



Protecting America's Future

Y/DZ-2720

## Packaging Materials Outgassing Study Final Report

**Y-12  
NATIONAL  
SECURITY  
COMPLEX**

**R. A. Smith**  
Compatibility and Surveillance  
Technology Development

Issue Date: September 26, 2006

Prepared by the  
Y-12 National Security Complex  
Oak Ridge, TN 37831  
Managed by  
BWXT Y-12, L.L.C.  
for the  
U. S. DEPARTMENT OF ENERGY  
under contract DE-AC05-00OR22800

MANAGED BY  
BWXT Y-12, L.L.C.  
FOR THE UNITED STATES  
DEPARTMENT OF ENERGY

UCN-13672 (11-03)

#### **DISCLAIMER**

This work of authorship and those incorporated herein were prepared by Contractor as accounts of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Contractor, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, use made, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency or Contractor thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency or Contractor thereof.

**PACKAGING MATERIALS OUTGASSING STUDY FINAL REPORT**

R. A. Smith  
Compatibility and Surveillance  
Technology Development  
Building 9202, MS 8097, 576-0615

Issue Date: September 26, 2006

Prepared by the  
Y-12 National Security Complex  
Oak Ridge, TN 37831  
Managed by  
BWXT Y-12, L.L.C.  
for the  
U. S. DEPARTMENT OF ENERGY  
under contract DE-AC05-00OR22800



## TABLE OF CONTENTS

LIST OF FIGURES.....	v
LIST OF TABLES .....	v
ABBREVIATIONS, ACRONYMS, AND INITIALISMS.....	vii
ABSTRACT .....	ix
INTRODUCTION.....	1
DIFFERENTIAL SCANNING CALORIMETRY .....	2
THERMOGRAVIMETRIC ANALYSIS.....	2
OUTGASSING STUDIES.....	3
EXPERIMENTAL .....	3
Materials.....	3
Equipment and Procedure .....	3
DATA AND RESULTS.....	5
BLANK OUTGASSING RESULTS .....	6
FOAM OUTGASSING RESULTS.....	6
TEFLON AND POLYETHYLENE OUTGASSING RESULTS .....	6
OUTGASSING COMPARISONS.....	7
CONCLUSIONS.....	7
REFERENCES.....	22
APPENDIX 1: DATA ANALYSIS .....	23



## LIST OF FIGURES

<u>Figure</u>	<u>Page</u>
1. Stainless steel vacuum container or <i>retort</i> .....	4
2. Red PU thermogram showing thermal transitions at 200°C and 490°C .....	8
3. White PU thermogram showing thermal transitions at 325°C and 560°C .....	9
4. Red PU foam showing three regions of thermal decomposition .....	10
5. White PU foam showing two regions of decomposition .....	11
6. Variation in heating profile from oven may lead to variation in outgassing results .....	12
7. Outgassing pressures from two stainless steel retorts .....	13
8. Outgassing of two red PU foam specimens (8.88 g and 2.98 g) .....	14
9. Outgassing of an 11.06-g specimen of white PU foam .....	15
10. Outgassing of two polytetrafluoroethylene (Teflon) specimens (8.14 g and 12.41 g) competes with measurement noise .....	16
11. Outgassing of an 8.18-g specimen of polyethylene bottle is at noise level and decreases rapidly upon cooling .....	17
12. Outgassing of an 8.3-g specimen of an HDPE bottle lid .....	18
13. Outgassing of an 8.90-g specimen of a black plastic bottle lid, possibly polyethylene .....	19
14. Relative outgassing by polymer types examined .....	20
15. Polyurethane molecular structure .....	21
16. Polyethylene molecular structure .....	21
17. Polytetrafluoroethylene (Teflon) molecular structure .....	21

## LIST OF TABLES

1. Characteristic values for polymer resins and PU foam in this study (Fried, Gibson, and MatWeb) .....	1
2. Heating and cooling profile (Profile 5) for outgassing tests .....	4





## ABBREVIATIONS, ACRONYMS, AND INITIALISMS

PE	polyethylene
PTFE	polytetrafluoroethylene
HAC	Hypothetical Accident Conditions
HDPE	high-density polyethylene
NCS	Normal Condition for Storage
PU	polyurethane
DSC	differential scanning calorimetry
TGA	thermogravimetric analysis
ppm	parts per million
STP	standard temperature and pressure
NRC	Nuclear Regulatory Commission



## ABSTRACT

An outgassing study was conducted on two polyurethane packaging foams, two polymer bottles (polytetrafluoroethylene and polyethylene), and two polymer lids. The purpose was to measure the volume of gases that diffuse from these packaging materials at a maximum of 400°F when stored in ambient air within sealed containers. A specific heating profile was used to measure the offgassing quantities in a set of accelerated aging tests. This set of experiments was designed to duplicate an earlier study conducted in 1991. Thermogravimetric analysis and differential scanning calorimetry tests were conducted to obtain basic information about the polyurethane foams. The polyurethane foams demonstrated the largest degree of outgassing per mass; specifically, the white foam outgassed 50% less than the red foam. The polytetrafluoroethylene and polyethylene materials provided relatively small amounts of outgassing. The polyethylene materials appeared to react further upon cooling, leading to negative outgassing values due to consumption of gas in the container.



## INTRODUCTION

Various materials are required for safely packaging items for transport or storage. Polymeric foams are a common means of protecting items from impact damage. The use of the foams in this study has the added requirement of minimal outgassing such that the closed container is not breached if exposed to fire. The experiments completed here provide measurements of the gases per polymer mass that would be released at elevated temperatures. It is assumed that the major constituent of such gases is water, as polymers have a tendency to adsorb water, particularly if a filler is compounded into the polymeric matrix. Fillers, processing aids, colorants, stabilizers, and other additives are typically added to polymers for mechanical property enhancement (Fried). Little information is available about the composition of the materials in this study.

Another packaging application for polymers includes plastic bottles, used to contain liquids and solid powders. The current study measures outgassing from a Teflon (polytetrafluoroethylene or PTFE) and a polyethylene (PE) bottle, as well as their respective lids. The latter are unknown polymer types, although one is assumed to be high-density polyethylene by its manufacturer's stamp. Table 1 lists some characteristic average values for the polymer resins under study. The polyurethane (PU) foam, also listed in this table, has a significantly low moisture absorption level due to its probable closed cell configuration (MatWeb). PU resin properties vary widely according to the formulation and processing.

**Table 1. Characteristic values for polymer resins and PU foam in this study (Fried, Gibson, and MatWeb)**

Polymer	T <sub>g</sub> (°C)	T <sub>m</sub> (°C)	Density (g/cm <sup>3</sup> )	Water absorption (%)
Polytetrafluoroethylene	-73 (-99°F)	327 (621°F)	2.1	0.01
Polyethylene	-120 (-184°F)	98-135 (208-275°F)	1.0	0.03
Polyurethane	-70 (-94°F)	177 (350°F)	1.2	1.0-38.0
Polyurethane foam	-70 (-94°F)	177 (350°F)	0.45	1.0-5.0

The objective of this project is to heat plastic materials in ramped stages up to 400°F (204°C) and measure outgassing quantities within sealed containers. The goal is to reproduce test results from similar tests done in 1991, as reported in a letter authored by earlier researchers (Tinnel). Data from that document were used in safety documentation submitted in 1991 as characterization for the scenarios called Hypothetical Accident Conditions (HAC) and Normal Condition for Storage (NCS). Starting with the assumption that an item being shipped is contained in a polyethylene bag, it is then cushioned in PU foam. The foam is sealed in a can that is insulated by a lightweight concrete. The concrete is packaged in an outer steel drum that is vented. According to standards set forth by the U. S. Nuclear Regulatory Commission,

- In the HAC scenario, the drum is assumed to burn in a fire for 30 min, and the foam reaches a 300°F (149°C) temperature.
- In the NCS situation, a drum is assumed to sit out in the sun for several days and nights, which means that it is subject to continual temperature excursions between cool and 180°F (82°C).

In both cases, the PU foam will outgas over a short or long time, and it is required not to exceed a pressure that will damage the shipping container and cause the container to be breached. It is assumed that moisture is the major offgassed constituent from this polymer structure, which only degrades beyond temperatures higher than 250°C (Hobbs).

PU foams are typically formulated from a polyol and an isocyanate component, adding a gas or blowing agent to one of these components to achieve the cellular structure. As stated earlier, additional constituents may be among the starting materials, as required in various applications. The original PU foam is a reddish-orange polyurethane formulated from Dow Chemicals components and was used for shipping protection until Dow decided to no longer manufacture this material. A white PU foam is now being considered to replace the earlier type and has components produced by BJB Enterprises, Inc. Both PU foams are tough and rigid and feature a nonporous skin where the foam apparently contacted the mold walls. There was random variability between the ratio of foam to skin in the specimens cut initially; smaller samples tended to have a larger fraction of skin. Care was taken to cut specimens from the mass of the foam, as the skin can demonstrate different properties; these foams are essentially composite materials (Broos). The density of the red foam specimens ranged from 0.45 to 0.50 g/cm<sup>3</sup> in the experiments discussed here. The density of the white foam material ranged from 0.27 to 0.49 g/cm<sup>3</sup>. The polyethylene bottle is an opaque white material and has a density typically similar to water (1.0 g/cm<sup>3</sup>). Teflon material typically has a density of 2.1 g/cm<sup>3</sup>; this bottle has a smooth waxy texture.

Preliminary examination of the two foams was done using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) in order to characterize some thermal properties. Figures 2 through 5 present the data. Figures 6 through 13 provide the outgassing data in this study. Figures 14, 15, and 16 comprise the basic molecular structures of these polymers.

## DIFFERENTIAL SCANNING CALORIMETRY

DSC is an analytical method that measures the quantity of heat flow required to maintain a reference and sample at a particular temperature. The specific heat of the sample is then determined over a temperature range, giving information about phase transitions, kinetic processes, and other thermal attributes (Kämpf). The PU foams undergo some type of transition, cell softening or a glass transition, near 200°F (93°C); however, the presence of additives such as flame retardants, catalysts, or antioxidants could also have an effect on the DSC output. The red foams and white foams begin melting at 480°F and 560°F, respectively (250°C and 293°C).

