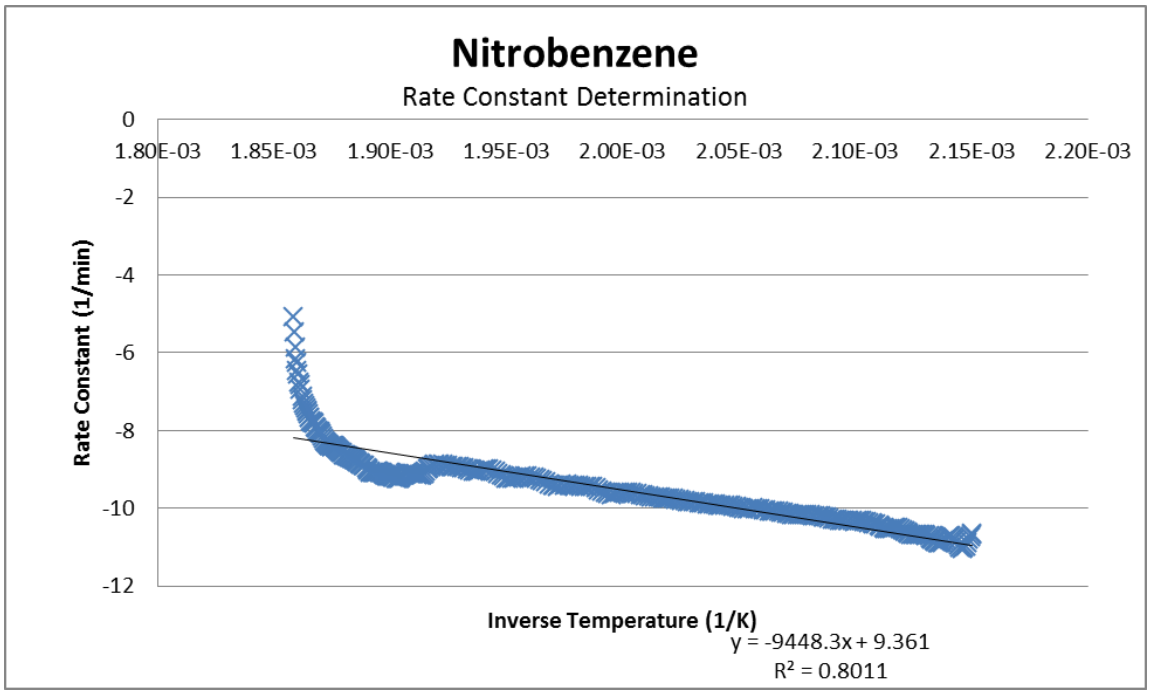

Fig. B.74 Rate Constant Determination - Nitrobenzene

B.16 Nitroethane

Table B.61
Material Properties - Nitroethane

Property	Value
m_s (g)	5.46
ρ_s (g/mL)	1.045
C_s (J/(g*K))	1.792
MW (g/mol)	75.07

Table B.62
Cell Properties - Nitroethane

Property	Value
m_{cell} (g)	52.43
V_{cell} (mL)	92.36
φ	5.501

Table B.63
IPD Properties - Nitroethane

Property	Value
A (1/s)	2.886E+09
E_A (J/(mol*K))	1.258E+05
T_{onset} (°C)	160
T_{max} (°C)	350
ΔH (J/g)	1.873E+03
IPD (W/ml)	1.558E+00

Table B.64
Gas Properties - Nitroethane

Property	Value
n_{max} (mol)	1.729E-02
dn/dt_{max} (mol/min)	9.433E-04
n_{maxn}	2.378E-01
dn/dt_{maxn} (1/min)	1.297E-02
GGP (1/min)	3.084E-03

Note – This compound exhibited a unique series of exotherms.

