PAT-1 SAR Addendum Section 4 teleconference

Questions 2 & 3 talking points

Comments

2) 4-9: “The three SC-1……yielded the highest pressure rise of 572 psia” – should be corrected to 598.94 psia (based on the Table on page 4-42).

RHY: Discussion item. The discussion on Page 4-9 for pressure referenced Section 2.12.8, which included a 70 gram quantity of HDPE for labeling/tagging. The assumptions are different for the LANL and SNL decomposition calculations.

3) 4-9a: “the total pressure within TB-1 is 615 psia” – should be corrected to 641.56 psia (based on the Table on page 4-42).

RHY: Discussion item. Same comment as 2).

Recommendation

- Add impact to TB-1 final pressure of ancillary plastic
- Continue LANL assumption of no char – despite limitations (reduced allowable weight) of no char assumption on ancillary plastic

Discussion:

The pressure differences arise because of differing assumptions between SNL and LANL:

1. The SNL analysis includes the impact of plastic labels and bags (ancillary plastic) on interim and final pressure.
2. SNL Analysis assumed limited oxygen available for oxidation of O-ring char and ancillary plastic pyrolysis. LANL assumed package had an infinite supply of O_2.

Ancillary Plastic

- Impact of ancillary plastic must be included in analysis – how depends on treatment of oxygen.
- Sources of Ancillary Plastic:
  - TID labels -- typically metalized Poly(Ethylene terephthalate) or PET (Example is Mylar™)
  - Polyethylene bags
  - Poly Vinylchloride or PVC labels
  - Poly(TetraFluoroEthylene or PTFE (example is Teflon™)
- Ancillary Plastic is a customer Requirement