## THERMOGRAVIMETRIC ANALYSIS

TGA was run on each polymer, and weight loss was tracked as a function of temperature. The structure of PUs typically begins degradation between 250 and 350°C (480–660°F). The red PU demonstrates three regions of decomposition at 480°F, 553°F, and 696°F. The white PU only gives evidence of two decomposition processes, at 562°F and 689°F. The 550–560°F temperature is where polymer bridges begin to break and re-form into a secondary polymer structure; over 600°F, the secondary polymer structure breaks down as well. In the case of the red PU, the early decomposition is possibly loss of some additive. In both cases, the initial 1–2% weight loss corresponds well with the loss of moisture.

## OUTGASSING STUDIES

During the outgassing study, samples of polymeric packaging materials were placed in vacuum-sealed stainless steel containers (retorts). Each retort was then attached to a capacitance manometer or "baratron" for direct measurement of the internal container pressure as the temperature was increased. This method allows tracking of the volatiles emitted from the materials, which are thought to mainly comprise moisture but also decomposition products at sufficiently high temperatures. While absorbed moisture is not immediately apparent under ambient conditions, the water contained in packaging is available to diffuse out over long time frames, such as years. Controlled heating provides a method to ascertain the maximum amount of outgassing from a material mass. This study provides information about the outgassing of volatiles in the situation combining elevated temperatures with the presence of air.

After the polymer specimens were loaded into retorts, the open or "free" volume within the containers was calculated. This study was initiated in the presence of atmospheric moisture and air pressure with a single absolute pressure gauge established to monitor the pressure as the temperature was ramped to a 204°C (400°F) maximum. Outgassing pressures are the sum of those gases emitted from the polymer specimen and retort, in addition to the air trapped inside the retort. The pressure gauge used has a maximum measurement range of 10,000 torr and was located outside the oven. The actual measurement volume included the retort headspace and the 24-in. flexible stainless steel hose used to connect the sample retort in the oven to the measurement device. An additional 1000-torr baratron was used as a reference to provide a measurement of the ambient pressure in the laboratory.

## EXPERIMENTAL

### Materials

The Packaging Engineering group provided the following test items for this study:

1. orange/dark red polyurethane foam in blocks (111.58 g)—this material had been formulated using components from Dow Chemical;
2. off-white polyurethane foam in blocks (168.8 g)—this material was formulated with components known as BJB280;
3. a clear/translucent Teflon (polytetrafluoroethylene) bottle capped with a white plastic lid labeled "Nalgene," possibly made of high-density polyethylene; and
4. an opaque polyethylene bottle capped with a black plastic lid, probably polyethylene.

Samples of random sizes and weights were cut using a blade or large scissors. Care was taken to exclude the skin from the foam materials being tested. Specimens were cut and weighed immediately before being sealed into a vacuum container. The total weight of pieces placed into a particular container was recorded in grams.

### Equipment and Procedure

Standard vacuum hardware was used to seal randomly sized specimens of each material (weighing from 8 to 12 g) in air after these were weighed on a calibrated scale. (For the two PU foams, the experiment had been repeated with smaller masses.) Additionally a "blank" container was tested over the temperature range. This blank served to provide a baseline outgassing level for the container. The oven was programmed to heat to specific temperature plateaus and hold for a specified time period

before ramping linearly to the next temperature. The temperature profile, named “Profile 5,” is described in Table 2. Despite the programming of the oven to cool to 50°F, its minimum temperature after heating was about 110°F; to cool the oven to room temperature the oven door was opened, which allowed free circulation of air into the heating zone.

**Table 2. Heating and cooling profile (Profile 5) for outgassing tests**

Temperature setting		Duration of ramp or hold
77–150°F	25–65°C	1-h ramp
150°F	65°C	2-h hold
150–200°F	65–93°C	1-h ramp
200°F	93°C	2-h hold
200–250°F	93–121°C	1-h ramp
250°F	121°C	2-h hold
250–300°F	121–149°C	1-h ramp
300°F	149°C	4-h hold
300–350°F	149–177°C	1-h ramp
350°F	177°C	4-h hold
350–400°F	177–204°C	1-h ramp
400°F	204°C	4-h hold
400–111°F	204–44°C	2-h ramp
111°F	44°C	Lower oven limit
77°F	25°C	Oven opened to lab

It should be noted that during the test period the test laboratory experienced continual temperature swings between 56 and 80°F (13–27°C). This range is typical for this laboratory and can cause random noise in the data under collection. For example, according to its specifications, the Despatch oven control stability is  $\pm 0.5^\circ\text{C}$  per  $5^\circ\text{C}$  change in ambient temperature. The signal conditioner and display have linearity and accuracies in the parts per million (ppm) range per degree  $^\circ\text{C}$ , but the combination of these small variations provides a visible noise level at extremely small outgassing levels.

The containers were constructed of stainless steel and bolted with the use of a copper gasket between 2.75-in. conflat flanges (Fig. 1). The assembly was completed with ¼-in. VCR® fittings and Swagelok or Nupro valves, using silver-plated nickel gaskets to seal interfaces.



**Fig. 1. Stainless steel vacuum container or retort.**



Pressure measurements were conducted using an MKS Instruments Type 690A14TRB 10,000-torr baratron providing output to an MKS 670 signal conditioner electronics unit. The baratron had an accuracy of 0.12% of reading and operates with a 59–104°F (15–40°C) ambient temperature span. The signal outputs were processed using a program called “Generic Application for Reading Pressure Gages for Import into Excel,” and data were collected using LabView software on a laboratory computer. Data were downloaded from this computer for storage and analysis on an office personal computer.

The heating procedure displayed in Table 2 was conducted in a Despatch LAC 1-67-6 programmable laboratory oven that uses a Protocol Plus microprocessor control. A thermocouple was used to separately track and write the oven temperature to the aforementioned LabView program.

#### Experimental Steps

- Clean stainless steel retorts using isopropanol and wipe dry. Allow to air dry for 24 h.
- Cut and weigh polymer samples in atmosphere.
- Document material type, sample name, and weight.
- Place polymer pieces in stainless steel retort; label retort with sample name.
- Bolt container to conflat flange using a copper gasket and six bolts.
- Store retorts near Despatch oven until testing could be conducted.
- Select random retort for test; use nickel gasket to connect container to flexible tubing inside oven.
- Record pressures from baratrons measuring ambient and experimental pressures; these should be equivalent before test.
- Open National Instruments program and establish data collection mode and sampling rate (in data points per minute).
- Check data readout from signal conditioner and thermocouple.
- Check data download to personal computer via Labview program using Excel.
- Open sample retort valve.
- Turn oven on and load Profile 5; select Run.
- Periodically check system to ensure that data are being collected as planned.
- At end of test, record pressures according to both ambient and experimental baratrons; note oven temperature.
- Turn off oven and open oven door.
- Allow pressure to reach a new “ambient” equilibrium, and again record pressures.
- Close sample retort valve.
- Unbolt sample retort, and reserve for possible headspace gas analysis.
- Download data immediately in Excel \*.csv format.
- Stop data collection program.

## DATA AND RESULTS

The data were collected, then downloaded and analyzed using Microsoft Excel. The raw data were recorded as pressure in units torr as a function of time; temperature in degrees centigrade was also tracked as a function of time. For all materials, charts were later calculated to provide outgassing volume in  $\text{cm}^3(\text{STP})/\text{g}$  and temperature in degrees Fahrenheit from ambient to 400°F, as a function of elapsed time (duration in hours). Blank data were used to calculate the moles of outgassed species

contributed by the sample container and other system components. Appendix 1, *Data Analysis*, provides additional detail on data processing.

## **BLANK OUTGASSING RESULTS**

Two empty containers (blanks 1 and 3) were subjected to the same temperature profile in separate tests. Outgassing patterns shown in Figs. 6 and 7 provide a guide to the variation in (a) oven runs at different times and (b) blank outgassing under identical temperature profiles. The oven temperature was observed to vary as much as 5% at the same temperature setting. In concert with this, the blank outgassing pressures varied from each other by -0.25 to 4.2% in these tests. An analysis shows a 0.58 correlation of pressure to temperature variation between these two experiments. The other significant variable that can cause variation in outgassing between the two seemingly identical blanks is dimensional variations. The container volume difference (observed to be <2%) will lead to pressure discrepancies for identical gas quantities. In the current tests, molar quantities were calculated using container data developed through successive gas expansions to measure their volumes.

## **FOAM OUTGASSING RESULTS**

The results from two red foam specimens are averaged in Fig. 8, where the specific volume of outgassing from each specimen is plotted with the temperature in degrees Fahrenheit. This normalized value is cited as specific volume at standard temperature and pressure (STP), providing the volume per specimen mass at standard temperature (273 K) and pressure (1 atm); the specific volume =  $V/g = (nRT/p)g^{-1}$ . It can be noted that the magnitude of outgassing is comparable to the 1991 data, but perhaps slightly less due to the material outgassing over time in storage. The experiment described here increases the temperature range and time of outgassing, so larger ultimate values than those of 1991 are observed. As well, the ramping and hold times were longer in the current experiment. The white foam outgassing quantities are shown in Fig. 7, and while on the same order of magnitude as the red PU, this material appears to produce only half the overall quantity of outgassed species. Both materials had continually increasing outgassing of volatiles at the highest test temperature, indicating that decomposition has started rather than outgassing has been seen at lower temperatures. The molecular structure of polyurethane includes an ester linkage that is subject to hydrolysis. Although some PU has a large moisture content, rigid foams typically have no more than 5% moisture. In this study, the red PU demonstrates about 1.2 wt % and the white foam 0.5 wt % moisture.