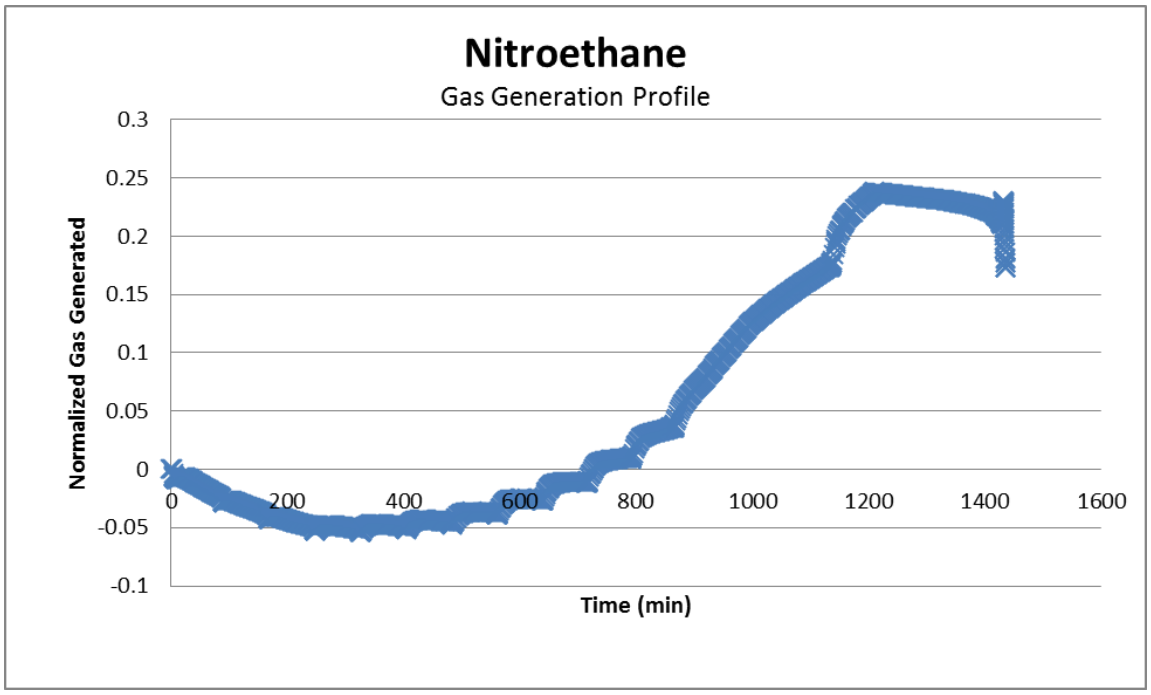

Fig. B.75 Normalized Gas Generation - Nitroethane

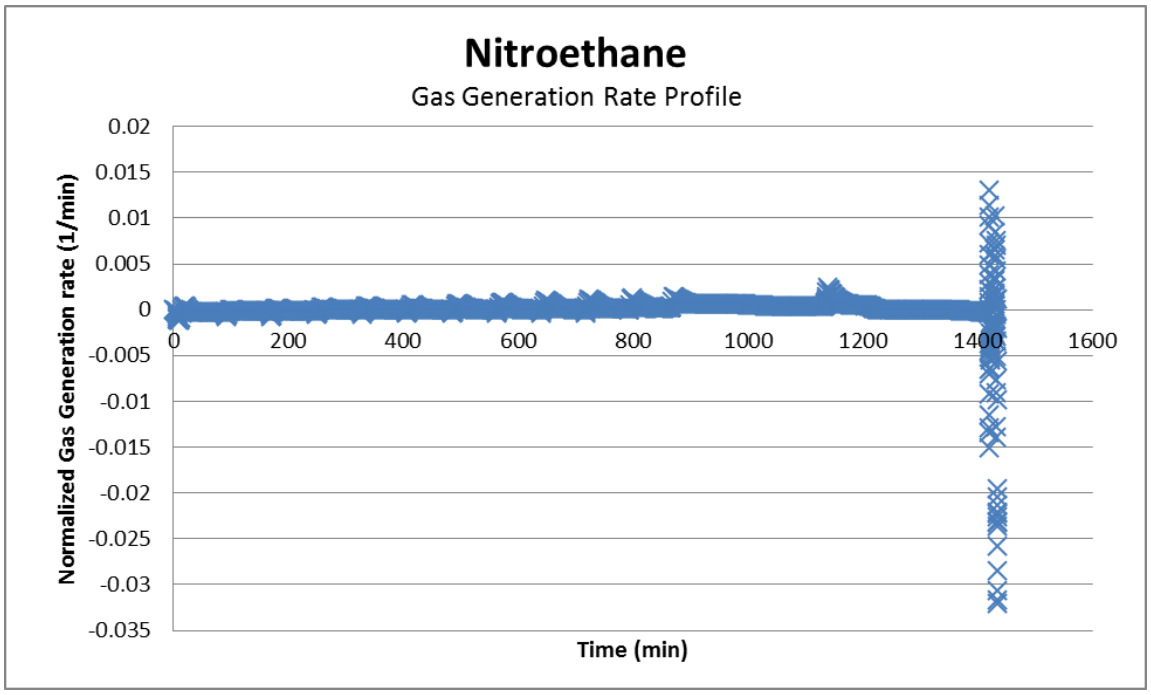

Fig. B.76 Normalized Gas Generation Rate - Nitroethane

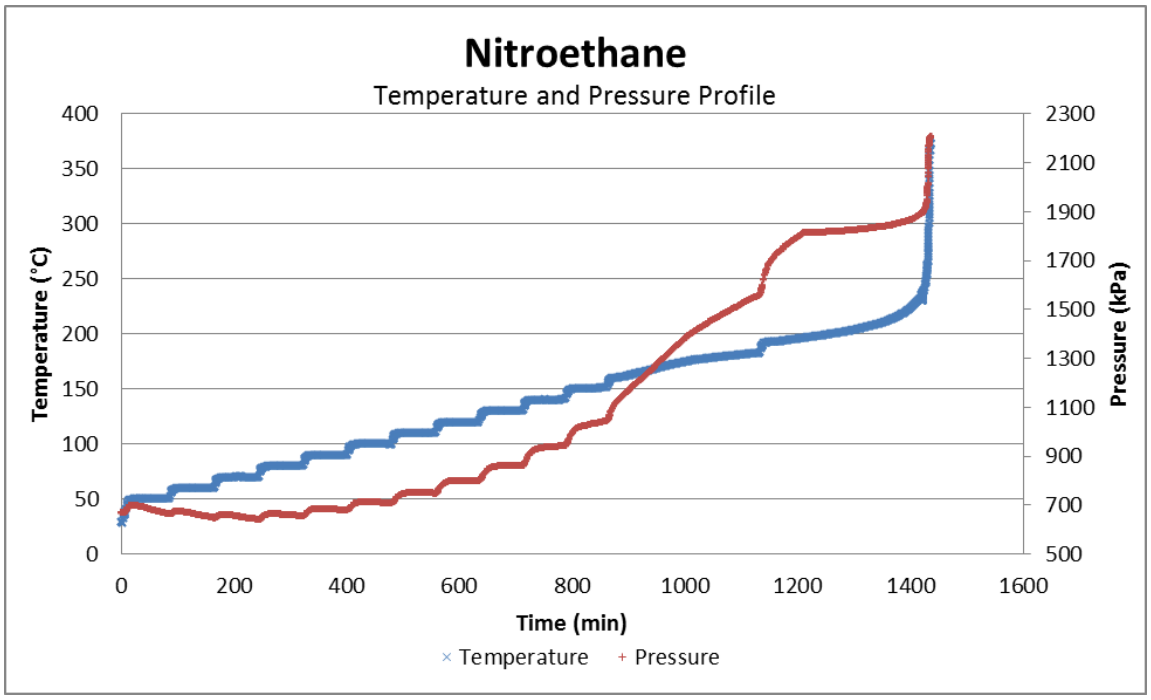

Fig. B.77 Temperature and Pressure Profiles - Nitroethane

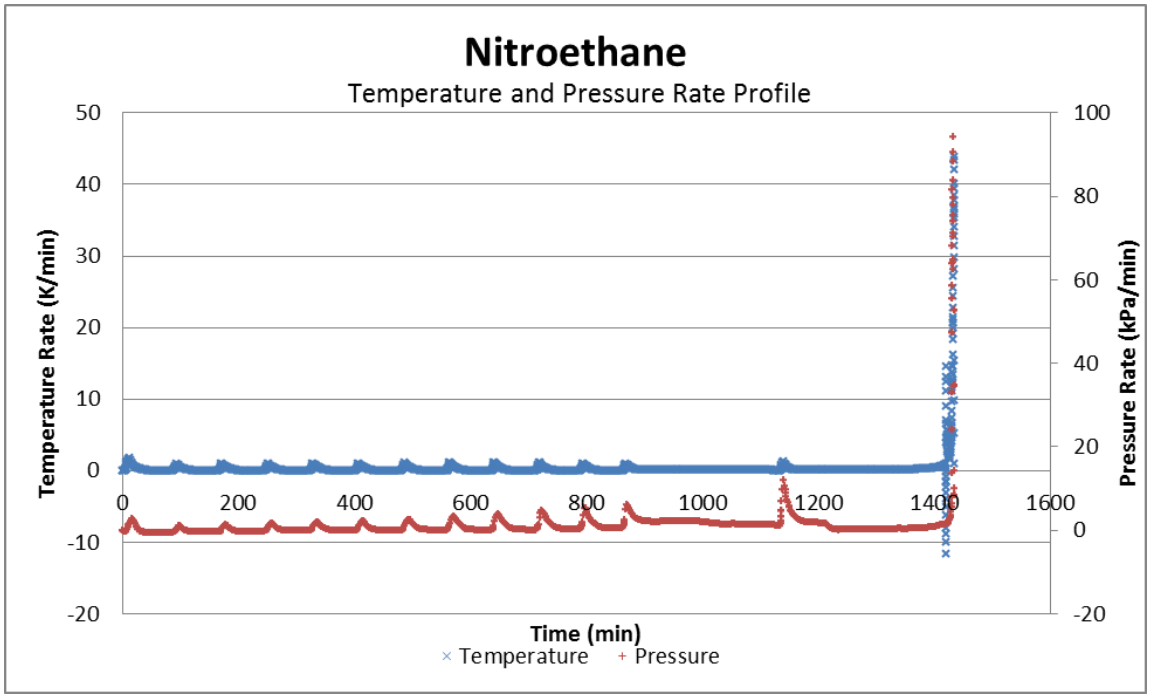

Fig. B.78 Temperature and Pressure Rate Profiles - Nitroethane

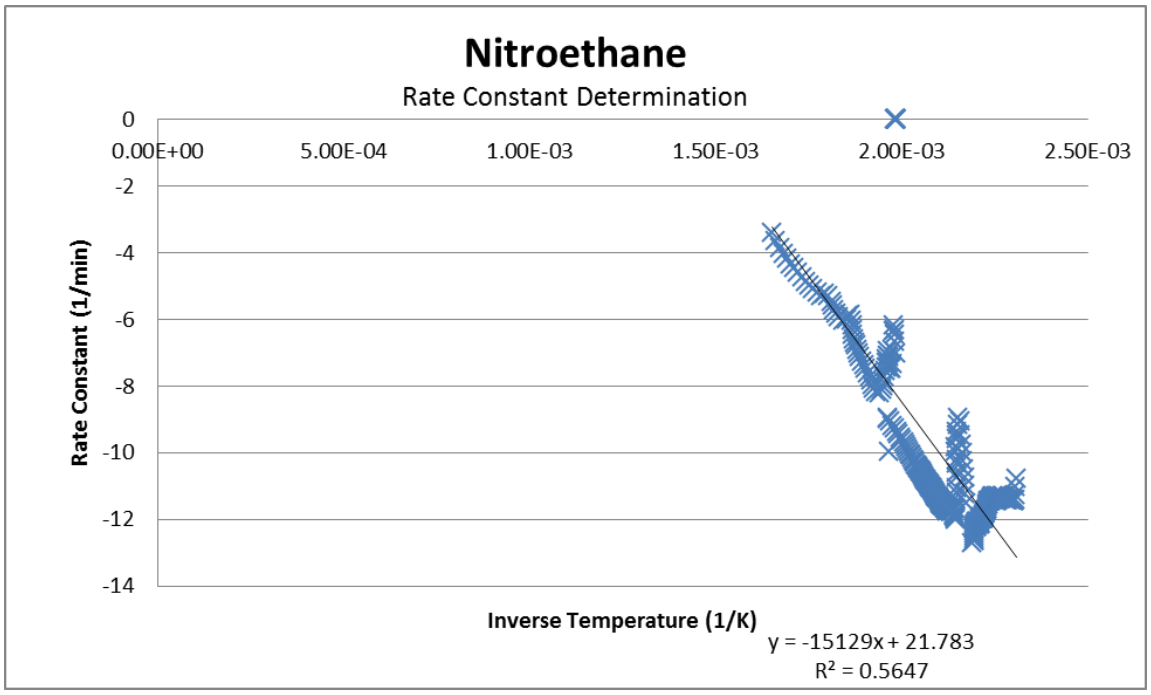

Fig. B.79 Rate Constant Determination - Nitroethane

B.17 Picoline

Table B.65
Material Properties - Picoline

Property	Value
m_s (g)	6.6
ρ_s (g/mL)	0.943
C_s (J/(g*K))	1.703
MW (g/mol)	93.13

Table B.66
Cell Properties - Picoline

Property	Value
m_{cell} (g)	57.85
V_{cell} (mL)	90.00
φ	5.323

Table B.67
IPD Properties - Picoline

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	N/A
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.68
Gas Properties - Picoline

Property	Value
n_{max} (mol)	4.991E-02
dn/dt_{max} (mol/min)	3.344E-04
n_{maxn}	7.043E-01
dn/dt_{maxn} (1/min)	4.718E-03
GGP (1/min)	3.323E-03

Note – This compound did not exhibit a decomposition reaction so does not include information to calculate IPD. It was run at atmospheric pressure (Saenz et al., 2009).

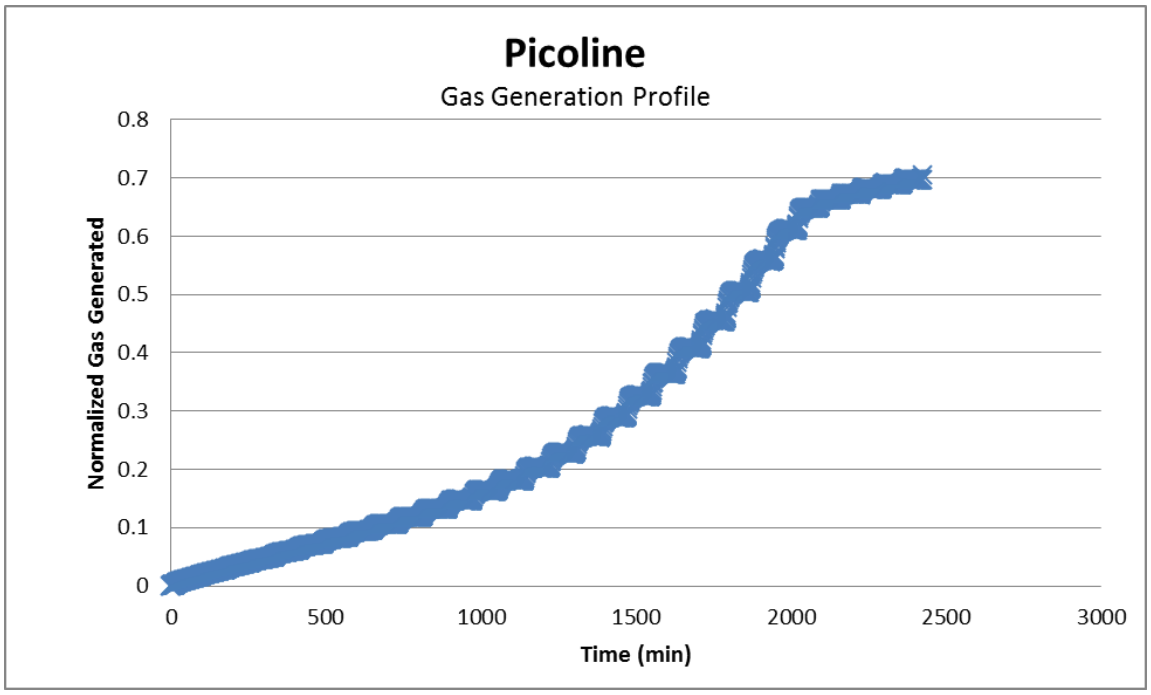

Fig. B.80 Normalized Gas Generation - Picoline

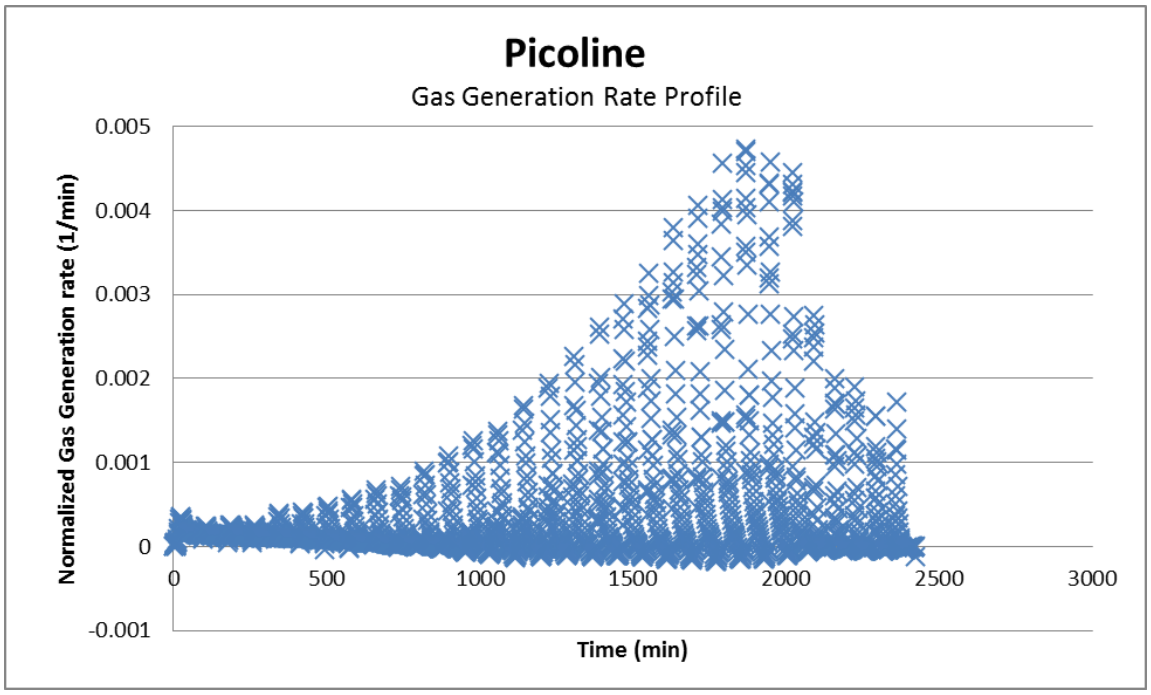

Fig. B.81 Normalized Gas Generation Rate - Picoline

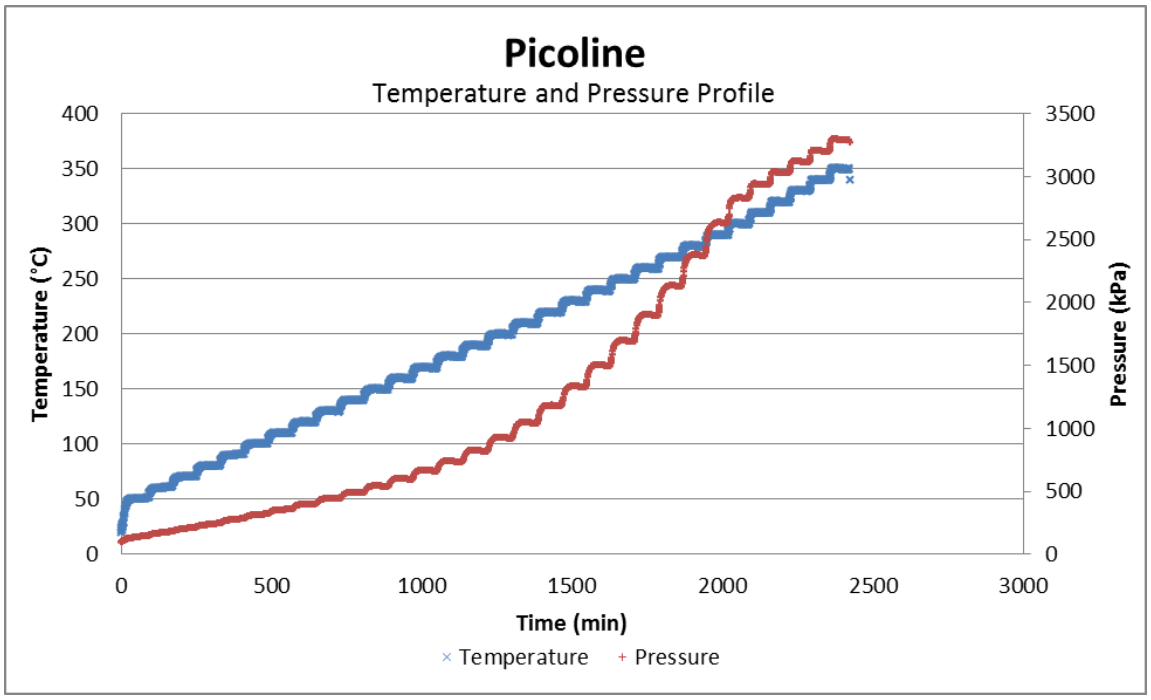

Fig. B.82 Temperature and Pressure Profiles - Picoline

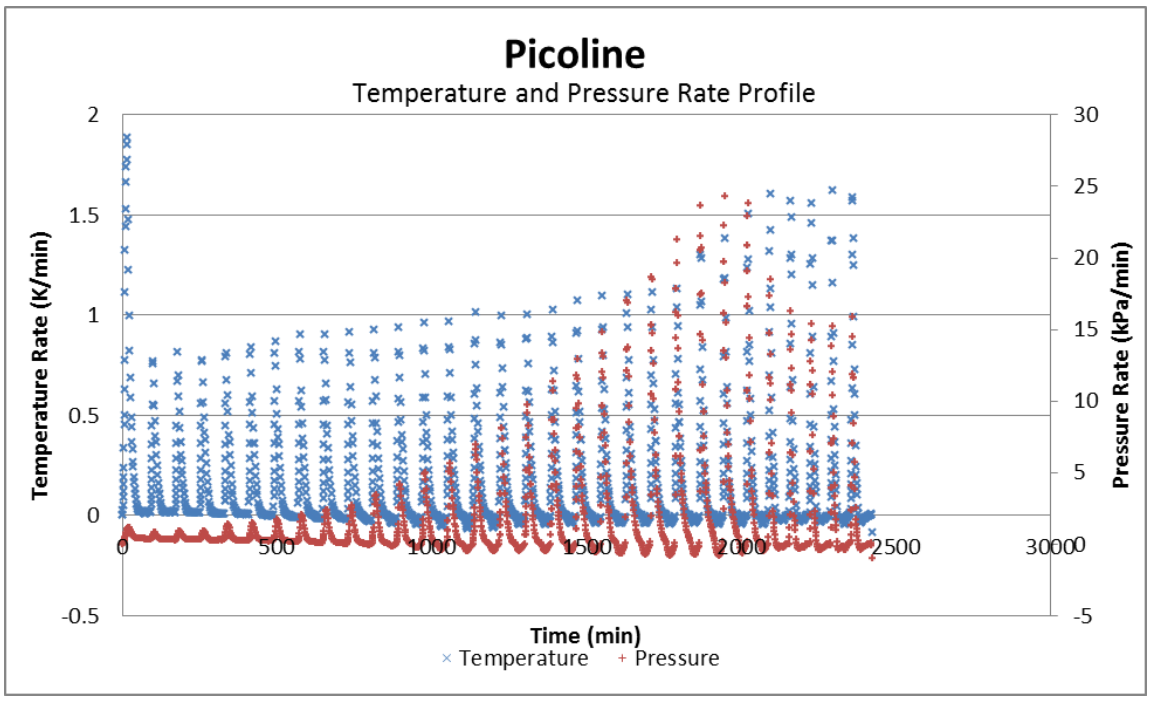

Fig. B.83 Temperature and Pressure Rate Profiles - Picoline

B.18 Polyacrylic Acid

Table B.69
Material Properties - Polyacrylic Acid

Property	Value
m_s (g)	4.48
ρ_s (g/mL)	1
C_s (J/(g*K))	2
Subunit MW (g/mol)	72.06

Table B.70
Cell Properties - Polyacrylic Acid

Property	Value
m_{cell} (g)	57.48
V_{cell} (mL)	92.15
φ	6.389

Table B.71
IPD Properties - Polyacrylic Acid

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	260
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.72
Gas Properties - Polyacrylic Acid

Property	Value
n_{max} (mol)	6.451E-02
dn/dt_{max} (mol/min)	2.536E-04
n_{maxn}	1.038E+00
dn/dt_{maxn} (1/min)	4.080E-03
GGP (1/min)	4.233E-03

Note – This compound was run at atmospheric pressure and did not exhibit a decomposition reaction. An IPD cannot be calculated. (Carreto-Vasquez et al., 2010).