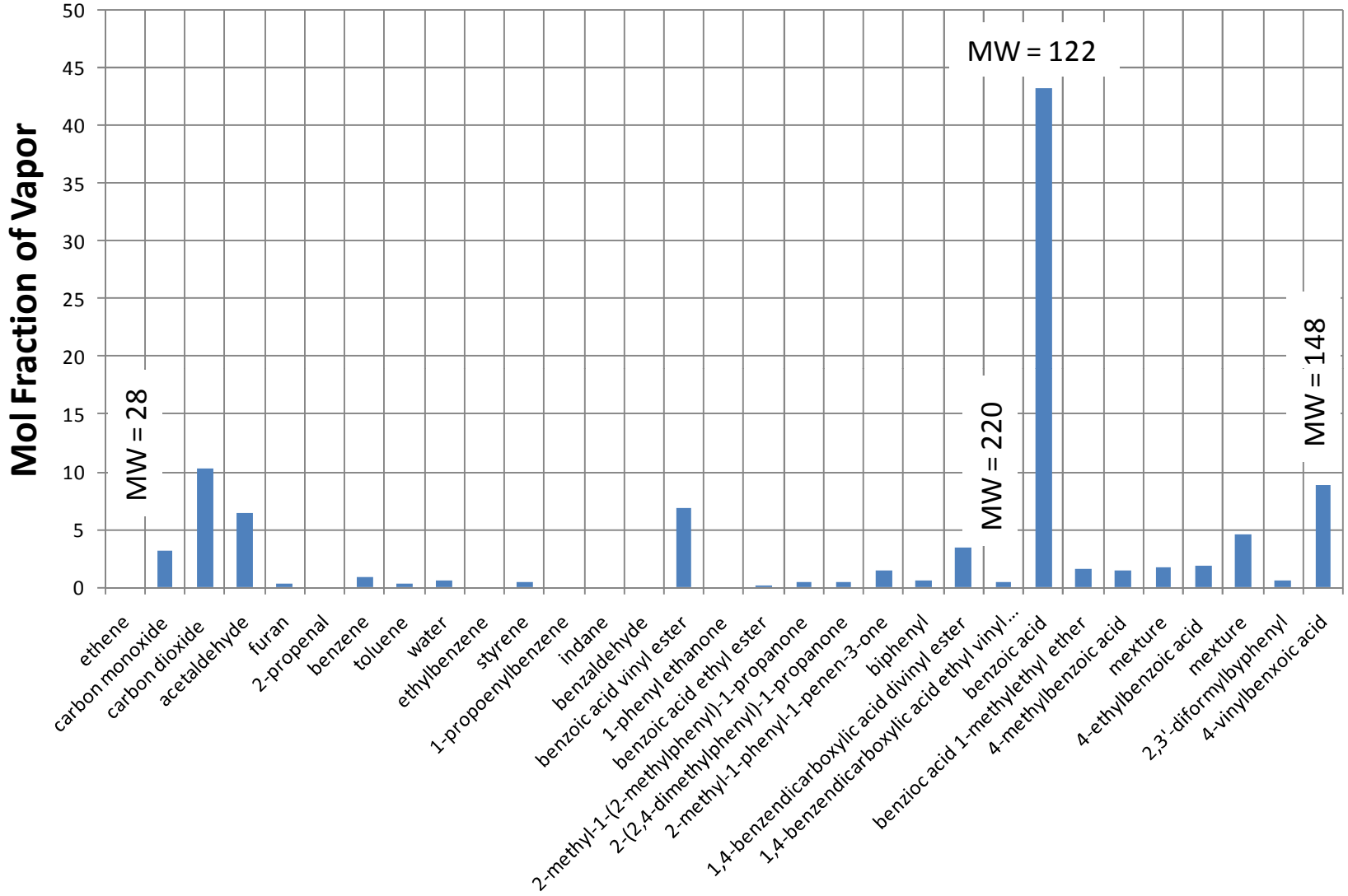
Metalized PET (Plastic #1) Example

- PET monomer: $C_{10}H_8O_4$
- Metal is aluminum and remains a solid.
- In an inert atmosphere at 1080 °F (Based on Experiment),
  - PET decomposes (via pyrolysis) into 31 hydrocarbon compounds with average MW of 107.6 g/mol.
  - Some char remains
  - 88.4 g PET required to achieve an Ultimate pressure of 1110 psia in TB-1. (Assumes TB-1 assembled in air – 21%)
- In an O_2 Saturated Atmosphere at 1080 °F (Hypothetical):
  - PET oxidizes into CO_2 and H_2O with an average MW of 36.6 g/mol

$$C_{10}H_8O_4 + 10O_2 \rightarrow 10CO_2 + 4H_2O$$

  - 6.278 g PET required to achieve an Ultimate pressure of 1110 psia in TB-1 . Equivalent to a 0.001” x 12.2” x 12.2” sheet
  - Oxidation requires 15 atmospheres of O_2

PET PYROLYSIS



Assuming Oxygen Saturation:

Common Name	Units	**Metalized PET**	**Polyethylene**	**PVC**	**Teflon (PTFE)**
Chemical name of monomer		ethylene terephthalate	ethylene	vinyl chloride	tetrafluoro-ethylene
Monomer formula		$C_{10}H_8O_4$	CH_2	C_2H_4Cl	C_2F_4
Monomer mol/mass ratio	g/mol	192.2	14.03	97.95	100.02
mol gas/monomer		14	2	4	6
mol O_2/monomer		10	1.5	5.5	1.5
Allowable mass (plastic only)	**g**	**6.278**	**3.208**	**11.2**	**7.924**
Size of 0.001 in thick square	in	16.5	11.8	22.1	18.2
Molar Contribution (mol)					
Original Atmosphere	mol	0.04481	0.04481	0.04481	0.04481
O-ring Thermal Decomposition					
HF	mol	0.2940	0.2940	0.2940	0.2940
CF_4	mol	0.0270	0.0270	0.0270	0.0270
CO_2 from char oxidation	mol	0.3200	0.3200	0.3200	0.3200
Helium generated from alpha decay	mol	0.00004615	0.00004615	0.00004615	0.00004615
Subtotal of all above sources	mol	**0.6859**	**0.6859**	**0.6859**	**0.6859**
Ancillary Plastic -- thermal decomposition and					
CO2	mol	0.3581	0.2507	0.2507	0.2507
H2O	mol	0.1432	0.2507	0.188	
Cl2	mol			0.06267	
F2	mol				0.2507
Total	mol	**1.187**	**1.187**	**1.187**	**1.187**

Molar Basis

Assuming Oxygen Saturation:

Common Name	Units	Metalized PET	Polyethylene	PVC	Teflon (PTFE)
Chemical name of monomer		ethylene terephthalate	ethylene	vinyl chloride	tetrafluoro-ethylene
Monomer formula		$C_{10}H_8O_4$	CH_2	C_2H_4Cl	C_2F_4
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mol gas/monomer		14	2	4	6
mol O_2/monomer		10	1.5	5.5	1.5
Allowable mass (plastic only)	**g**	**6.278**	**3.208**	**11.2**	**7.924**
Size of 0.001 in thick square	in	16.5	11.8	22.1	18.2
Pressure Contribution at 1080 °F					
Original Atmosphere	psia	41.34	41.9	41.9	41.9
O-ring Thermal Decomposition					
HF	psia	274.9	274.9	274.9	274.9
CF_4	psia	25.25	25.25	25.25	25.25
CO_2 from char oxidation	psia	299.2	299.2	299.2	299.2
Helium generated from alpha decay	psia	0.04316	0.04316	0.04316	0.04316
Subtotal of all above sources	psia	**641.4**	**641.4**	**641.4**	**641.4**
Ancillary Plastic -- thermal pyrolysis with oxidation					
CO2	psia	334.9	234.4	234.4	234.4
H2O	psia	133.9	234.4	175.8	
Cl2	psia			58.6	
F2	psia				234.4
Total Pressure	psia	1110	1110	1110	1110
Oxygen Required To support Saturation					
Oxygen required	mol	0.6781	0.6781	0.6781	0.6781
Ratio O_2/Argon		15.13	15.53	22.53	9.939

Pressure Basis