## **TEFLON AND POLYETHYLENE OUTGASSING RESULTS**

The polytetrafluoroethylene and polyethylene materials outgassed relatively little, making it difficult to detect outgassing due to the heated container and that arising from the polymer alone. In other words, the final plots (Figs. 11-13) show a great deal of noise. It could be concluded that these materials would not present a large consideration for their outgassing potential in a heated situation. Their polyolefin structure does not attract moisture to the degree of the ester group in the PU structure. An interesting feature of the polyethylene materials is observable as the test vessel is cooled to room temperature. These experiments actually went into a negative pressure status, indicating that a reaction was taking place that consumed the gas phase inside the container. It is recognized that polyolefins degrade in air by oxidative reactions (Boenig). A mechanism for pressure decrease occurs if oxygen present in the original headspace reacts with the polymer and suppresses outgassing, even

during the heating cycle. Polymers also degrade by fragmentation, producing free radicals, which can then continue to react with one another (cross-linking). During a cooling of this system, these moieties would have reduced mobility, thereby increasing the probability of reaction with the gas phase. An analysis of the headspace would provide a means to study the remaining constituents.

## OUTGASSING COMPARISONS

Figure 14 sets forth a straightforward comparison of outgassing quantities. The maximum and minimum amounts of gas are calculated for various samples after the background quantities are subtracted. These were weighted by the specimen mass and plotted on a bar chart as moles per gram of polymer specimen. The PUs demonstrated a larger outgassing of volatile species per mass, in comparison to PE and PTFE. Again, it is interesting to note the negative outgassing values in the case of PE minimums.

## CONCLUSIONS

The next experimental procedure would be to conduct a gas analysis of the headspace on each container. The Y-12 National Security Complex Plant Laboratory is the best resource to complete this task. This would pinpoint the identity of outgassed species and provide a guide to ascertaining chemical reactions taking place in the solid-gas interface. This certainly would verify that reactions between the oxygen and polymer fragments have occurred.

Another stage would be to clearly identify the identity and manufacturer of each material, including the age, ingredients, and processing steps. Processing information for each polymer would assist in explaining the DSC and TGA output, if such an effort is desired. The response of a polymer to its environment involves its constituents, processing history, and treatment in storage. The large range of polymer properties, including outgassing, is due to these variables.

It can be concluded that PU foams absorb and outgas moisture to a larger extent than the polyolefins, as expected according to their respective molecular structures. This is also reflected in the literature absorption values. The white PU outgassing is no more likely to cause a shipping container breach than the red PU outgassing in the Nuclear Regulatory Commission (NRC) scenarios. The red PU outgassed a specific volume per mass similar to that quantity derived in the 1991 study.

Sample: orange rose  
Size: 8.8200 mg

DSC

File: C:\ATAData\DSC\orange rose.001  
Operator: Lisa T  
Run Date: 12-Jan-06 08:21  
Instrument: 2920 MDSC V2.6A

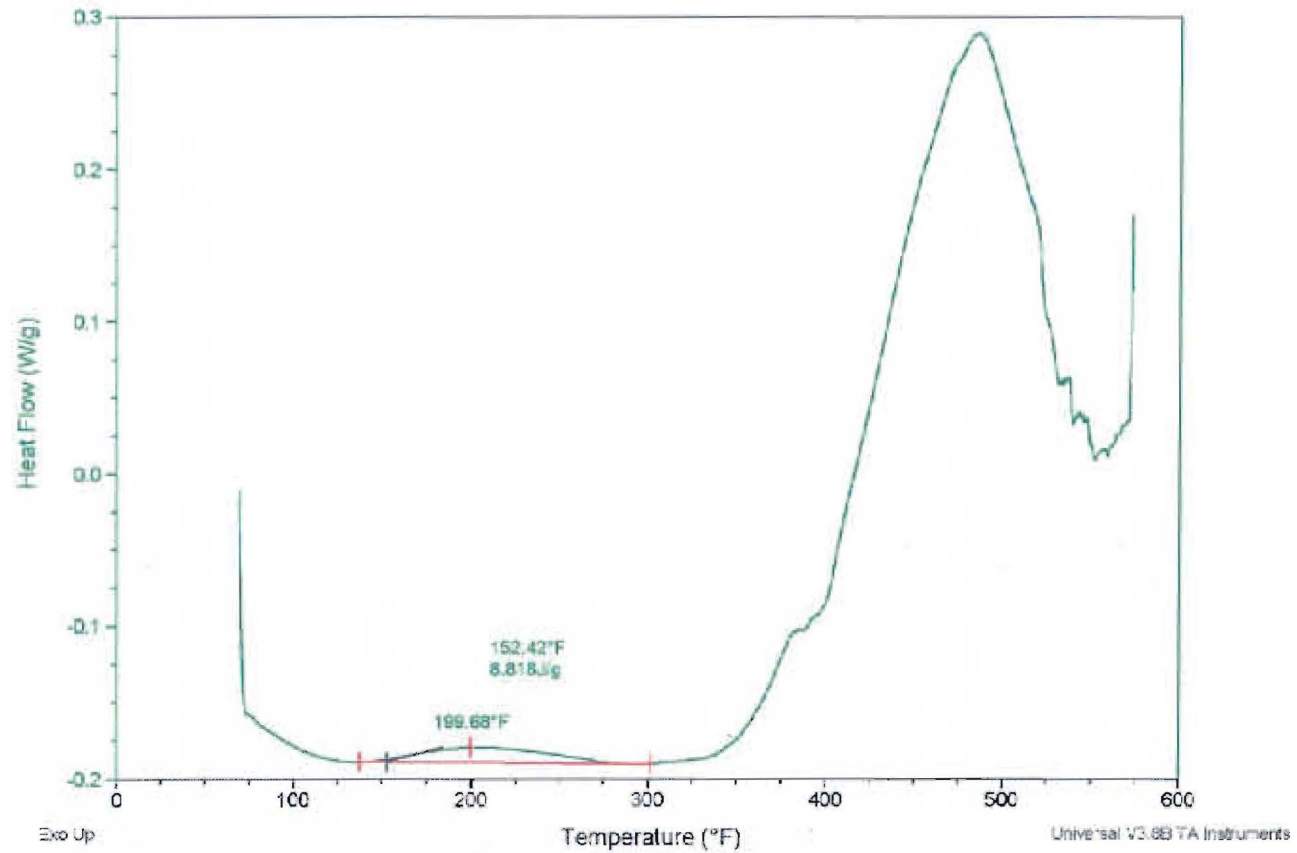


Fig. 2. Red PU thermogram showing thermal transitions at 200°C and 490°C.

Sample: white rose  
Size: 18.4400 mg

DSC

File: C:\TA\Data\DSC\white rose.001  
Operator: Lisa T  
Run Date: 11-Jan-06 12:48  
Instrument: 2920 MDSC V2.8A

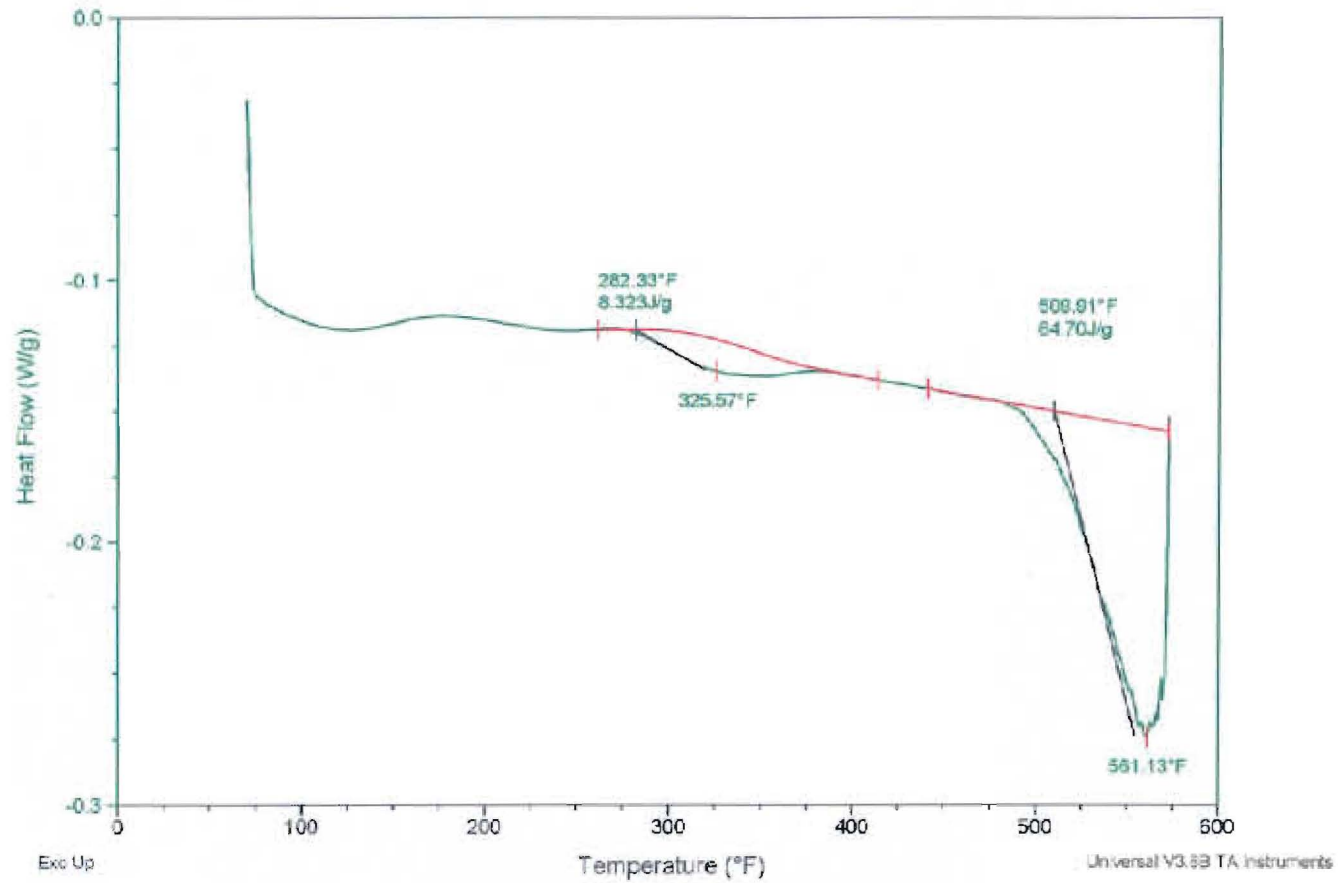


Fig. 3. White PU thermogram showing thermal transitions at 325°C and 560°C.