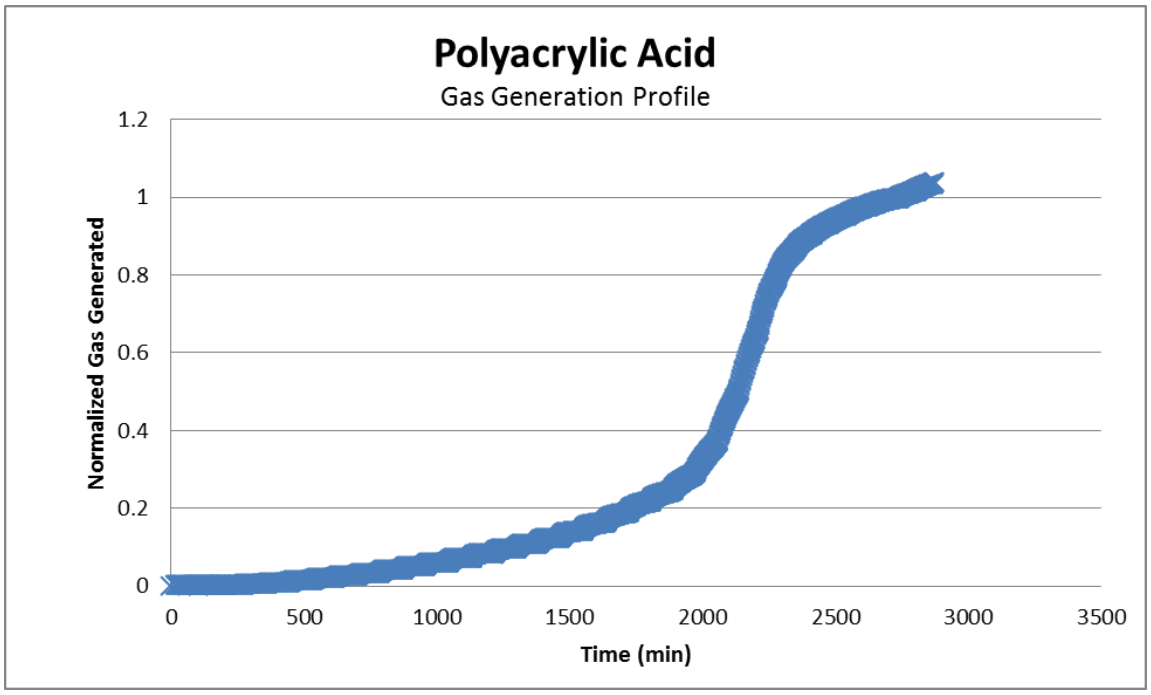

Fig. B.84 Normalized Gas Generation - Polyacrylic Acid

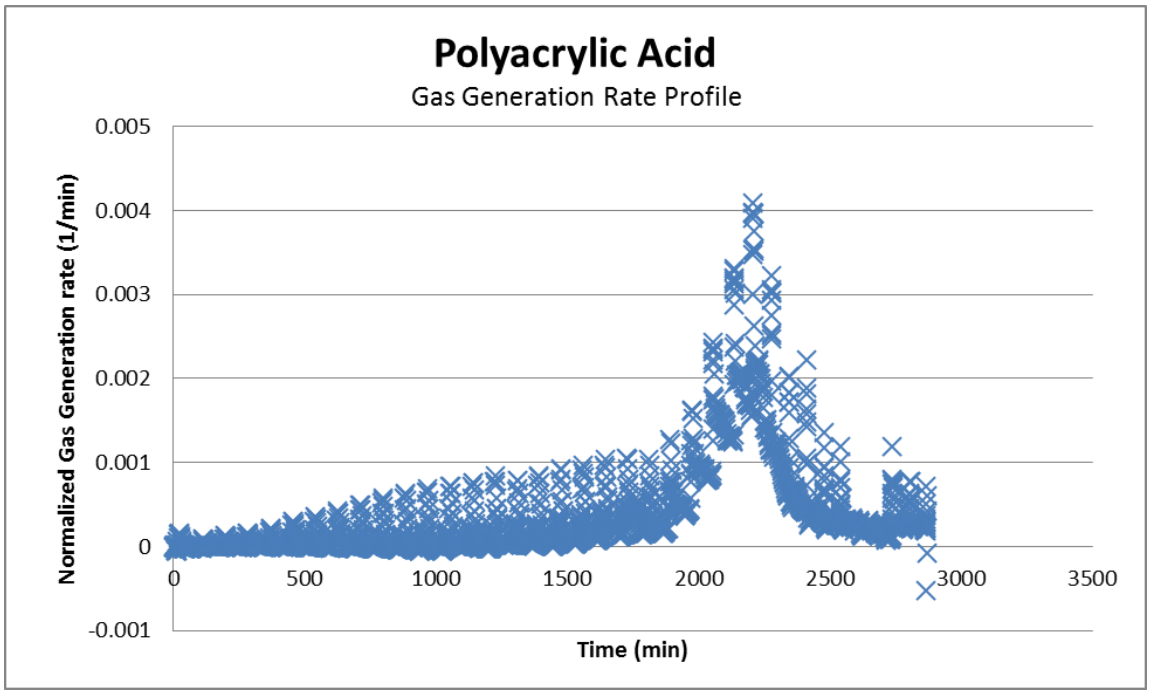

Fig. B.85 Normalized Gas Generation Rate - Polyacrylic Acid

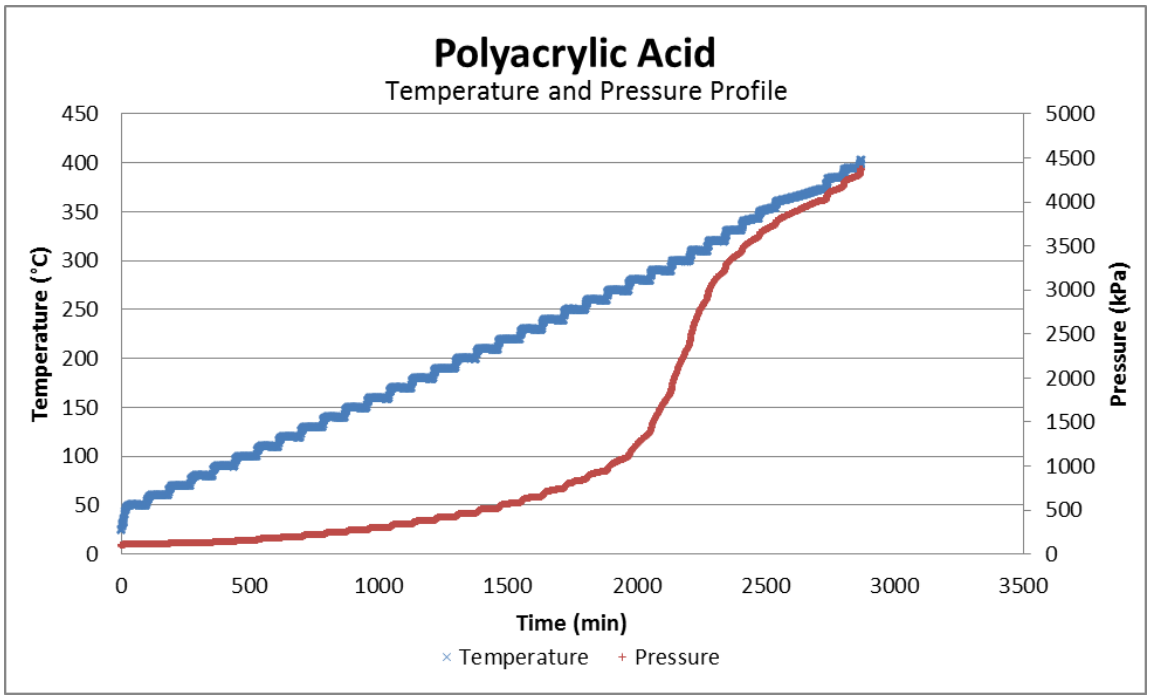

Fig. B.86 Temperature and Pressure Profiles - Polyacrylic Acid

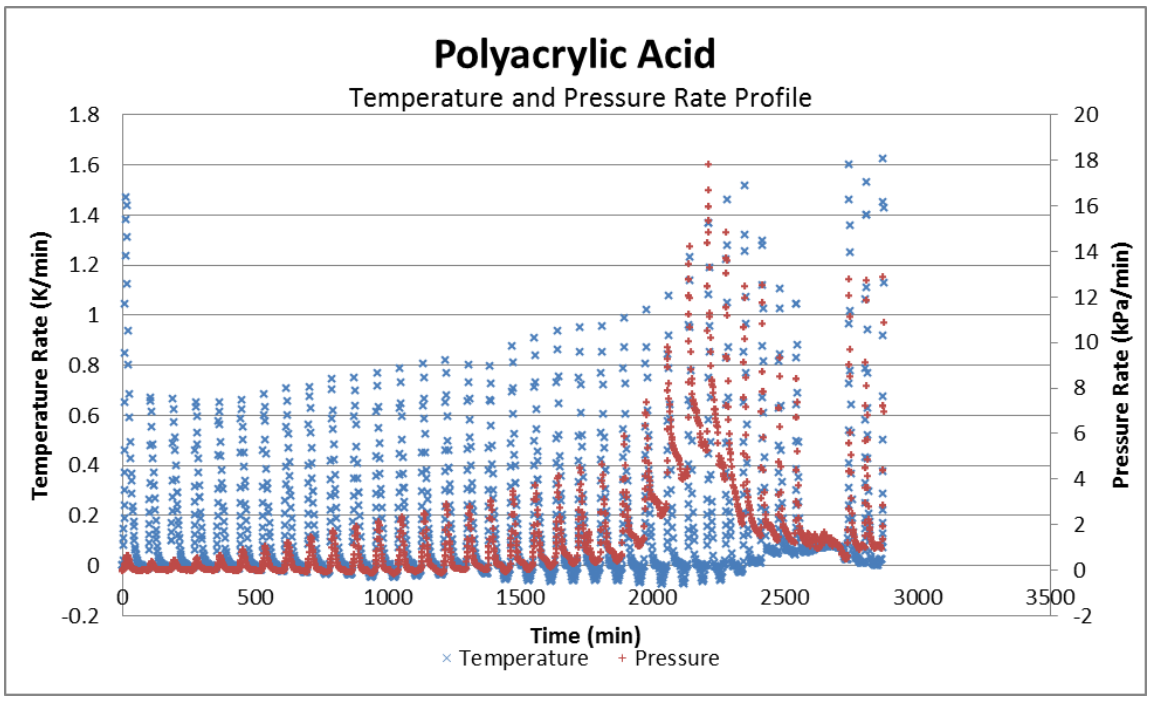

Fig. B.87 Temperature and Pressure Rate Profiles - Polyacrylic Acid

B.19 Polyarylamide

Table B.73
Material Properties - Polyarylamide

Property	Value
m_s (g)	12.53
ρ_s (g/mL)	1.1
C_s (J/(g*K))	2
Subunit MW (g/mol)	121.7

Table B.74
Cell Properties - Polyarylamide

Property	Value
m_{cell} (g)	58.63
V_{cell} (mL)	91.50
φ	2.965

Table B.75
IPD Properties - Polyarylamide

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	300
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.76
Gas Properties - Polyarylamide

Property	Value
n_{max} (mol)	6.045E-02
dn/dt_{max} (mol/min)	5.830E-04
n_{maxn}	5.871E-01
dn/dt_{maxn} (1/min)	5.663E-03
GGP (1/min)	3.325E-03

Note – This compound was run at atmospheric pressure and did not exhibit a decomposition reaction. An IPD cannot be calculated. (Carreto-Vasquez et al., 2010).

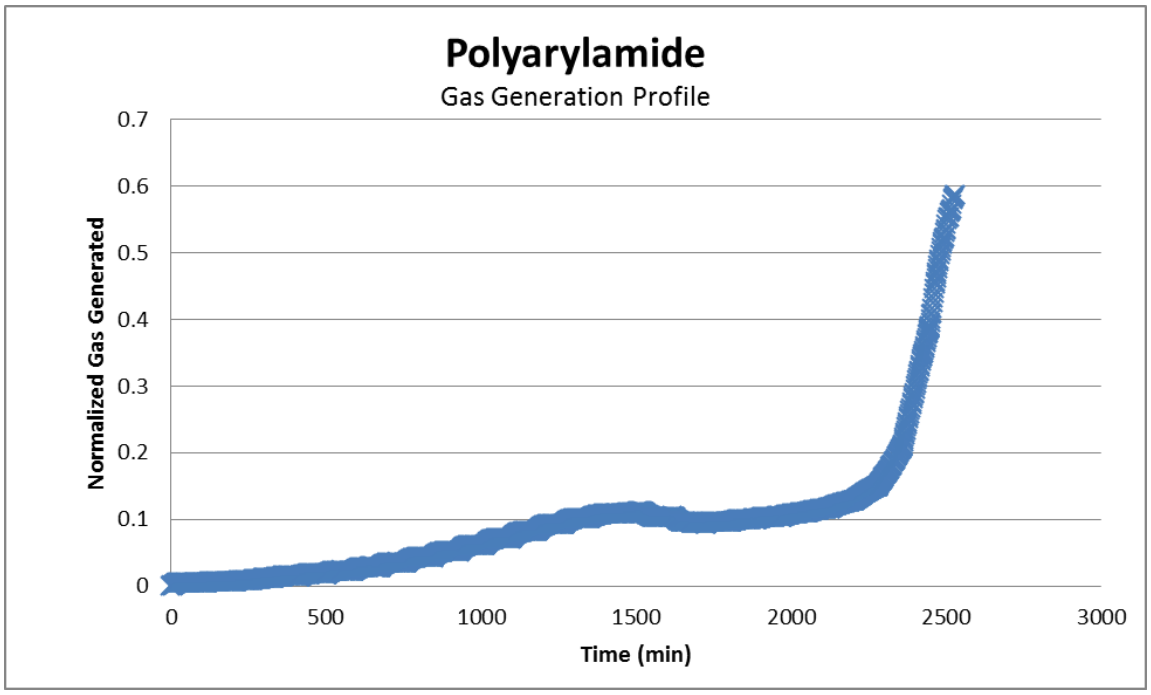

Fig. B.88 Normalized Gas Generation - Polyarylamide

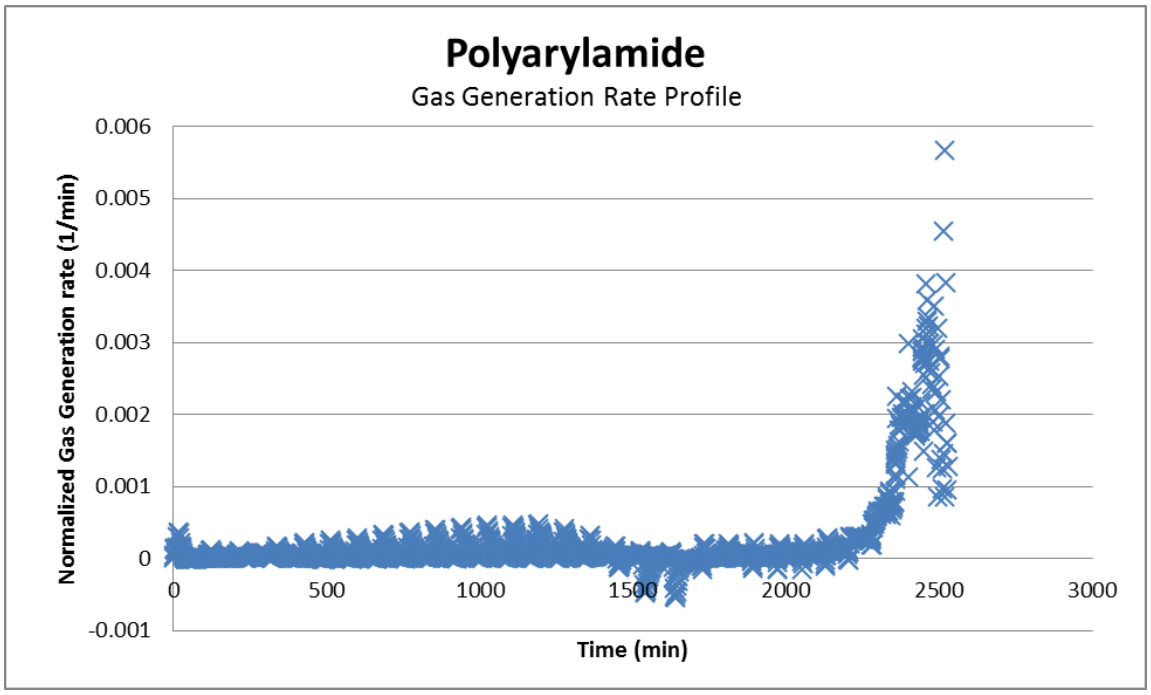

Fig. B.89 Normalized Gas Generation Rate - Polyarylamide

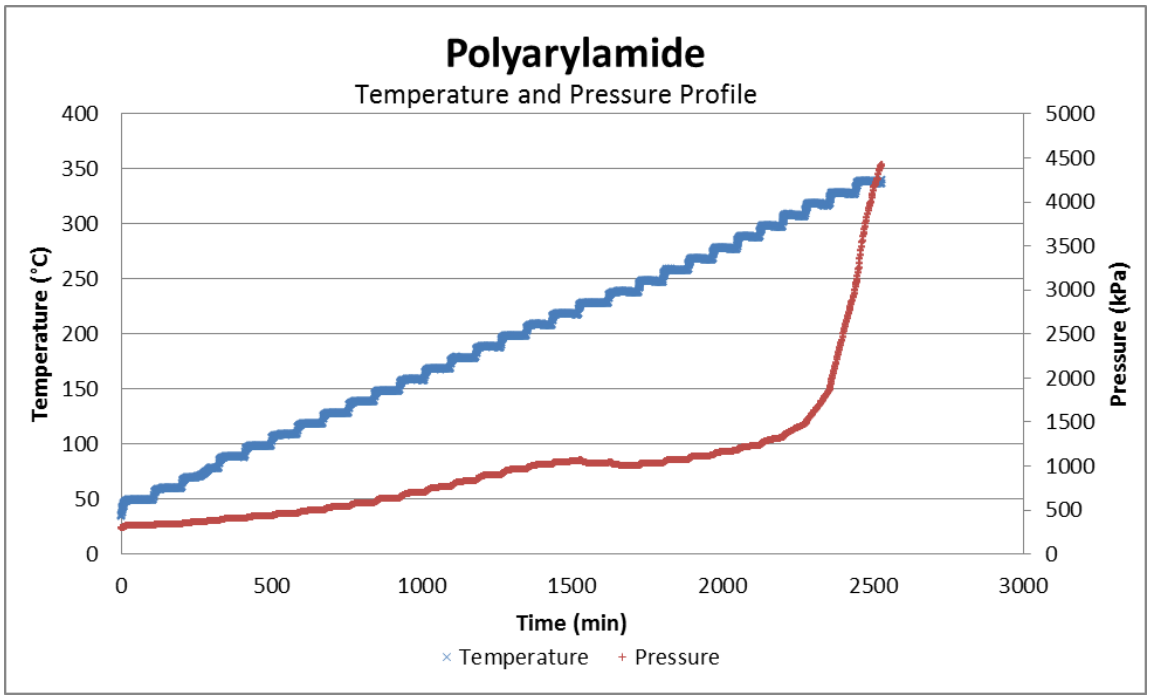

Fig. B.90 Temperature and Pressure Profiles - Polyarylamide

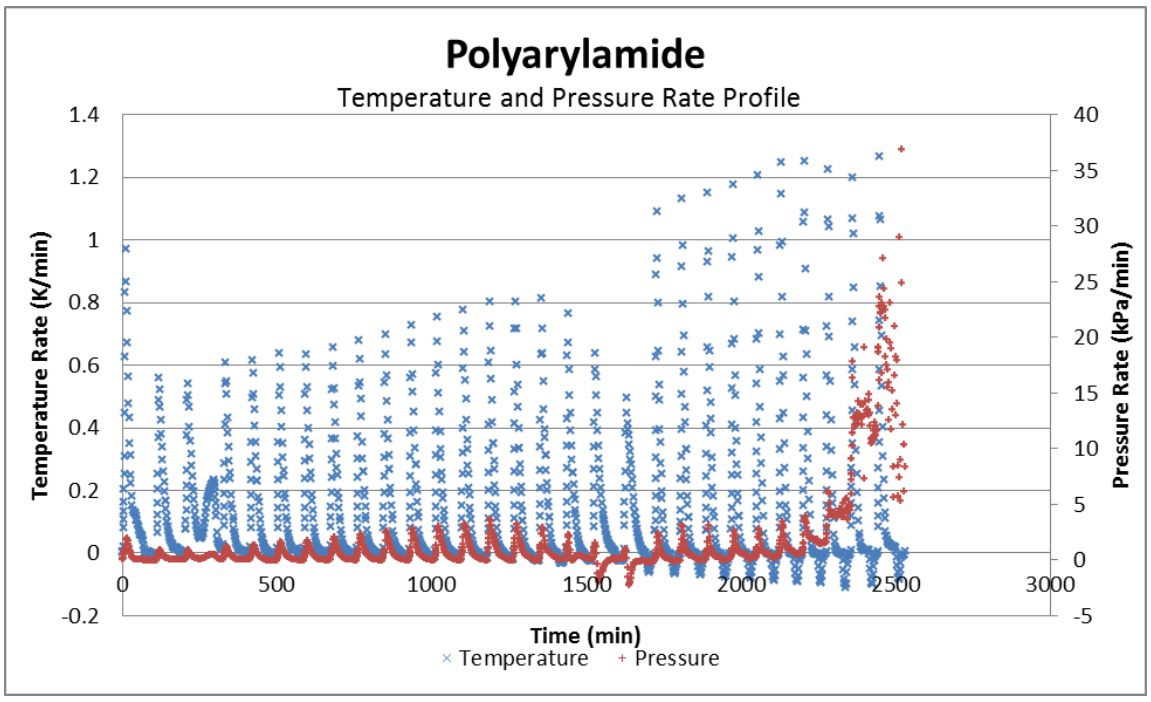

Fig. B.91 Temperature and Pressure Rate Profiles - Polyarylamide

B.20 Polyethylene Glycol

Table B.77
Material Properties - Polyethylene Glycol

Property	Value
m_s (g)	5.21
ρ_s (g/mL)	1
C_s (J/(g*K))	3.322
Subunit MW (g/mol)	45

Table B.78
Cell Properties - Polyethylene Glycol

Property	Value
m_{cell} (g)	54.71
V_{cell} (mL)	92.00
φ	3.655

Table B.79
IPD Properties - Polyethylene Glycol

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	290
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.80
Gas Properties - Polyethylene Glycol

Property	Value
n_{max} (mol)	3.680E-04
dn/dt_{max} (mol/min)	1.383E-04
n_{maxn}	3.179E-03
dn/dt_{maxn} (1/min)	1.194E-03
GGP (1/min)	3.796E-06

Note – This compound did not exhibit a decomposition reaction. An IPD cannot be calculated.