Sample: orange rose  
Size: 11.9360 mg

### TGA

File: C:\TA\Data\TGA\orange rose 001

Run Date: 12-Jan-06 08:22  
Instrument: 2950 TGA HR V6.1A

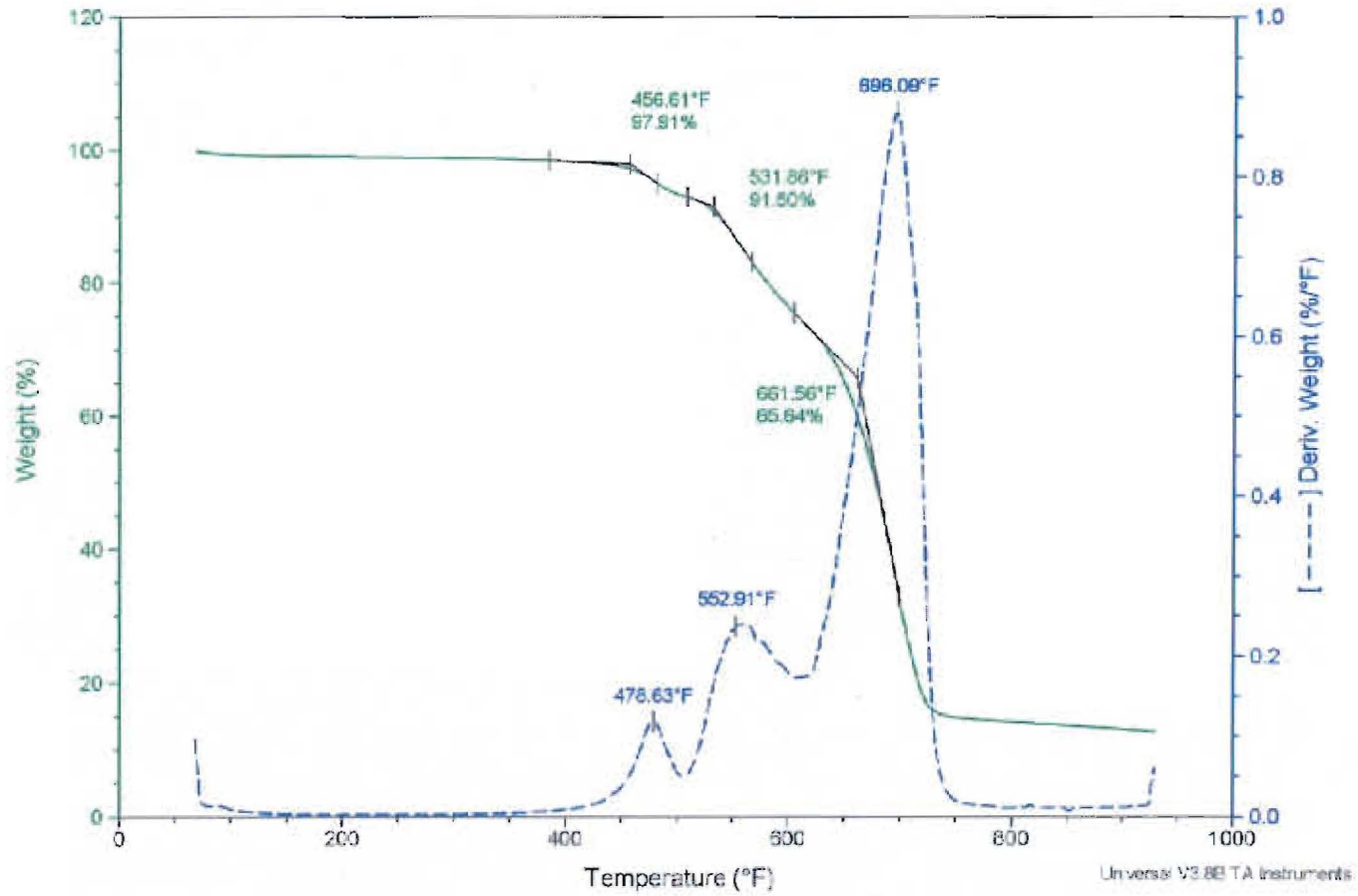


Fig. 4. Red PU foam showing three regions of thermal decomposition.

Sample: white rose  
Size: 23.4890 mg

### TGA

File: C:\TA\Data\TGA\white rose 001

Run Date: 11-Jan-06 12:48  
Instrument: 2950 TGA HR V6.1A

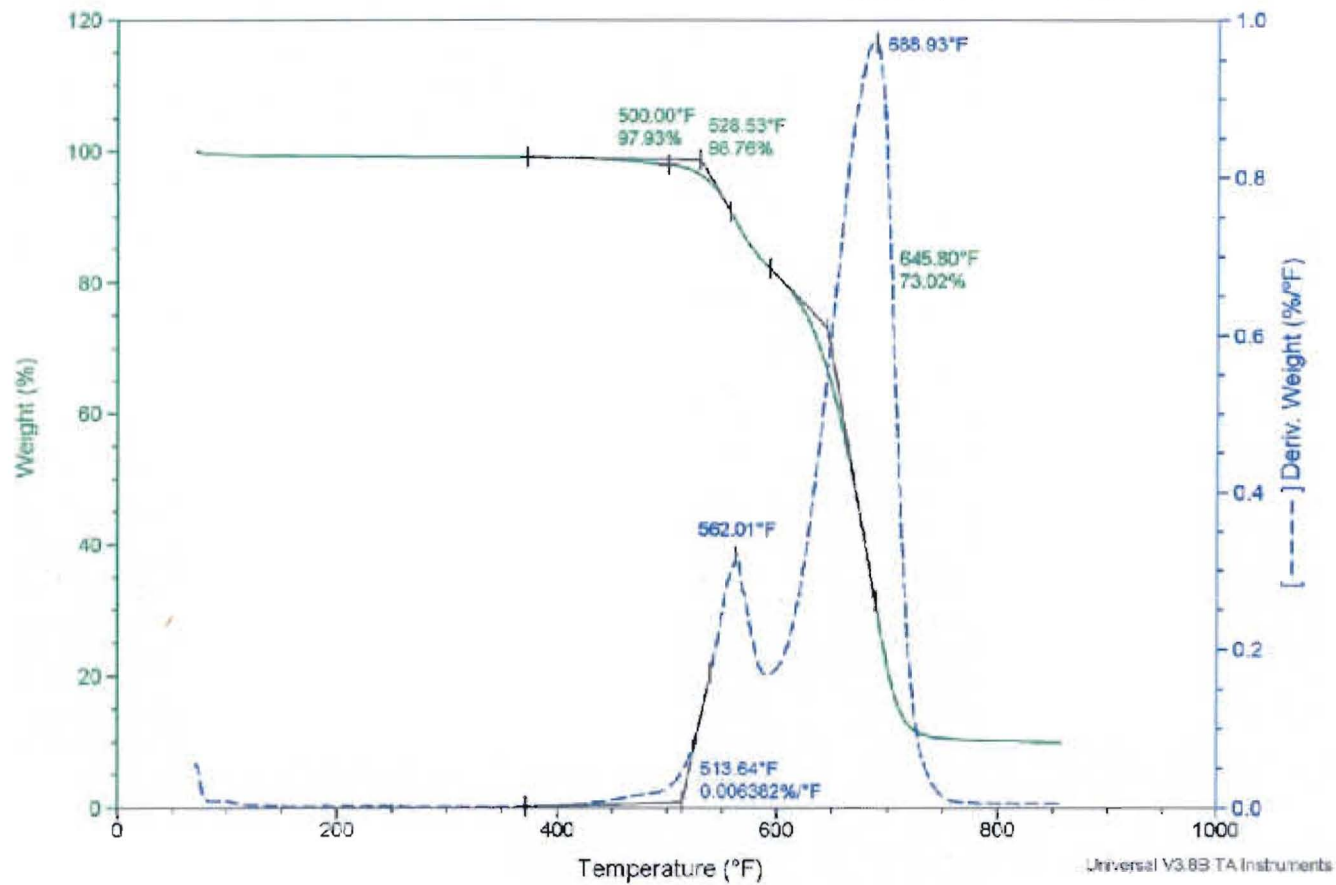


Fig. 5. White PU foam showing two regions of decomposition.