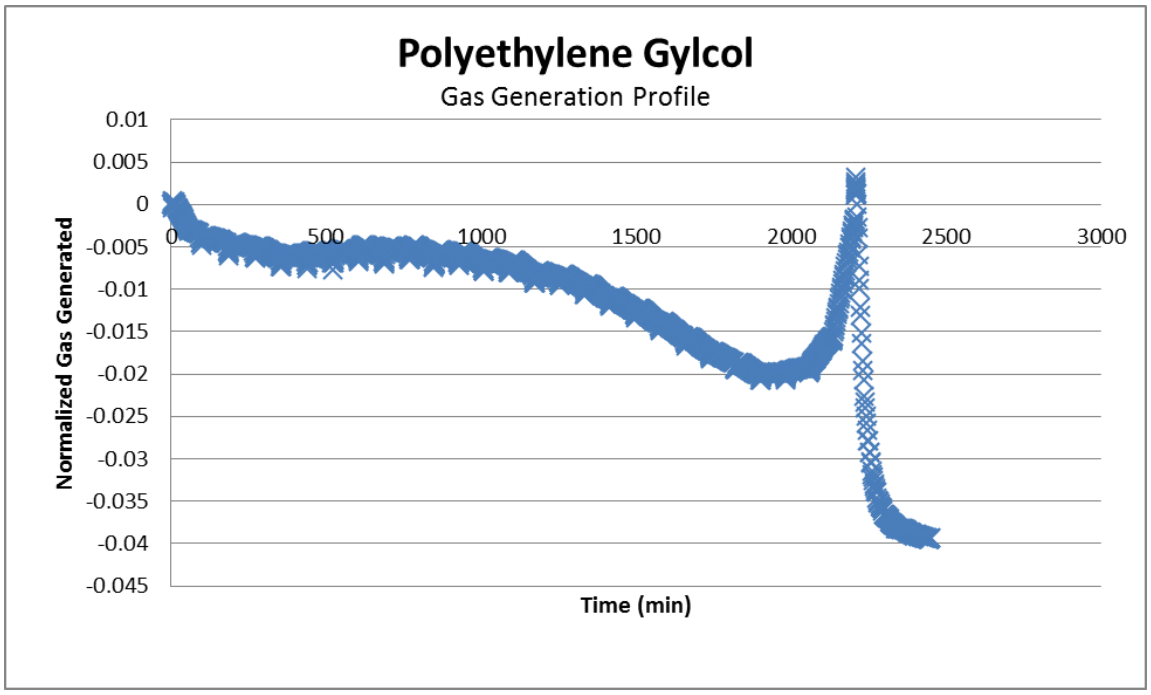

Fig. B.92 Normalized Gas Generation - Polyethylene Glycol

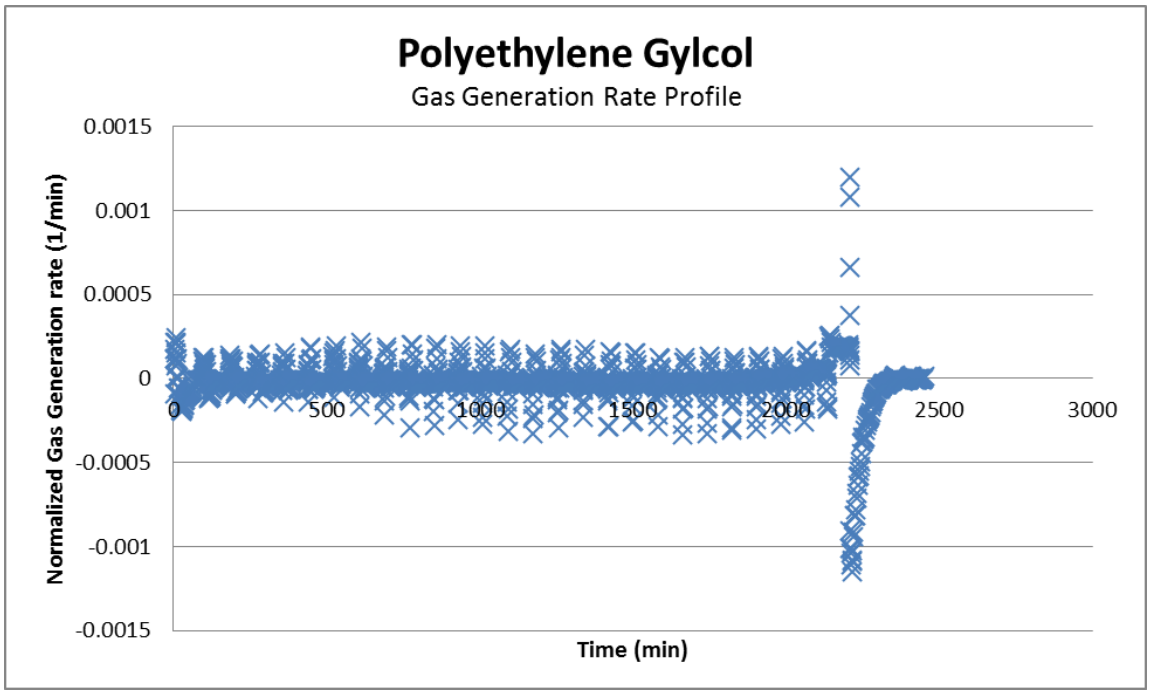

Fig. B.93 Normalized Gas Generation Rate - Polyethylene Glycol

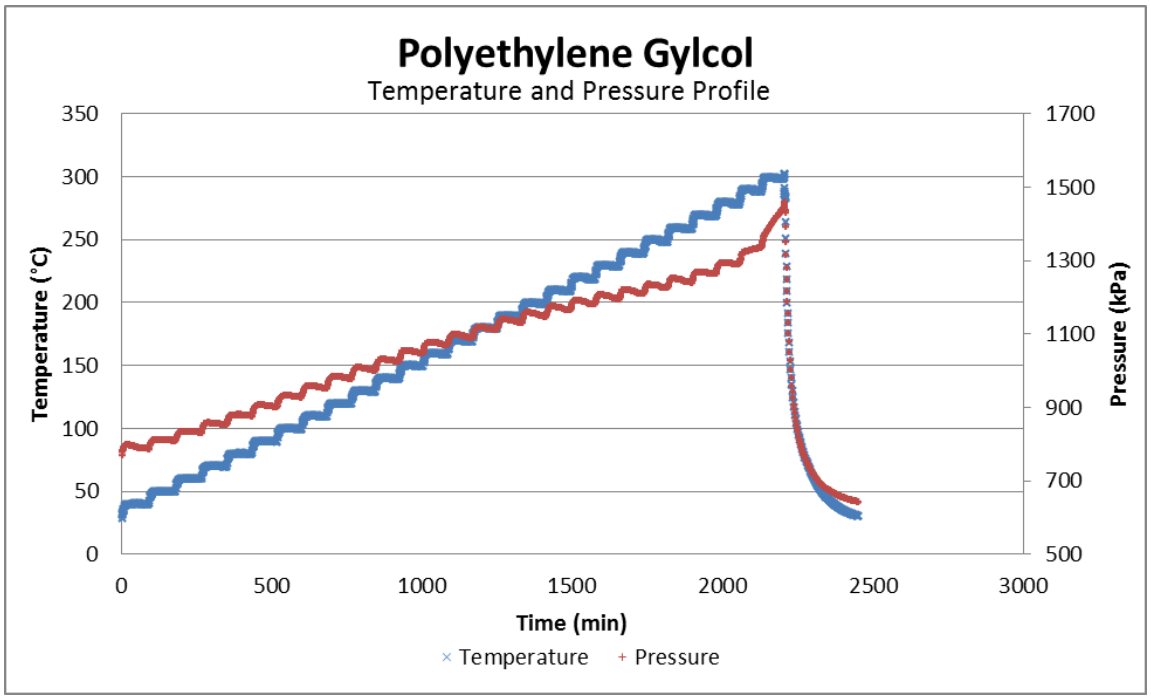

Fig. B.94 Temperature and Pressure Profiles - Polyethylene Glycol

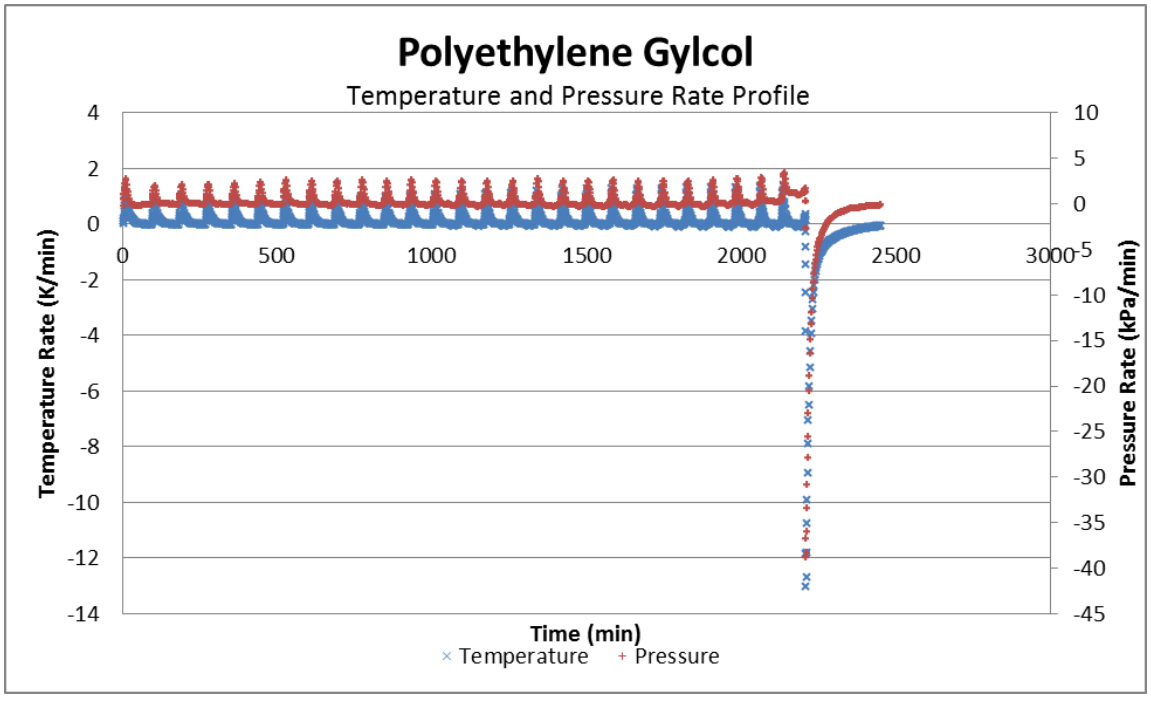

Fig. B.95 Temperature and Pressure Rate Profiles - Polyethylene Glycol

B.21 Polyvinyl Acetate

Table B.81
Material Properties - Polyvinyl Acetate

Property	Value
m_s (g)	11.07
ρ_s (g/mL)	1.19
C_s (J/(g*K))	2
Subunit MW (g/mol)	86.09

Table B.82
Cell Properties - Polyvinyl Acetate

Property	Value
m_{cell} (g)	58.83
V_{cell} (mL)	91.48
φ	3.232

Table B.83
IPD Properties - Polyvinyl Acetate

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	240
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.84
Gas Properties - Polyvinyl Acetate

Property	Value
n_{max} (mol)	9.833E-02
dn/dt_{max} (mol/min)	4.922E-04
n_{maxn}	7.647E-01
dn/dt_{maxn} (1/min)	3.828E-03
GGP (1/min)	2.927E-03

Note – This compound was run at atmospheric pressure and did not exhibit a decomposition reaction. An IPD cannot be calculated. (Carreto-Vasquez et al., 2010).

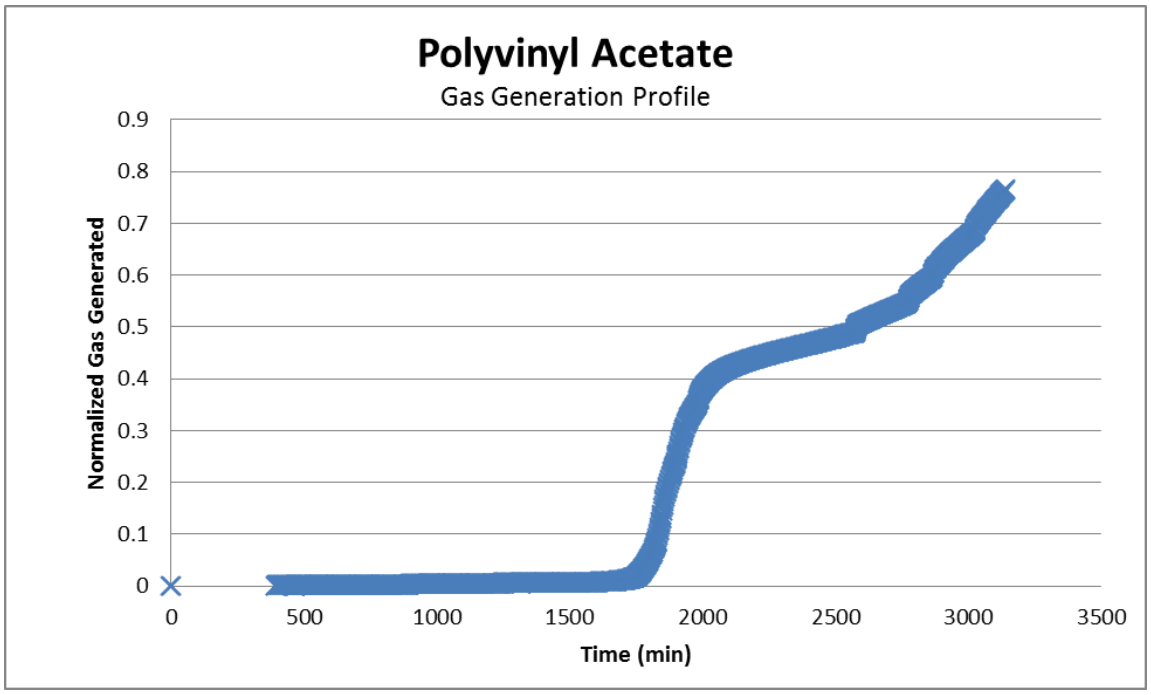

Fig. B.96 Normalized Gas Generation - Polyvinyl Acetate

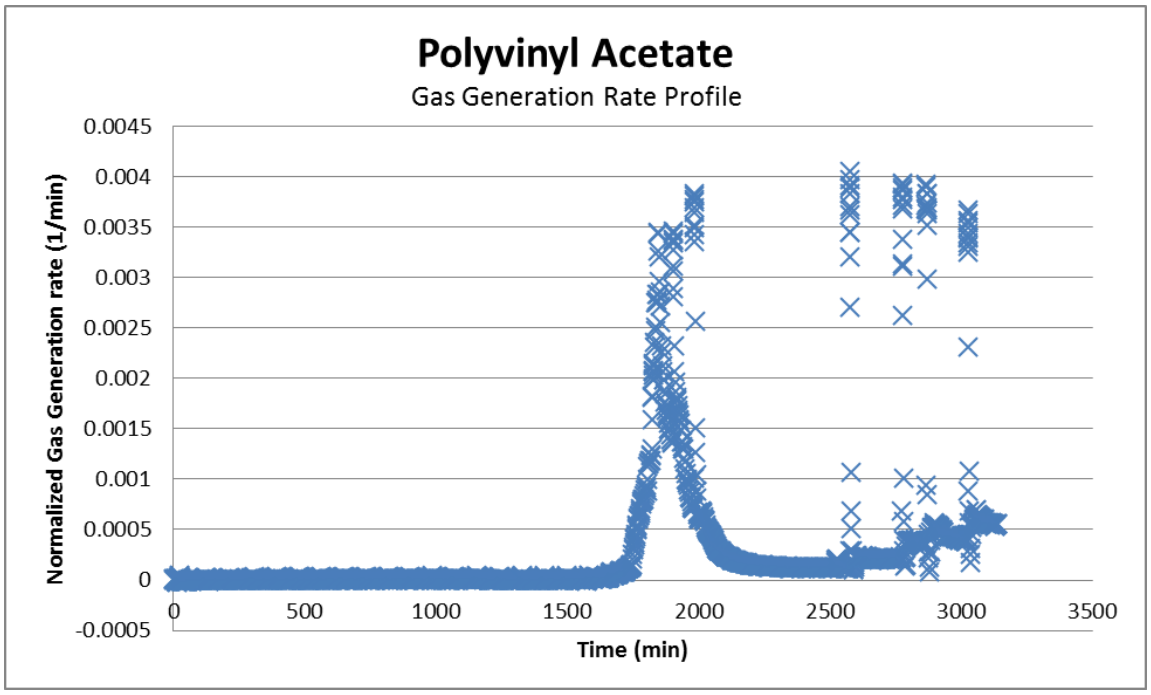

Fig. B.97 Normalized Gas Generation Rate - Polyvinyl Acetate

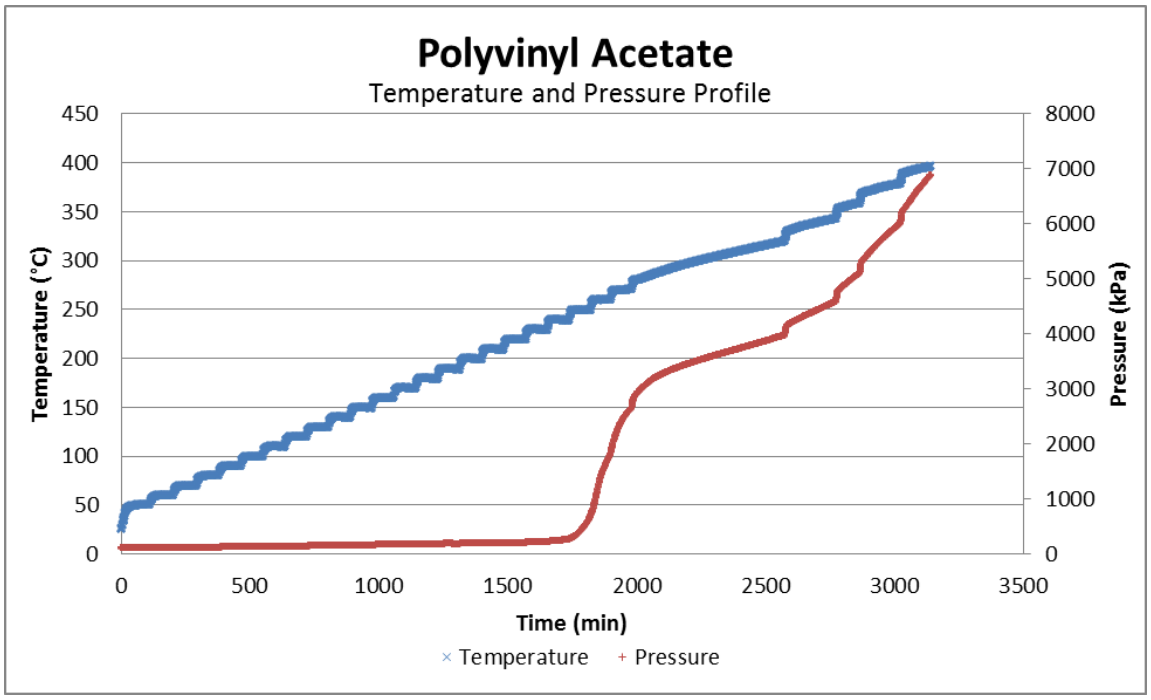

Fig. B.98 Temperature and Pressure Profiles - Polyvinyl Acetate

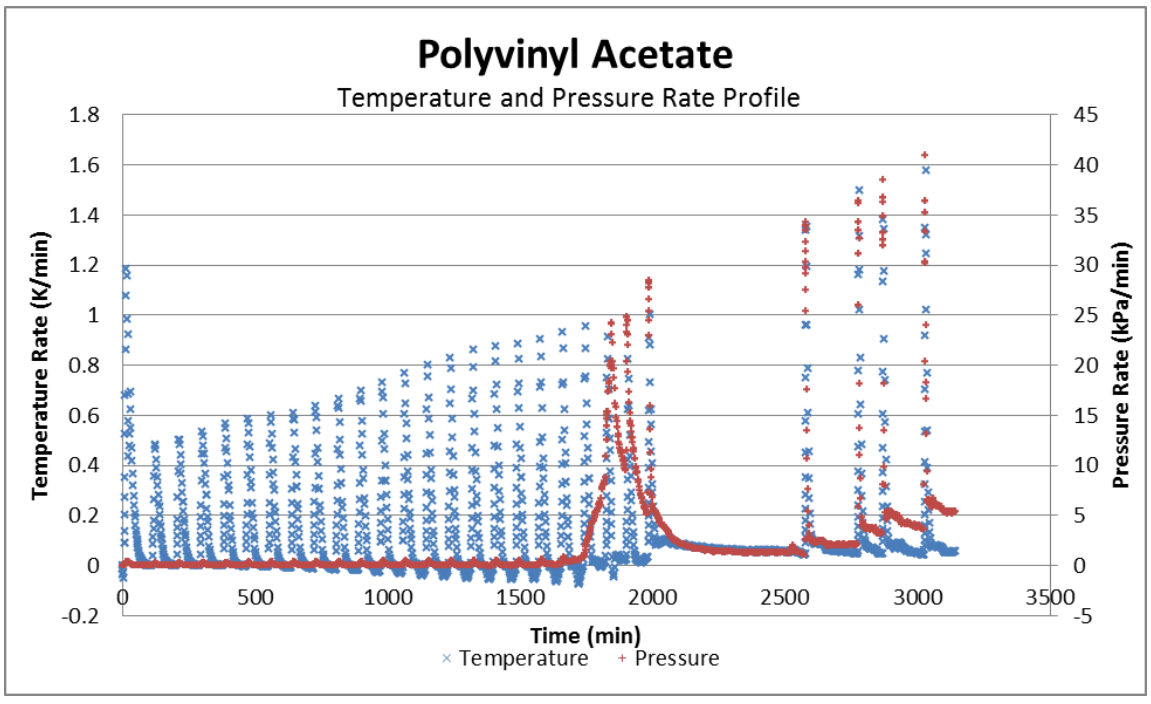

Fig. B.99 Temperature and Pressure Rate Profiles - Polyvinyl Acetate

B.22 Styrene

Table B.85
Material Properties - Styrene

Property	Value
m_s (g)	5.46
ρ_s (g/mL)	0.906
C_s (J/(g*K))	1.800
MW (g/mol)	104.15

Table B.86
Cell Properties - Styrene

Property	Value
m_{cell} (g)	51.09
V_{cell} (mL)	93.47
φ	5.366

Table B.87
IPD Properties - Styrene

Property	Value
A (1/s)	1.593E+08
E_A (J/(mol*K))	9.635E+04
T_{onset} (°C)	120
T_{max} (°C)	235
ΔH (J/g)	1.111E+03
IPD (W/ml)	3.847E+01

Table B.88
Gas Properties - Styrene

Property	Value
n_{max} (mol)	6.525E-03
dn/dt_{max} (mol/min)	5.072E-04
n_{maxn}	1.245E-01
dn/dt_{maxn} (1/min)	9.674E-03
GGP (1/min)	1.204E-03