### Temperature Profile Variations for Blank 1 and Blank 3 Tests

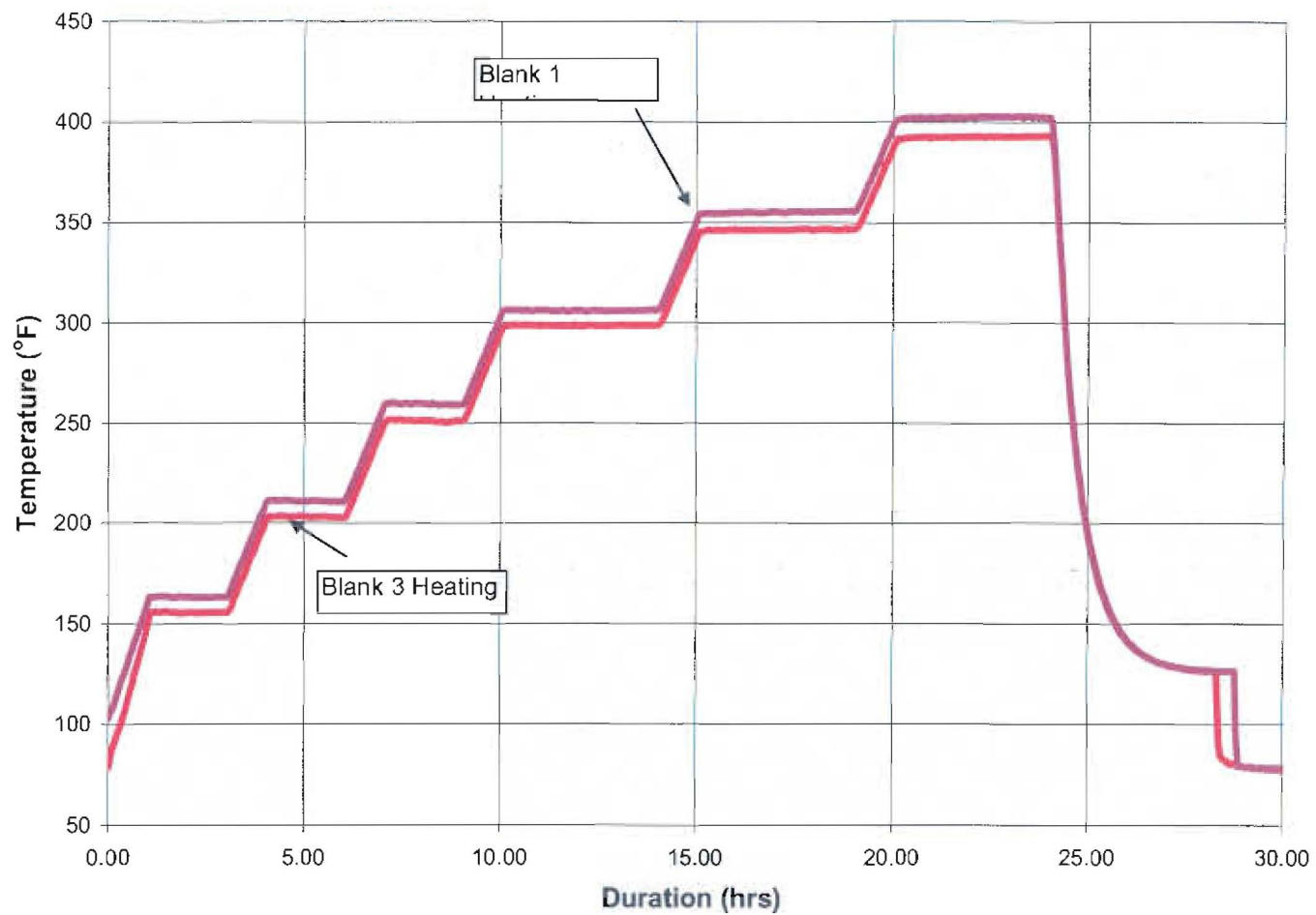


Fig 6. Variation in heating profile from oven may lead to variation in outgassing results.



### Outgassing Pressure from Empty Stainless Steel Retorts

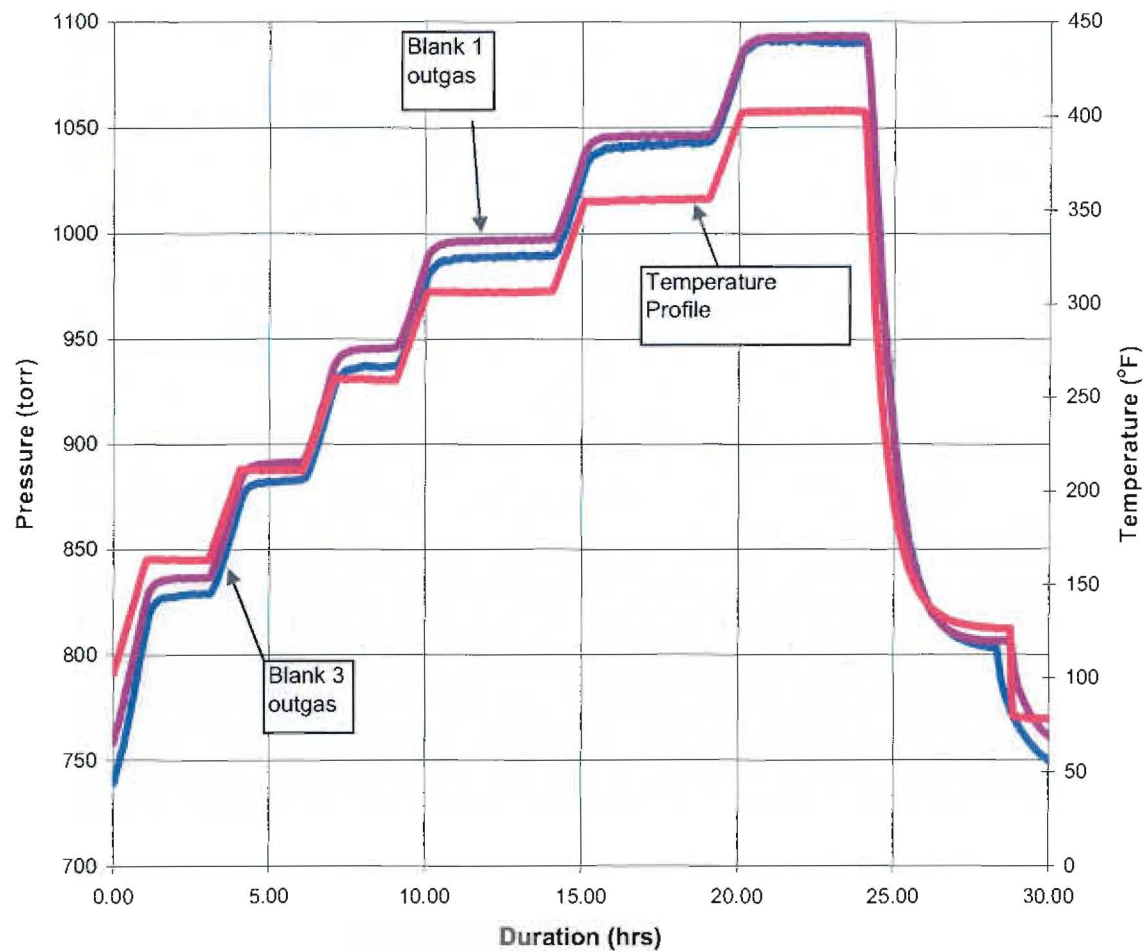


Fig. 7. Outgassing pressures from two stainless steel retorts.

### Red Foam Outgassing Quantities

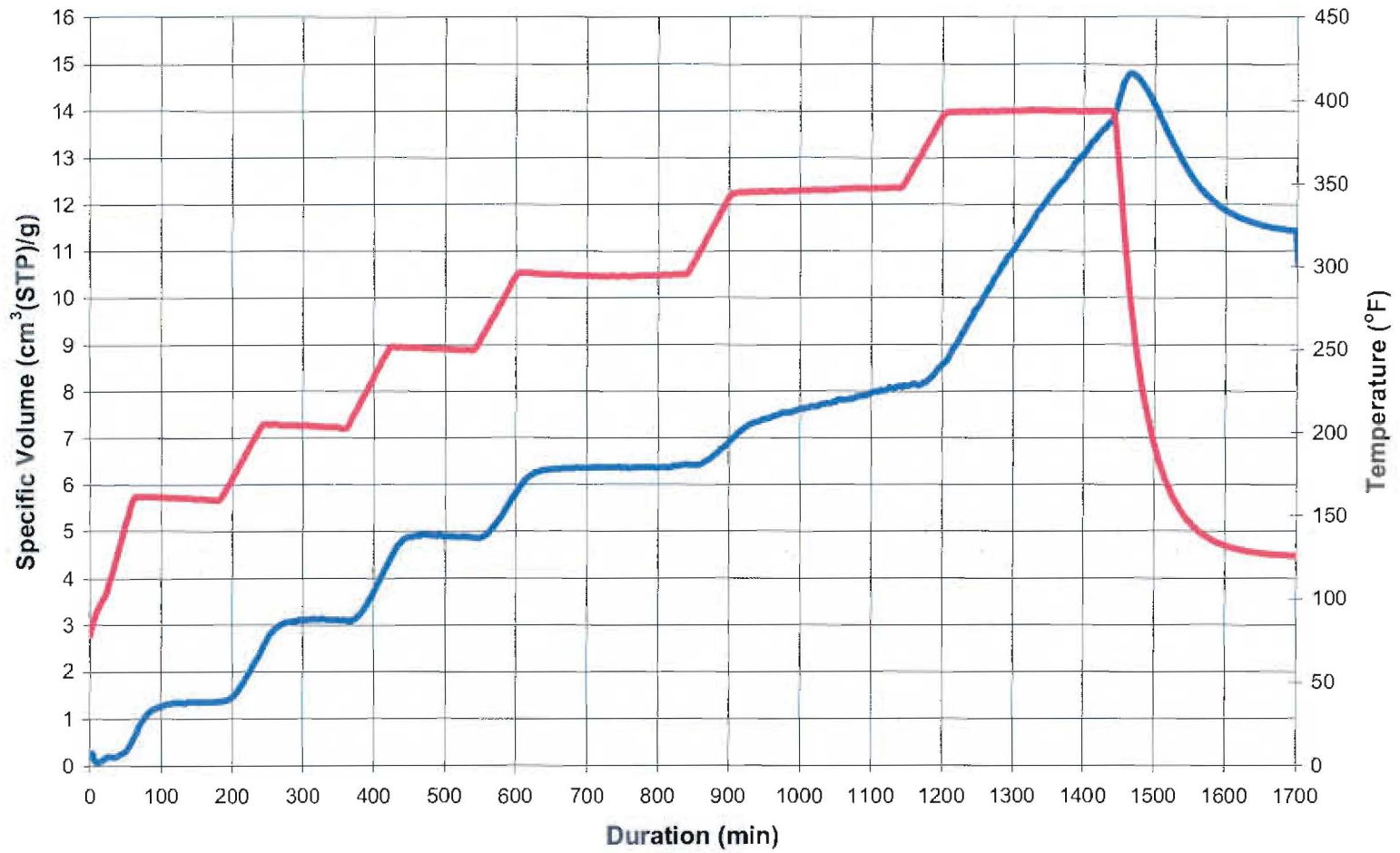


Fig. 8. Outgassing of two red PU foam specimens (8.88 g and 2.98 g).