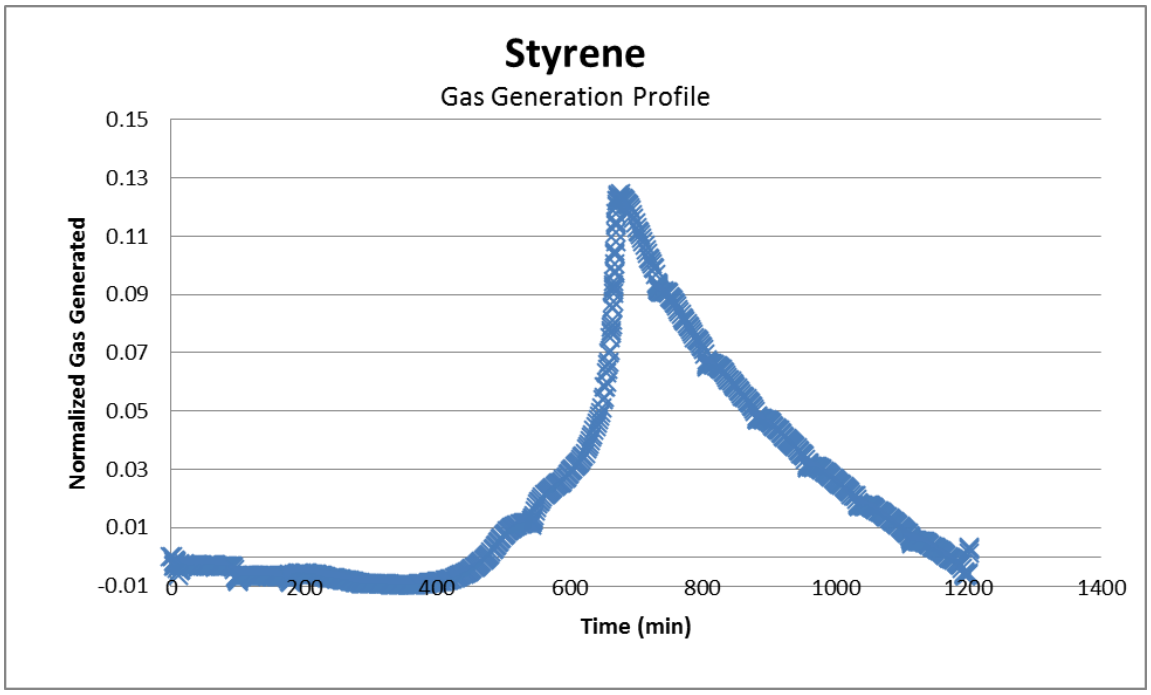

Fig. B.100 Normalized Gas Generation - Styrene

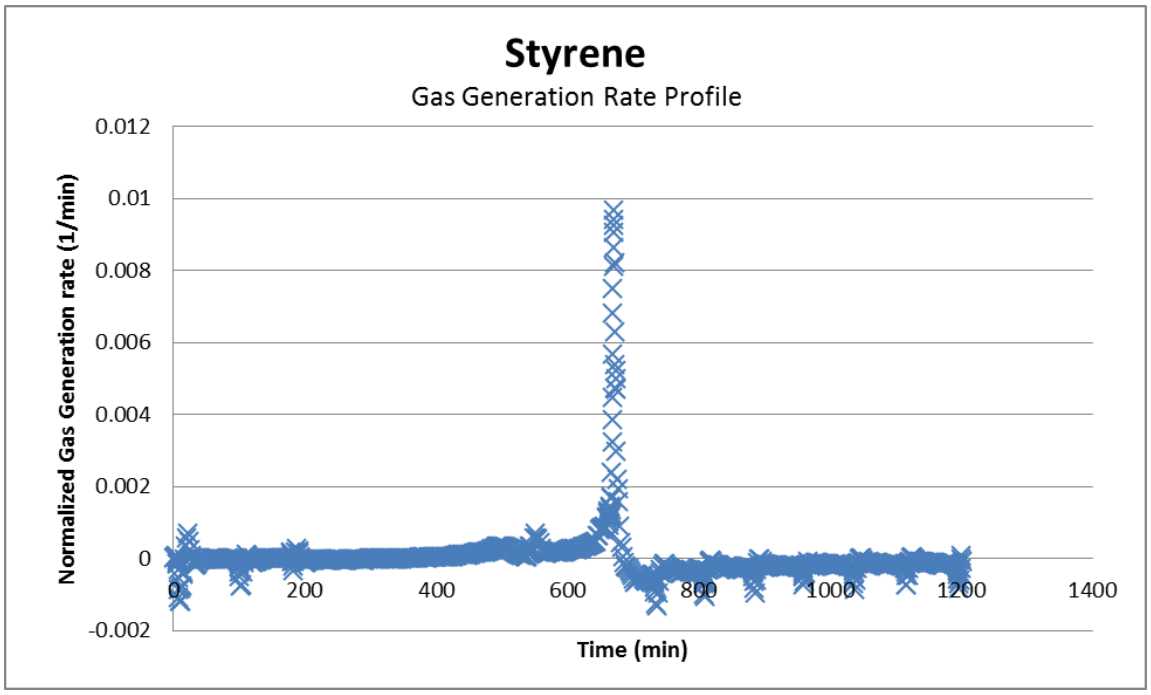

Fig. B.101 Normalized Gas Generation Rate - Styrene

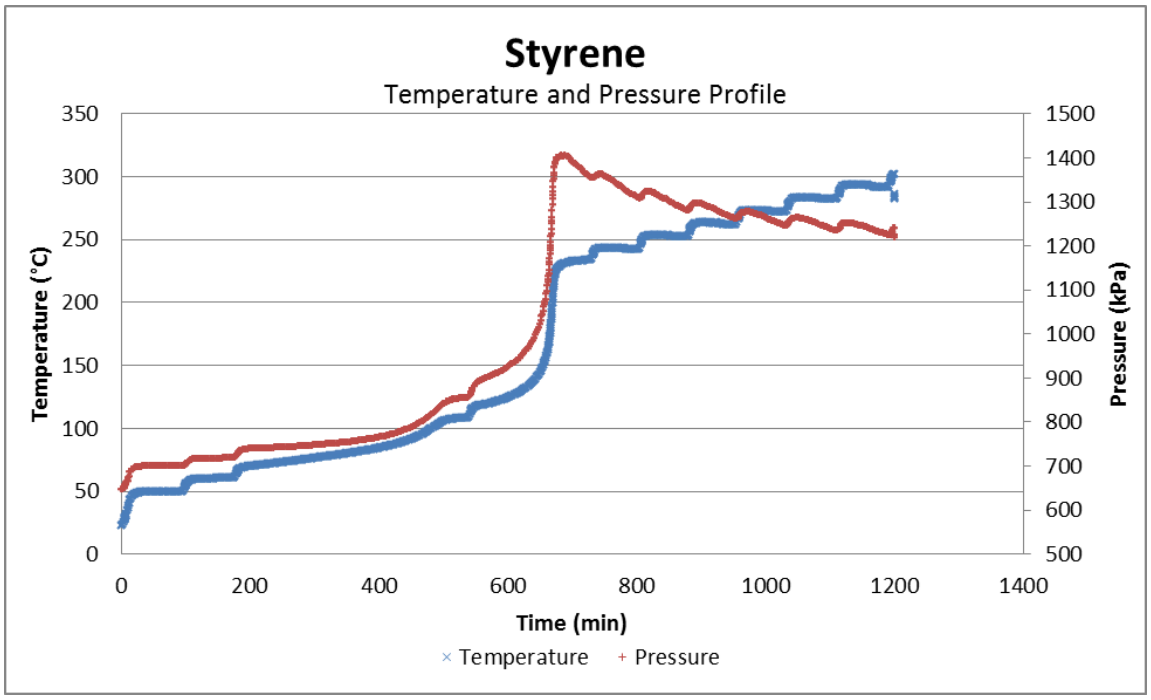

Fig. B.102 Temperature and Pressure Profiles - Styrene

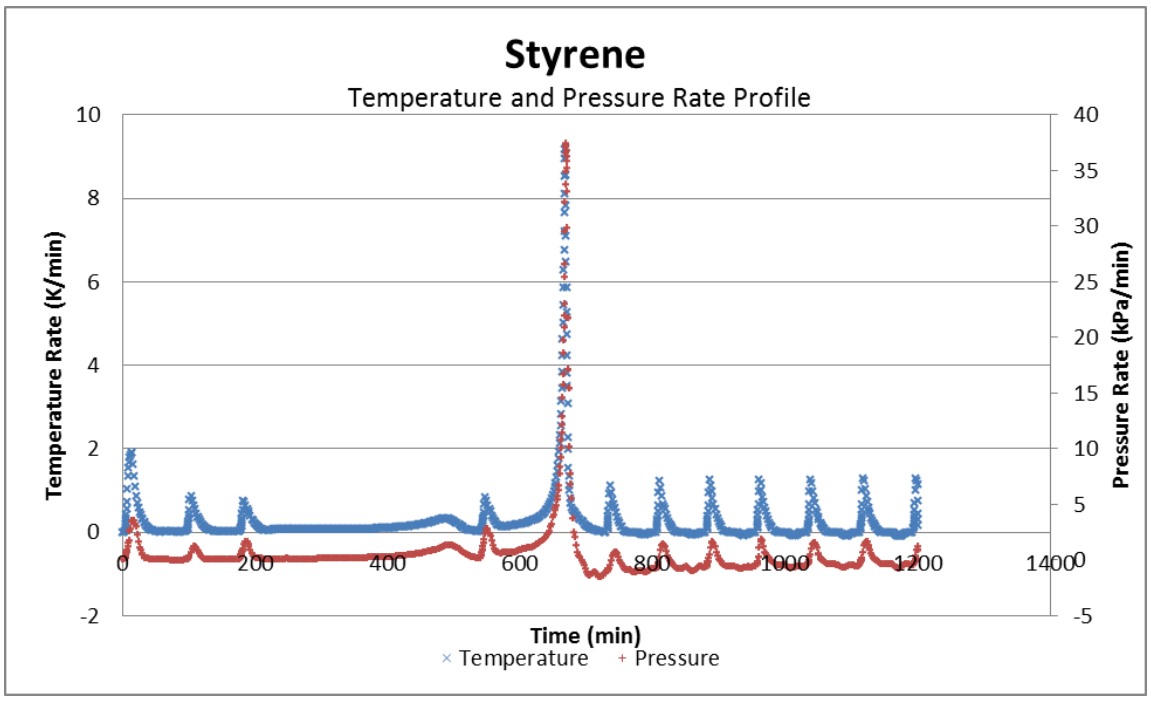

Fig. B.103 Temperature and Pressure Rate Profiles - Styrene

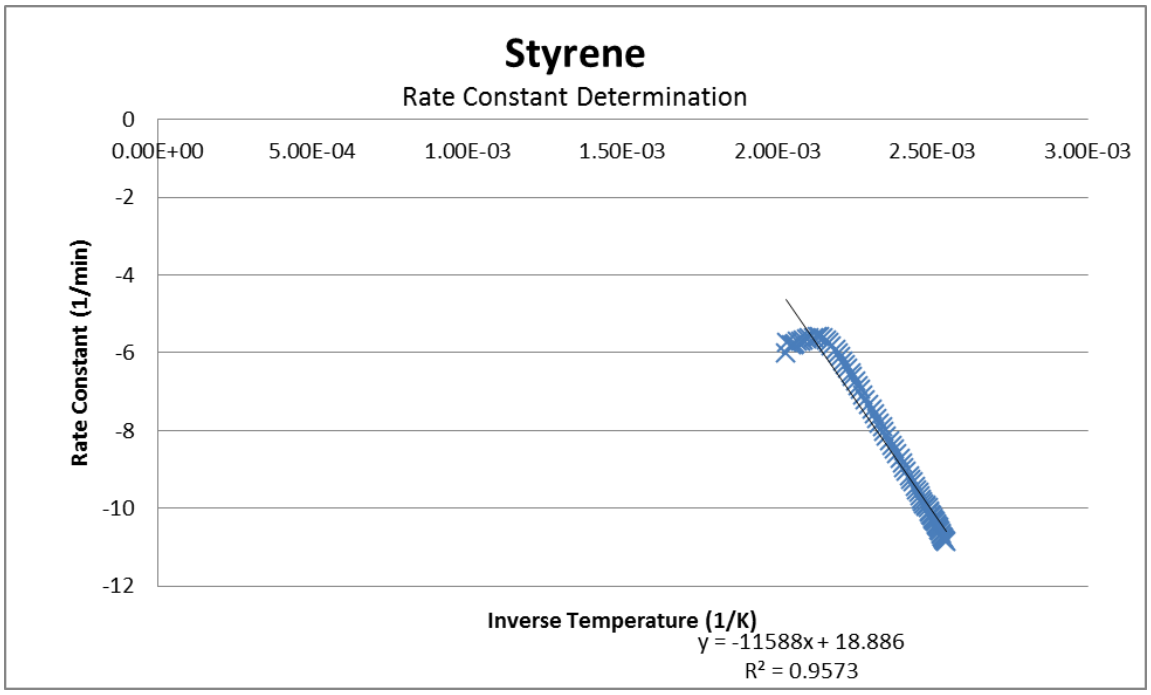

Fig. B.104 Rate Constant Determination - Styrene

B.23 Tertbutyl Peroxide 1.3g-avg

Table B.89
Material Properties - Tertbutyl Peroxide 1.3g-avg

Property	Value
m_s (g)	1.3
ρ_s (g/mL)	0.796
C_s (J/(g*K))	1.499
MW (g/mol)	146.23

Table B.90
Cell Properties - Tertbutyl Peroxide 1.3g-avg

Property	Value
m_{cell} (g)	51.74
V_{cell} (mL)	96.90
φ	22.80

Table B.91
IPD Properties - Tertbutyl Peroxide 1.3g-avg

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	100
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	8.88E+01

Table B.92
Gas Properties - Tertbutyl Peroxide 1.3g-avg

Property	Value
n_{max} (mol)	2.04E-02
dn/dt_{max} (mol/min)	2.01E-04
n_{maxn}	2.20E+00
dn/dt_{maxn} (1/min)	2.17E-02
GGP (1/min)	4.79E-02

Note – This is an averaged value based on the five 1.3g samples of tertbutyl peroxide.

B.24 Vinyl Acetate

Table B.93
Material Properties - Vinyl Acetate

Property	Value
m_s (g)	6.9
ρ_s (g/mL)	0.934
C_s (J/(g*K))	1.708
MW (g/mol)	86.09

Table B.94
Cell Properties - Vinyl Acetate

Property	Value
m_{cell} (g)	52.29
V_{cell} (mL)	93.06
φ	4.727

Table B.95
IPD Properties - Vinyl Acetate

Property	Value
A (1/s)	9.147E+18
E_A (J/(mol*K))	1.880E+05
T_{onset} (°C)	160
T_{max} (°C)	195
ΔH (J/g)	2.826E+02
IPD (W/ml)	4.048E+02

Table B.96
Gas Properties - Vinyl Acetate

Property	Value
n_{max} (mol)	4.427E-02
dn/dt_{max} (mol/min)	6.290E-04
n_{maxn}	5.523E-01
dn/dt_{maxn} (1/min)	7.848E-03
GGP (1/min)	4.335E-03

Note – This compound exhibited two exotherms.