### White Foam Outgassing Quantities

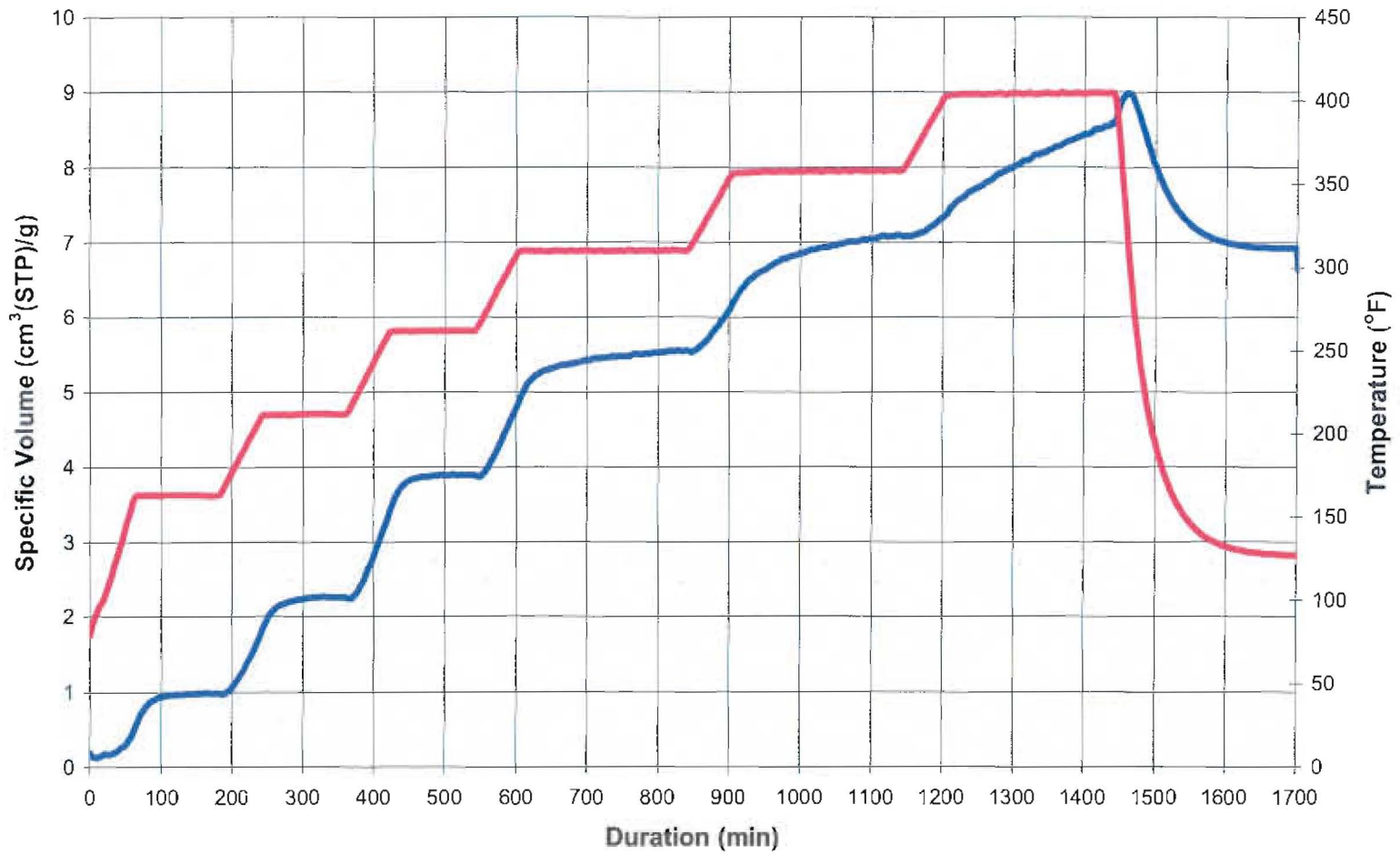


Fig. 9. Outgassing of an 11.06-g specimen of white PU foam.

### Polytetrafluoroethylene "Teflon" Outgassing Quantities

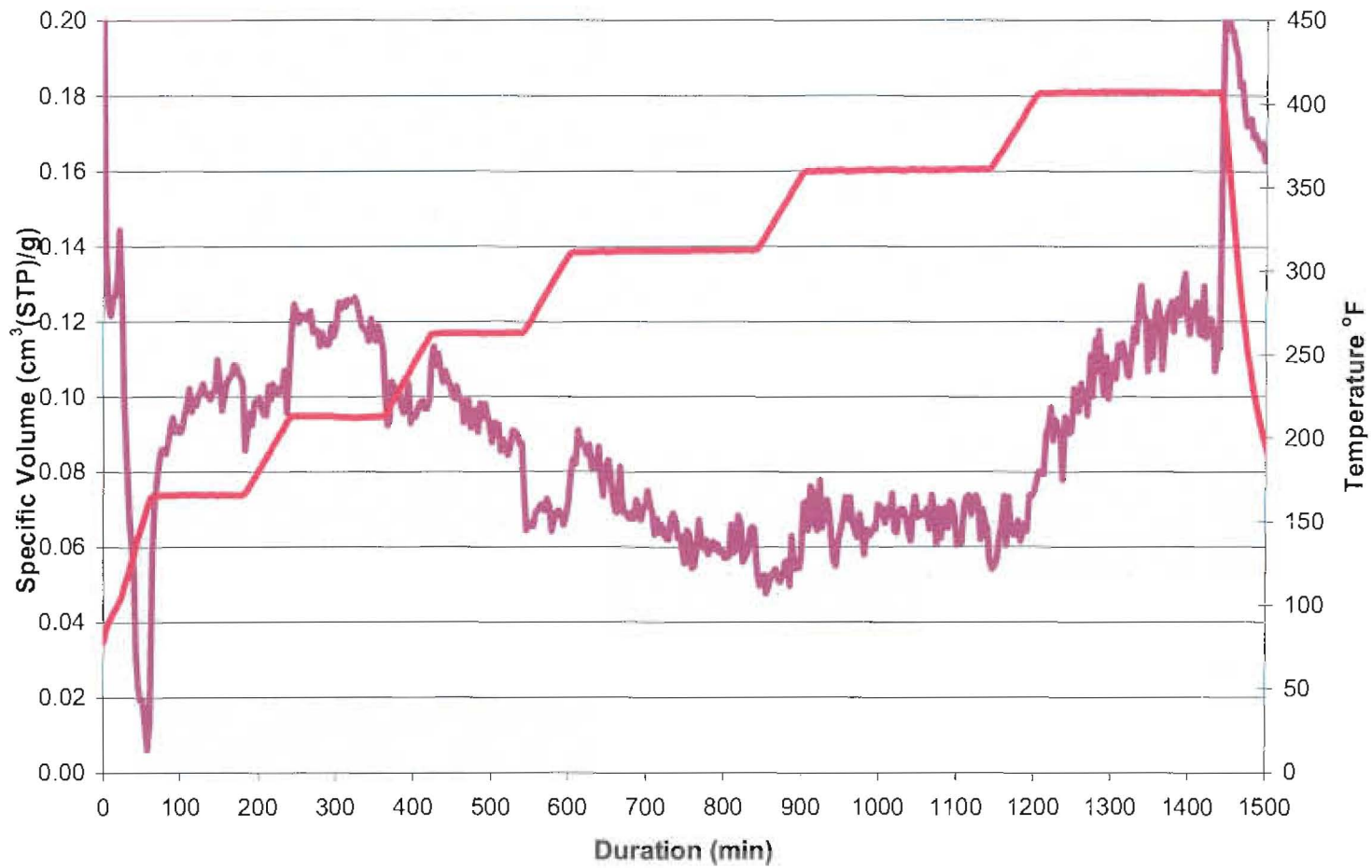


Fig 10. Outgassing of two polytetrafluoroethylene (Teflon) specimens (8.14 g and 12.41 g) competes with measurement noise.