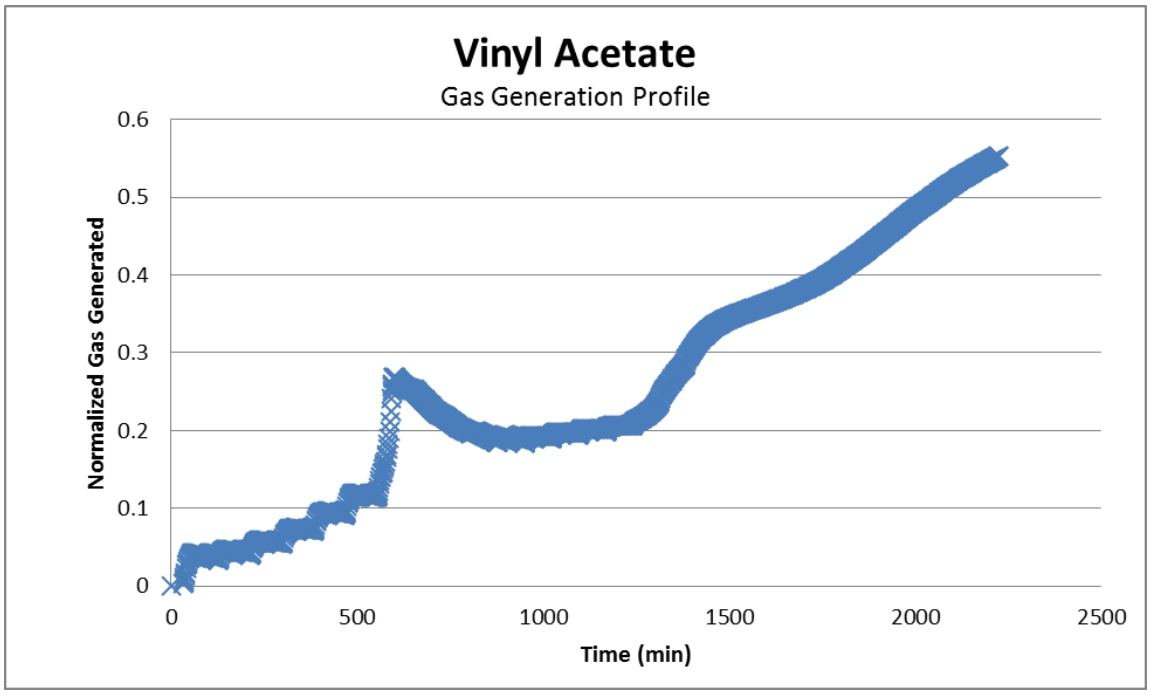

Fig. B.105 Normalized Gas Generation - Vinyl Acetate

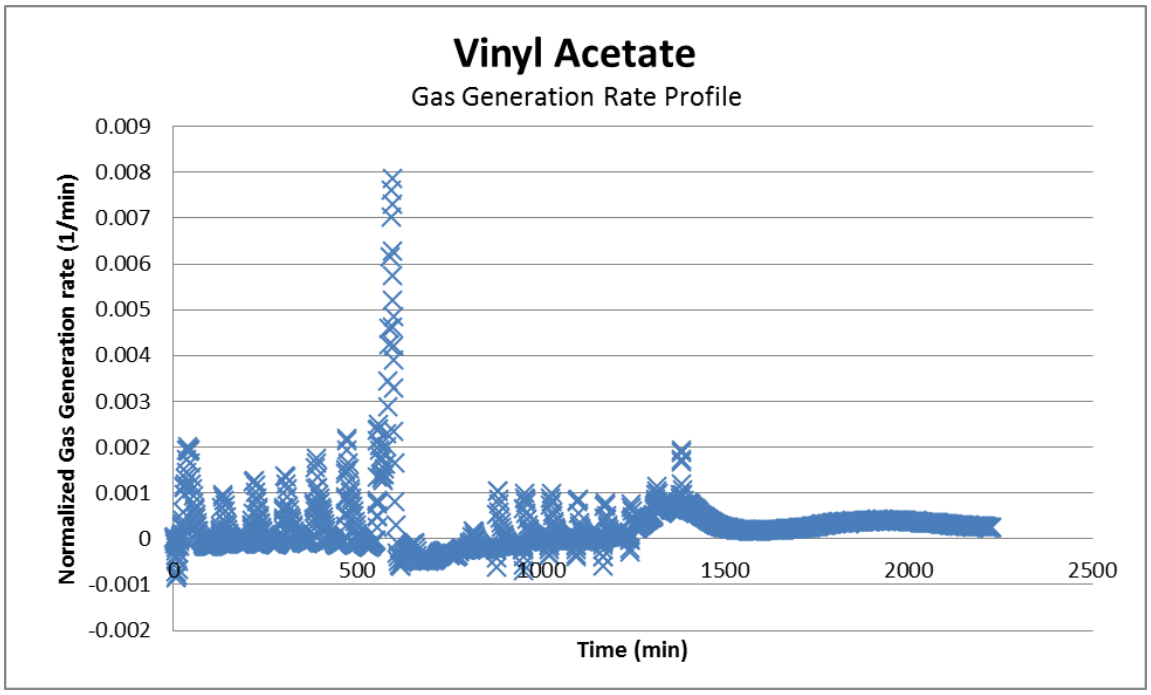

Fig. B.106 Normalized Gas Generation Rate - Vinyl Acetate

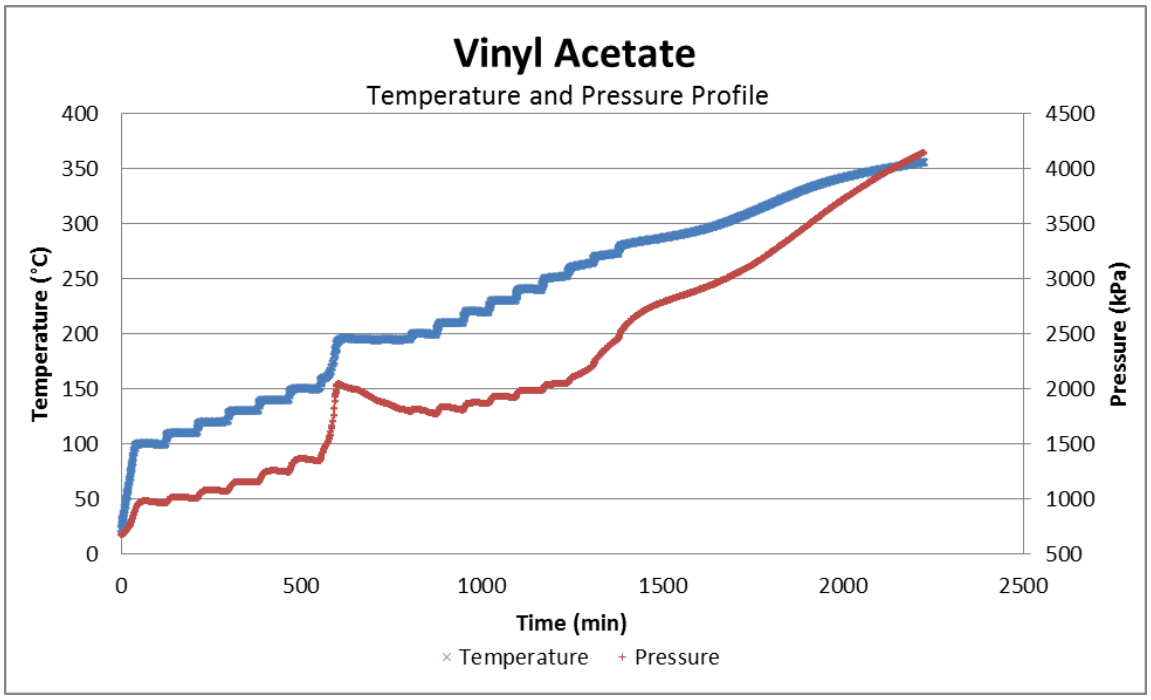

Fig. B.107 Temperature and Pressure Profiles - Vinyl Acetate

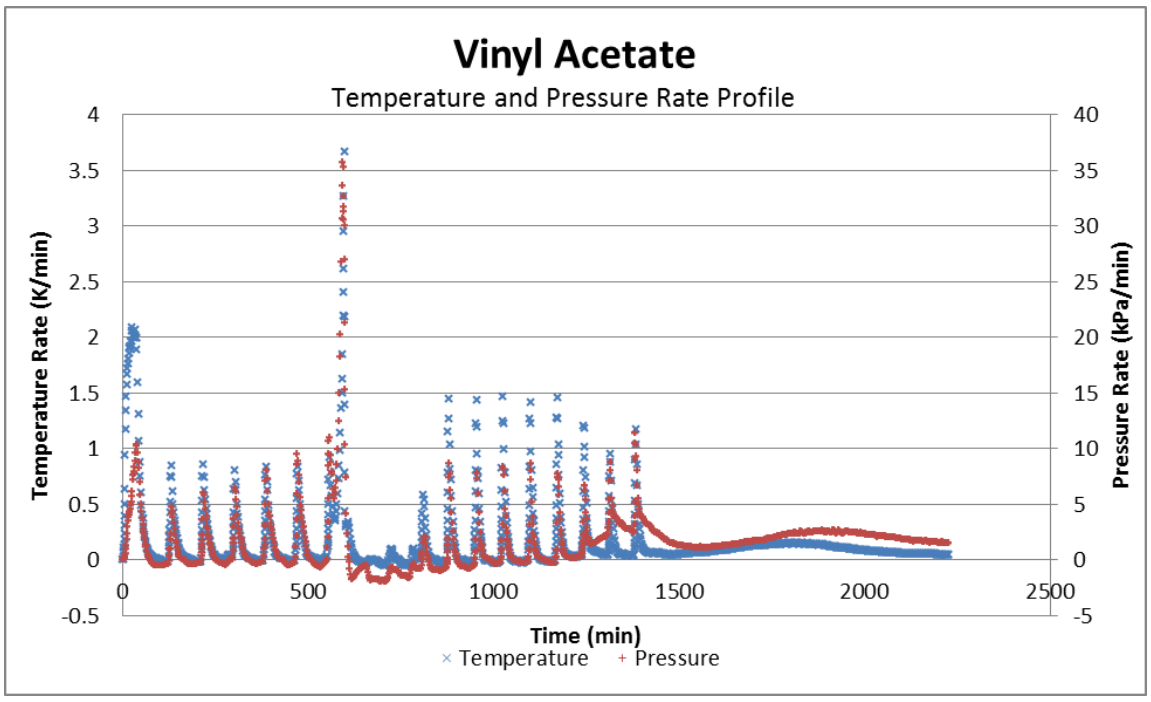

Fig. B.108 Temperature and Pressure Rate Profiles - Vinyl Acetate

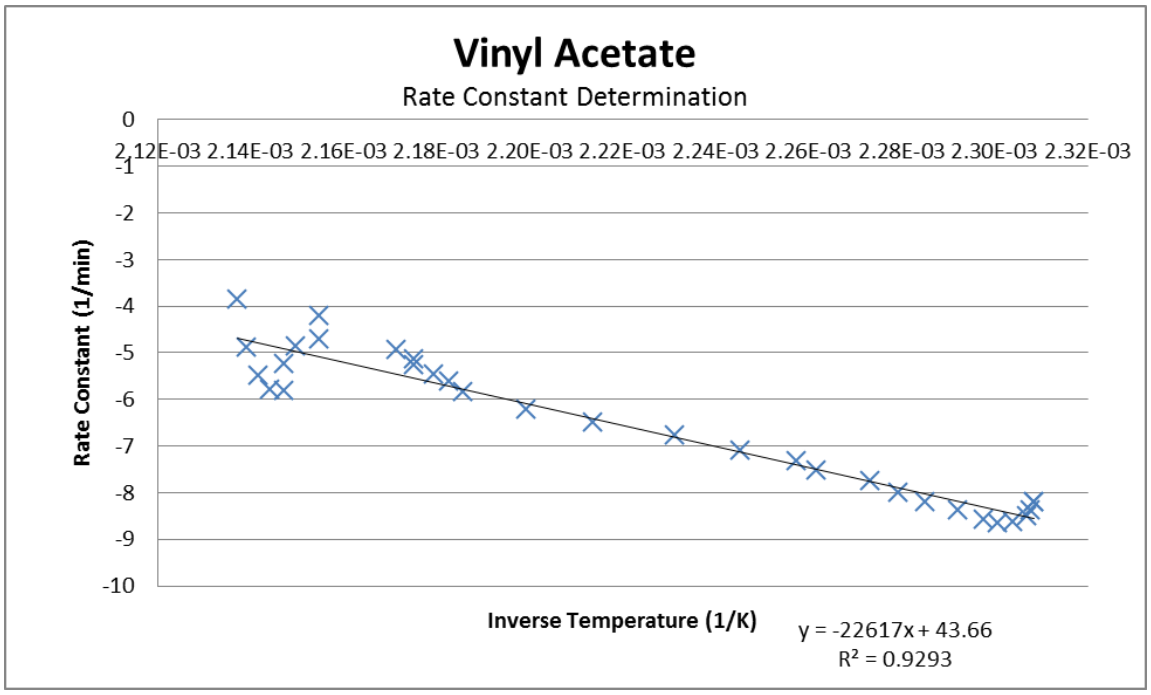

Fig. B.109 Rate Constant Determination - Vinyl Acetate

B.25 Water

Table B.97
Material Properties - Water

Property	Value
m_s (g)	12.82
ρ_s (g/mL)	1
C_s (J/(g*K))	4.184
MW (g/mol)	32

Table B.98
Cell Properties - Water

Property	Value
m_{cell} (g)	51.77
V_{cell} (mL)	96.85
φ	1.811

Table B.99
IPD Properties - Water

Property	Value
A (1/s)	N/A
E_A (J/(mol*K))	N/A
T_{onset} (°C)	N/A
T_{max} (°C)	N/A
ΔH (J/g)	N/A
IPD (W/ml)	N/A

Table B.100
Gas Properties - Water

Property	Value
n_{max} (mol)	4.475E-02
dn/dt_{max} (mol/min)	1.377E-03
n_{maxn}	1.117E-01
dn/dt_{maxn} (1/min)	3.437E-03
GGP (1/min)	3.839E-04

Note – This compound did not exhibit a decomposition reaction so does not include information to calculate IPD.

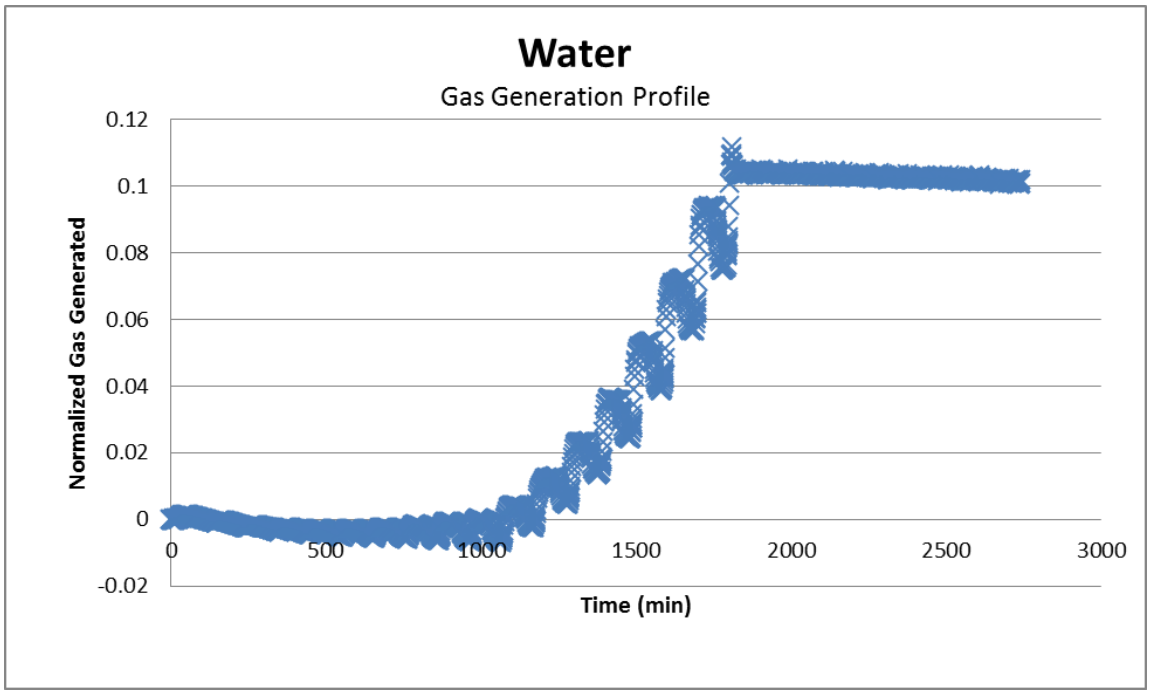

Fig. B.110 Normalized Gas Generation - Water

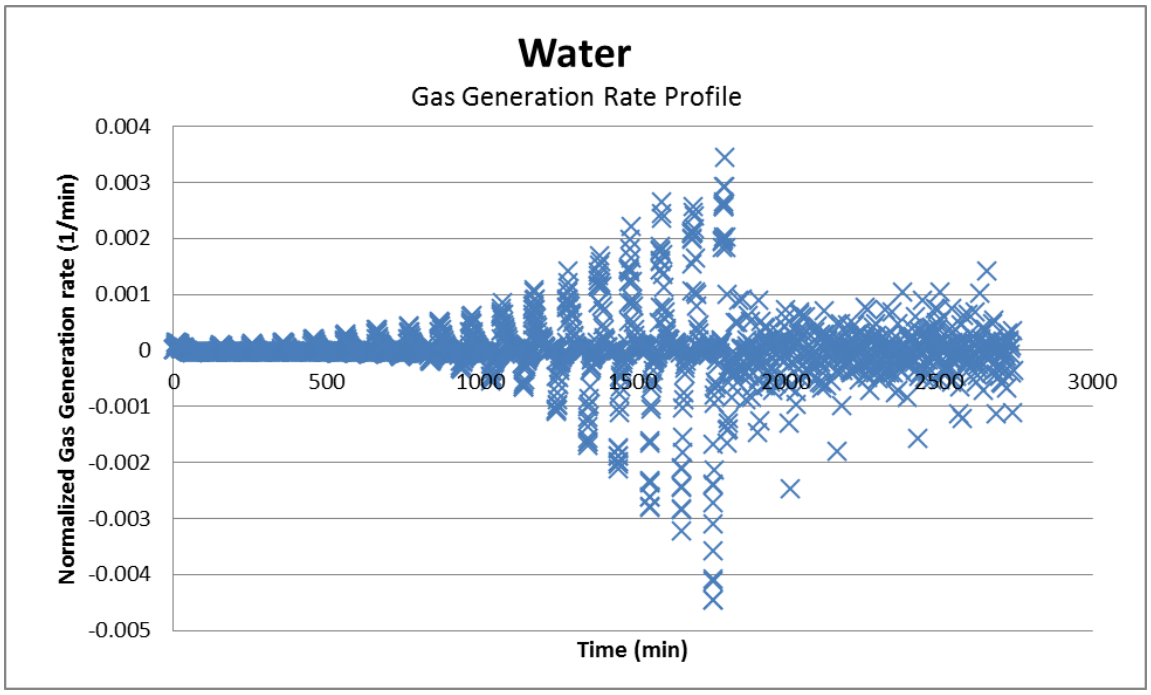

Fig. B.111 Normalized Gas Generation Rate - Water

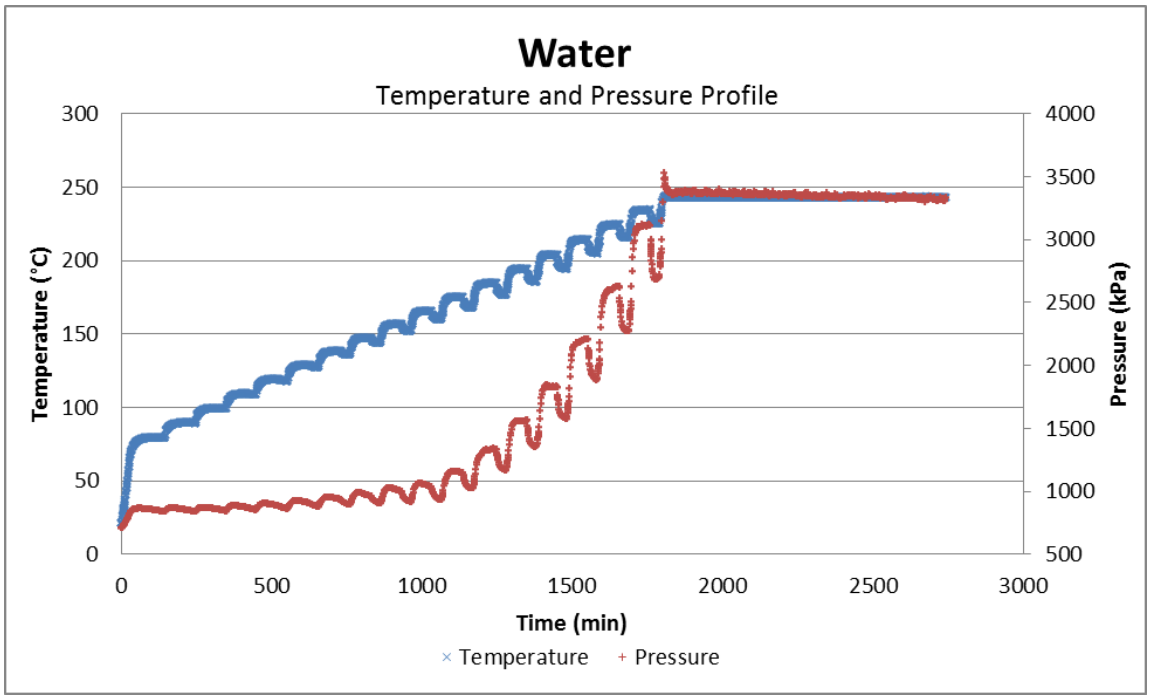

Fig. B.112 Temperature and Pressure Profiles - Water

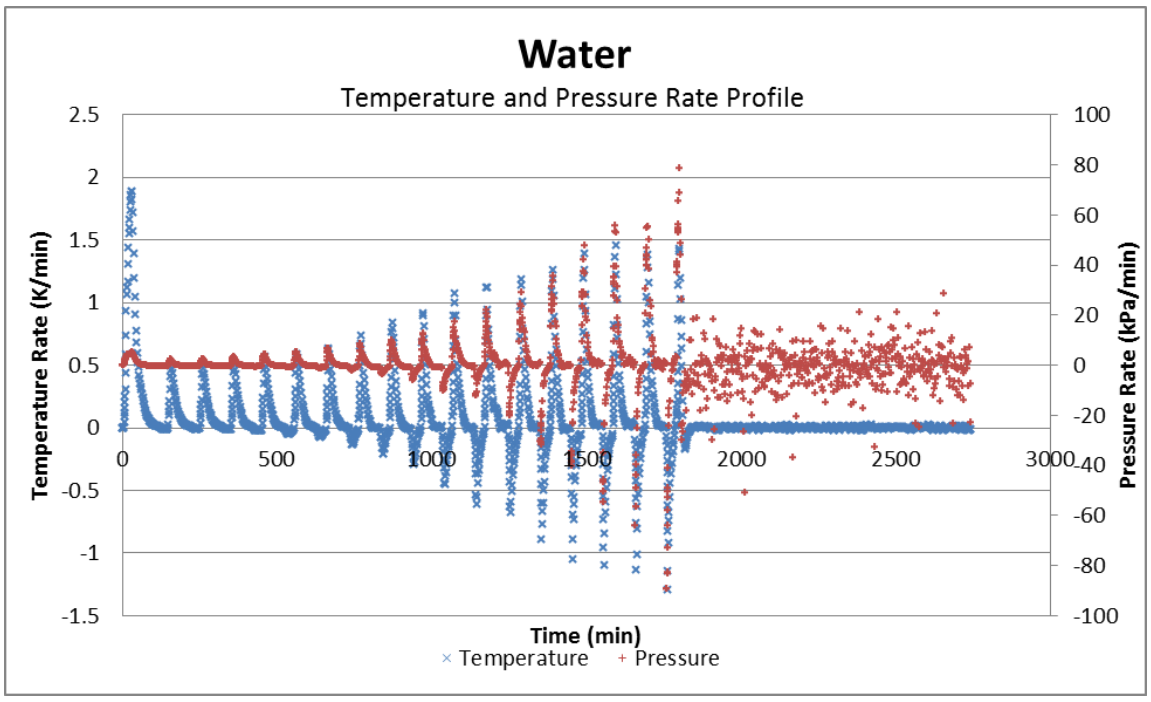

Fig. B.113 Temperature and Pressure Rate Profiles - Water

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