### Polyethylene Outgassing Quantities

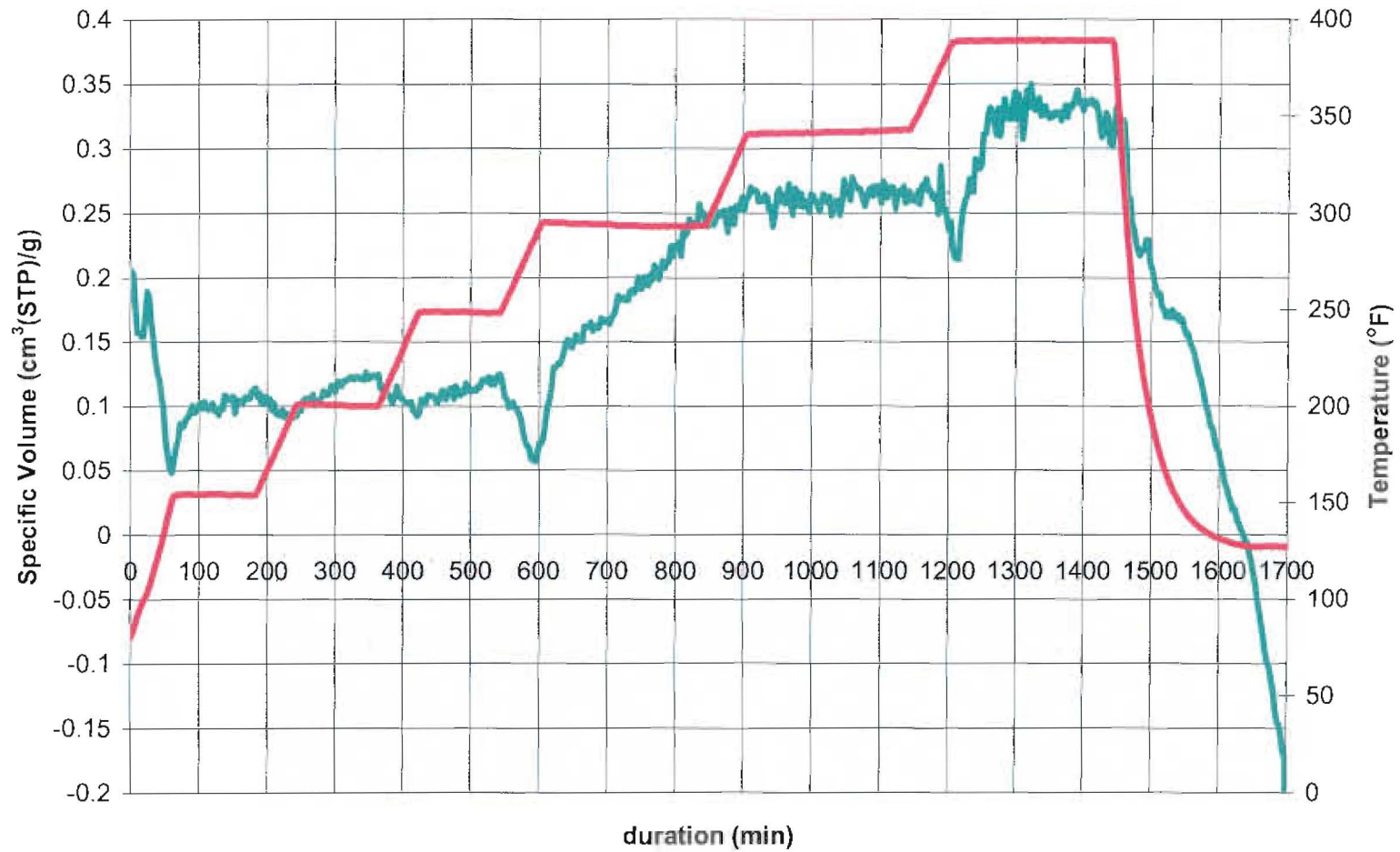


Fig. 11. Outgassing of an 8.18-g specimen of polyethylene bottle is at noise level and decreases rapidly upon cooling.

### High Density Polyethylene Outgassing Quantities

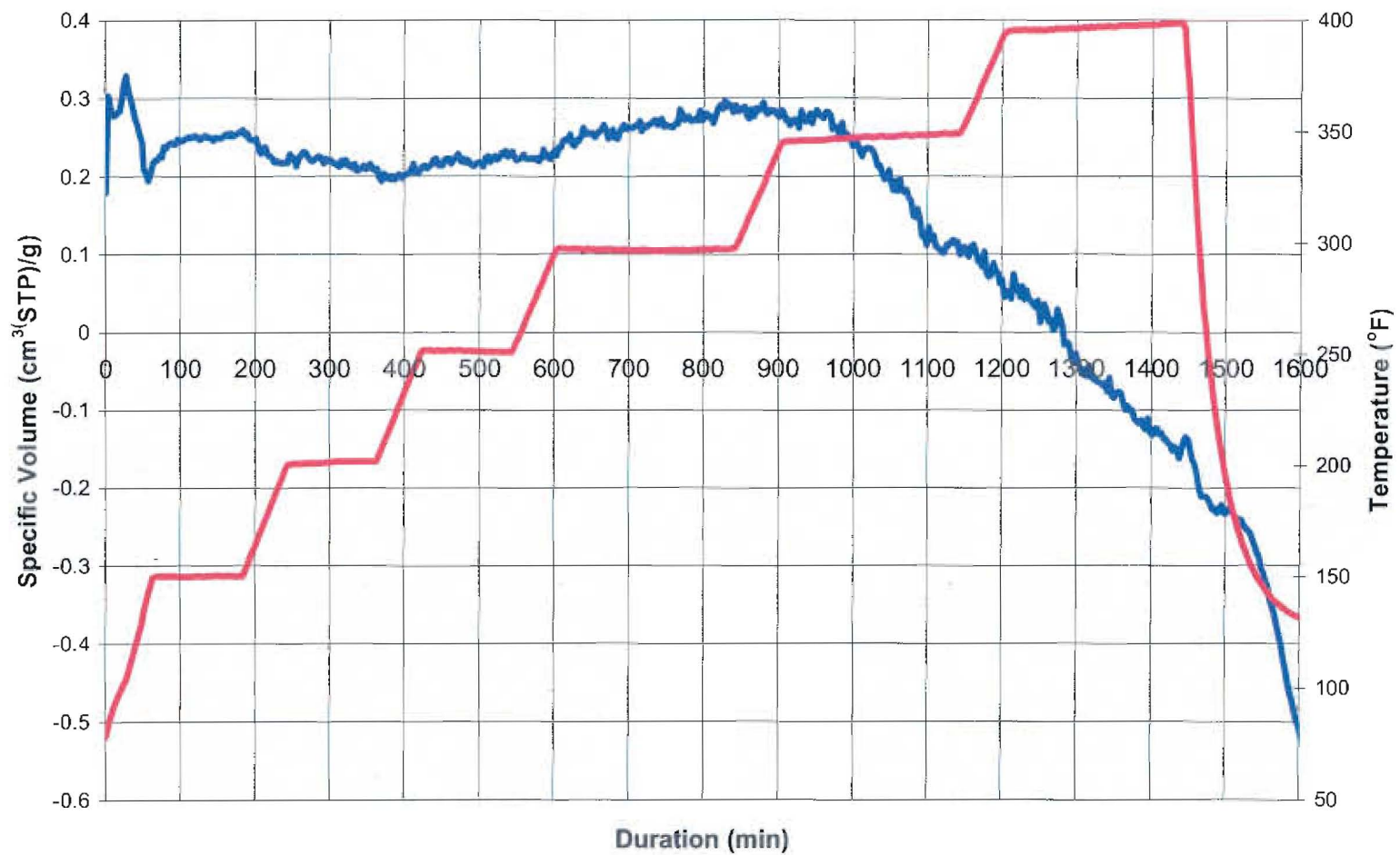


Fig. 12. Outgassing of an 8.3-g specimen of an HDPE bottle lid.

### Black Lid Outgassing Quantities

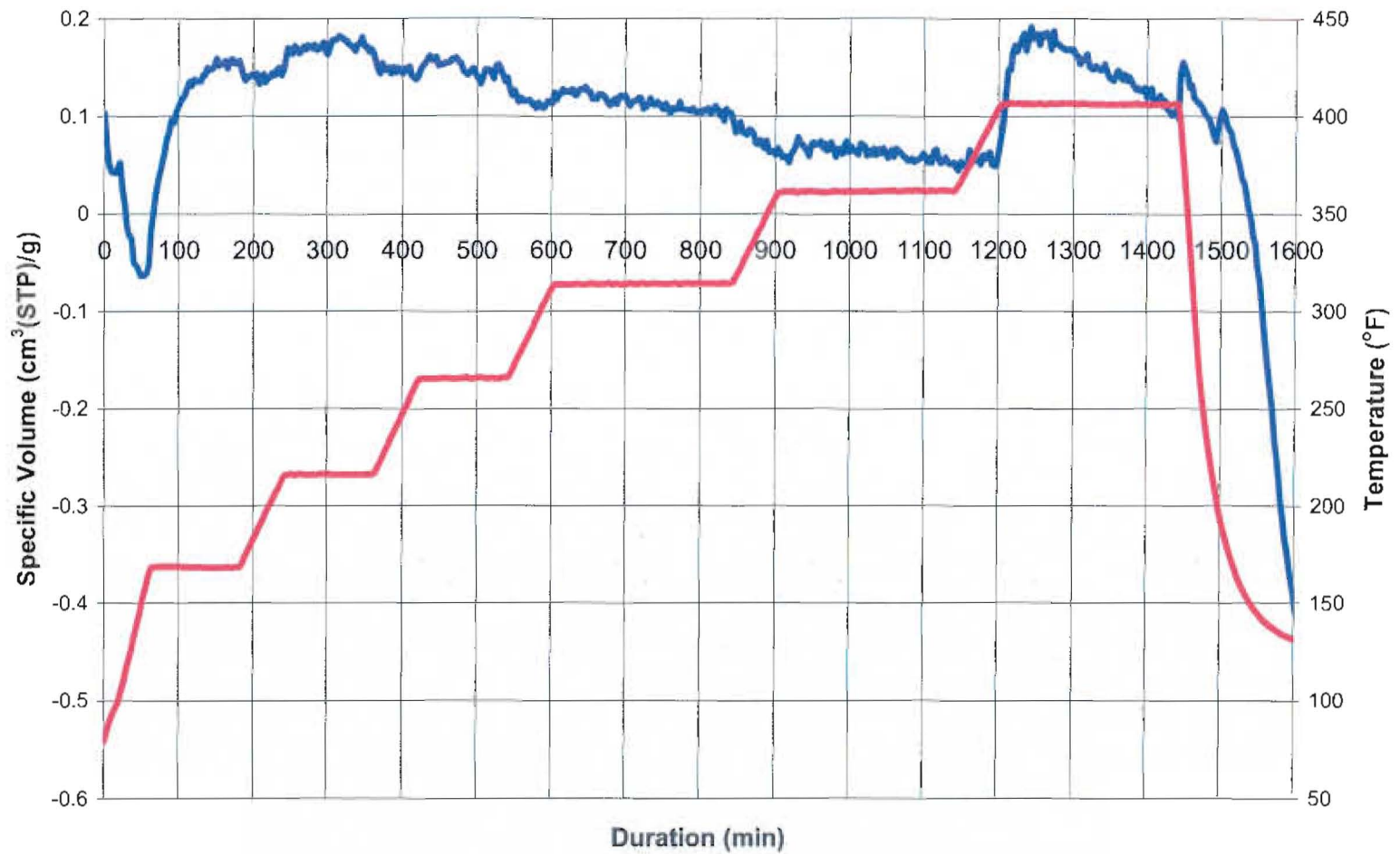


Fig. 13. Outgassing of an 8.90-g specimen of a black plastic bottle lid, possibly polyethylene.

Relative Outgassing Maximum and Minimum Per Polymer Mass in grams  
(Background Outgassing Subtracted)

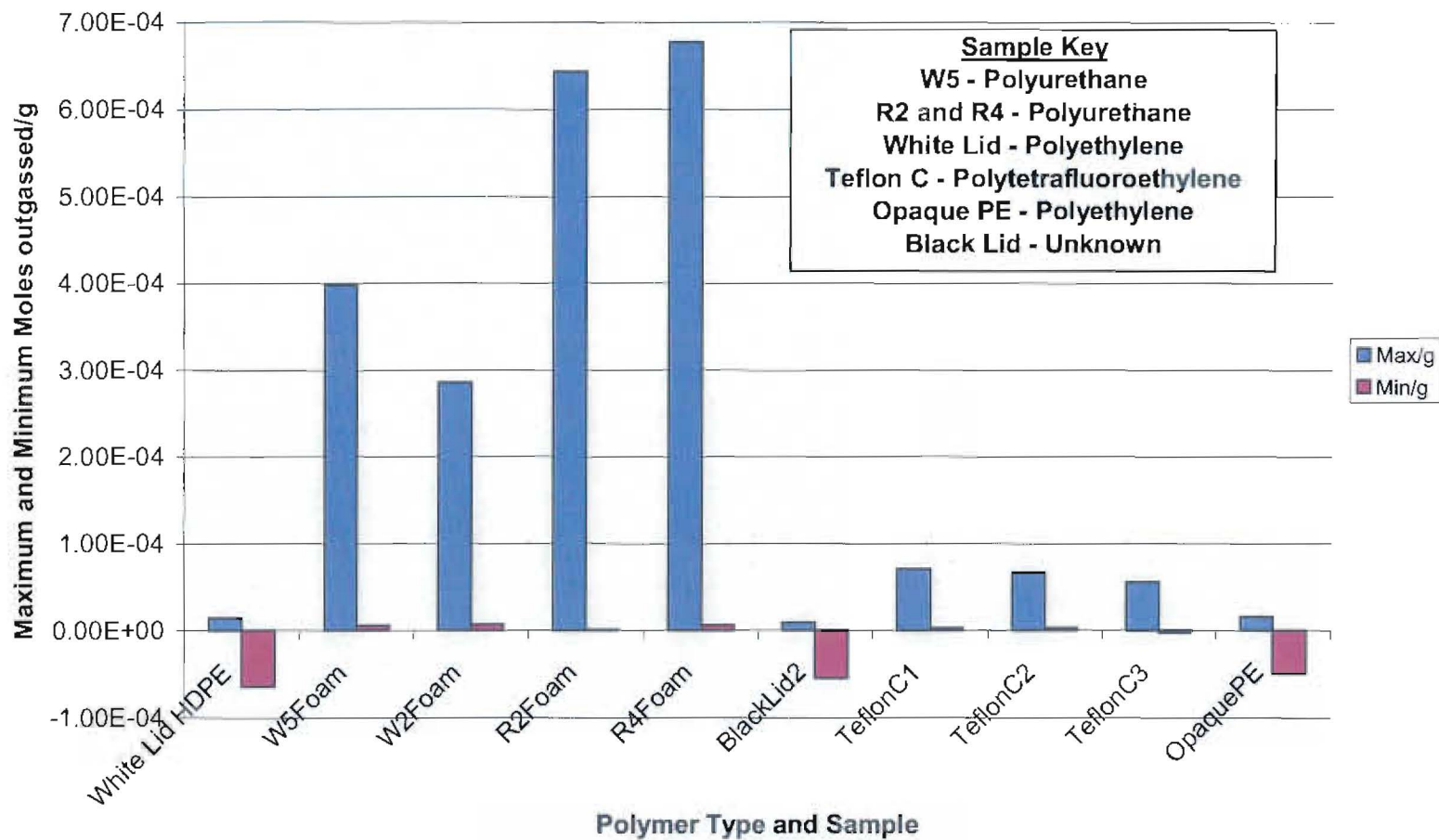
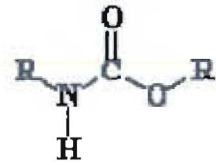
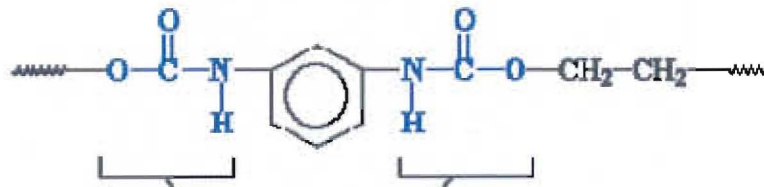


Fig. 14. Relative outgassing by polymer types examined.





a urethane



the urethane linkages  
in a polyurethane

Fig. 15. Polyurethane molecular structure.

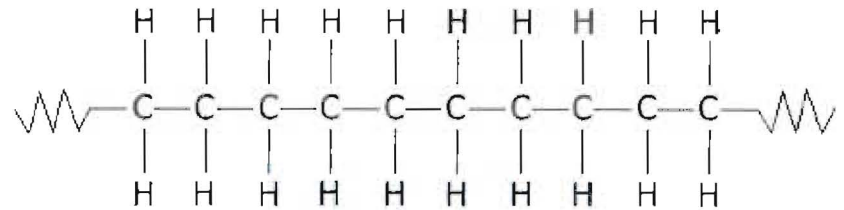


Fig. 16. Polyethylene molecular structure.

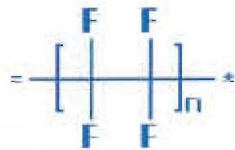


Fig. 17. Polytetrafluoroethylene (Teflon) molecular structure.

## REFERENCES

- BJB Enterprises, Inc., *Technical Datasheet for TC-280 A/B 8 Lb. Self Skinning Flexible Foam*, August 26, 2004.
- H. V. Boenig, *Polyolefins: Structure and Properties*, pp. 234–235, Elsevier Publishing Co., Amsterdam, 1966.
- R. Broos, J.-M. Sonney, H. P. Thanh, and F. M. Casati, “Polyurethane Foam Molding Technologies for Improving Total Passenger Compartment Comfort,” p. 348, from <http://www.polyurethane.org/conferences/expo/2004/proceedings/2000/contents.pdf>.
- J. R. Fried, *Polymer Science and Technology*, pp. 252–263, 473, Prentice Hall PTR, New Jersey, 1995.
- L. J. Gibson and M. F. Ashby, *Cellular Solids—Structure and Properties*, pp. 56–57, 2<sup>nd</sup> ed., Cambridge University Press, Cambridge, 1997.
- M. L. Hobbs, K. L. Erickson, , and T. Y. Chu, *Modeling Decomposition of Unconfined Rigid Polyurethane Foam*, Sandia Report SAND99-2758, Sandia National Laboratories, Albuquerque, New Mexico, November 1999.
- P. I. Tinnel and J. H. Leckey, internal correspondence to distribution, entitled “Rate of Generation of Volatile Components,” February 25, 1991.
- G. Kämpf, *Characterization of Plastics by Physical Methods*, pp. 175–196, Hanser Publishers, Munich, 1986.
- MatWeb, The Online Materials Database, <http://www.matweb.com>.
- U. S. Nuclear Regulatory Commission, “Hypothetical Accident Conditions,” U.S. NRC 10 CFR 71.73(c)(1-3) from [www.nrc.gov/reading-rm/doc-collections/cfr/part071/part071-0073.html](http://www.nrc.gov/reading-rm/doc-collections/cfr/part071/part071-0073.html).

## APPENDIX 1: DATA ANALYSIS

This is a description of steps taken in Excel software to process data downloaded in the form of \*.csv spreadsheets from National Instruments software. In general, new columns are set up for each calculation.

1. Open file
2. Data columns appear including Date and Time, Temperature, Pressure (torr)
3. Input sample name and weight (in grams) above pressure column
4. Insert column for duration—units can include days, hours, or minutes
5. Use CONVERT function to establish column of Fahrenheit temperatures
6. Input values for  $R$  (gas constant) and  $V$  (volume of container and flex hose) into cells on top of spreadsheet
7. Set up column to calculate the number of moles according to the Ideal Gas Law:
  - a.  $N = \{p(\text{torr})V(\text{cm}^3)/[R (82.057 \text{ atm}\cdot\text{cm}^3/\text{K}\cdot\text{mol})\cdot T (T^{\circ}\text{C} + 273)\text{K}]\} \cdot (1 \text{ atm}/760 \text{ torr})$   
using cell addresses for  $p$ ,  $V$ ,  $R$ , and  $T$  values
8. Paste column of blank outgassed moles
9. Subtract column of blank moles outgassed from specimen moles outgassed; this eliminates initial air and system outgassing
10. Calculate the volume of outgassed species at standard temperature and pressure (273 K and 1 atm) or by assuming an ideal gas that will have a volume of 22.4 liters per mole
11. Divide  $V_{STP}$  by specimen weight in grams; this column is Specific Volume
12. Plot  $T (^{\circ}\text{F})$  and Specific Volume vs Time (min), created separate axes for temperature and volume variables
13. Apply appropriate titles and formatting.



## DISTRIBUTION\*

### Y-12 National Security Complex

C. M. Cecala *cm6*

J. H. Clinton *cjh*

C. Heatherly *cqh*

M. L. Goins *mlg*

J. H. Leckey *lec*

J. S. Morrell *jkr*

W. I. North *wno*

M. W. Richey *mwr*

R. A. Smith *rox*

Technology Development Archives

T. L. Warren *wte*

Y-12 Central Files—RC (hard copy only)

---

\* Electronic copy unless otherwise noted.

