1.0 Analysis Approach

The analysis approach was to compile a list of chemicals that will be used at the PDCF, estimate the maximum quantity of each chemical that might be involved in a release, estimate the airborne release, and, given the release, estimate the concentration at 30 meters from the release point using the *Areal Locations of Hazardous Atmospheres* (ALOHA) modeling program. If the concentration at 30 meters (m) exceeded the Emergency Response Planning Guideline (ERPG)-2 or Temporary Emergency Exposure Limit (TEEL)-2 value at that point, then the chemical warranted further analysis in the Emergency Preparedness Hazards Assessment (EPHA).

To ensure that no chemicals with very low vapor pressure were screened out, two release mechanisms were considered: the release when the material was spilled, and the release from an evaporating liquid pool formed after the spill. The first mechanism was considered for all the chemicals, the second just for the liquids in the chemical list. These were hydrochloric acid (HCl), hydrofluoric acid (HF), sulfuric acid (H_2SO_4), and nitric acid (HNO_3); the alcohols methanol, ethanol, and isopropanol and the base sodium hydroxide as a solution.

2.0 Inventory of Hazardous Chemicals

A chemical screening analysis was conducted for the hazardous chemicals that will be used at the PDCF. These chemicals are primarily present in six areas:

- Chemical Storage and Distribution System
- HVAC Chilled Water System
- Analytical Laboratory
- Process Gas Supply System
- Argon and Helium Supply System
- Nitrogen Supply System

The chemicals that will be used in the Chemical Storage and Distribution System and the HVAC Chilled Water System are listed in Table 1. Also listed in Table 1 are the amounts that will be supplied in a single delivery. In addition, the chemicals listed in Table 1 will be diluted for use, so analyzing the chemicals as they are delivered would bound releases from tanks and pipes.

Table 1. Chemicals Used in the Chemical Storage and Distribution System and the HVAC Chilled Water System

Chemical	Formula	CAS Registry No.	Amount Per Delivery
Sodium Hydroxide (25 weight percent)	NaOH	1310-73-2	55 gallons
Sulfuric Acid (95 weight percent)	H_2SO_4	7664-93-9	55 gallons
Sodium Sulfate (solid)	Na_2SO_4	7757-82-6	150 lbs.
Bleach (30 weight percent)	NaOCl	7681-59-9	55 gallons
Tolyltriazole (solid)	$C_7H_7N_3$	29385-43-1	50 lbs.

Table 2 lists the chemicals and chemical mixtures used in the analytical laboratory (first column) and their source (second column). As can be seen from the second column, many of the mixtures are prepared in the laboratory from pure chemicals. Others are procured as pure chemicals and used either at full strength or diluted, typically with water.

Table 2. Listing of Hazardous Chemical Inventories in PDCF

Chemical Present in PDCF	How Prepared or Procured
Acetone	Procured in 4-liter bottles, four at a time
Anhydrone (Magnesium perchlorate)	Procured as Magnesium Perchlorate (s)
Argon	Procured as liquid – stored in 900-gallon insulated tank
Ascorbic Acid	Procured as Ascorbic Acid (s)
Barium Chloride (0.5 M)	Prepared from Barium Chloride (s) and water
12 M HNO_3 – 0.1 M HF	Prepared from 68 wt % HNO_3, 49 wt. % HF and water
0.5 mg/ml Collodion in Alcohol	Prepared from Collodion (Nitrocellulose, Ethyl Ether - 60 to 70%, Ethyl Alcohol) and Ethyl Alcohol
Depleted U_3O_8	Procured as Depleted U_3O_8
Diphenylcarbazide Solution	Procured as Diphenylcarbazide (s) dissolved in Acetone to make solution, assume hazard bounded by Acetone
Eluant Solution ($NaHCO_3$, Na_2CO_3 and water)	Prepared from $NaHCO_3$ (s) and Na_2CO_3 (s) and water
F/Cl Standard	Prepared from 36 wt. % HCl and 49 wt. % HF and water
Ferrous Sulfamate 2 M	Prepared from Ferrous Sulfamate (s) and water
Ferrous Sulfate 1.5 M	Prepared from Ferrous Sulfate (s) and water
0.1 M HCl – 0.05 M HF	Prepared from 36 wt % HCl, 49 wt. % HF and water
HCl 5 M and Oxalic Acid 0.05 M	Prepared from 36 wt % HCl, Oxalic Acid (s) and water
HCl 6 M and Oxalic Acid 0.05 M	Prepared from 36 wt % HCl, Oxalic Acid (s) and water
Helium	Procured in Portable Gas Cylinder (291 SCF) [1]
12 M HNO_3 and 0.1 M HF	Prepared from 68 wt % HNO_3, 49 wt. % HF and water
Hydrochloric Acid 0.04 M	Prepared from 36 wt % HCl, and water
Hydrochloric Acid 9 M	Prepared from 36 wt % HCl, and water
Hydrogen 4% and Helium	Procured in Portable Gas Cylinder (291 SCF)
Hydrogen Peroxide 3%	Prepared from 30% Hydrogen Peroxide Solution
Hydrogen Peroxide 30%	Procured as 30% Hydrogen Peroxide Solution
0.02 M HNO_3 – 0.02 M HF, 0.02 M NH_4I	Prepared from 68 wt % HNO_3, 49 wt. % HF and NH_4I (s) and water
0.02 M HNO_3 – 0.005 M HF	Prepared from 68 wt % HNO_3, 49 wt. % HF and water
Liquid Scintillation Cocktail (Ultima Gold LT)	Procured as Ultima Gold LT
Methanol 95%, Ethanol 5%	Prepared by mixing Methanol and Ethanol
Nitric Acid (various molar concentrations)	Prepared from 68 wt. % Nitric Acid
3 M HNO_3 – 0.2 M HF and other molar ratios	Prepared from 68 wt % HNO_3, 49 wt. % HF and water
2.5 to 0.5 M $Al(NO_3)_3$	Prepared by dissolving solid $Al(NO_3)_3$ in water
3 M HNO_3 – 0.1 M $Fe(SO_3NH_2)_2$ (Ferrous Sulfamate)– 0.1 M $C_6H_8O_6$ (Ascorbic Acid)	Prepared from 68 wt % HNO_3, solid Ferrous Sulfamate, solid Ascorbic Acid and water
3 M HNO_3 – 0.01 M $Fe(SO_3NH_2)_2$ (Ferrous Sulfamate)	Prepared from 68 wt % HNO_3, solid Ferrous Sulfamate, and water
Nitrogen	Procured as liquid, stored in 1,500 gallon insulated tank
Oxygen	Procured in Portable Gas Cylinder (291 SCF)
Potassium Dichromate solutions	Prepared from Potassium Dichromate (s) and water
Potassium Oxalate 1 M	Prepared from Potassium Oxalate (s) and water
Propane	Procured as pressurized liquid, 50 pounds per tank
Sodium Hydroxide	Procured as wt. 25 % solution in water
Sodium Nitrate 3 M	Prepared from Sodium Nitrate (s) and water
Potassium Chloride 4 M	Prepared from Potassium Chloride (s) and water
Sulfate standard	Prepared from Sodium Sulfate and water
Sulfuric acid solutions (various molarities)	Prepared from 95 wt. % Sulfuric Acid and water
Tetrasodium Pyrophosphate Decahydrate ($Na_4P_2O_7 \cdot 10H_2O$)	Prepared by dissolving $Na_4P_2O_7 \cdot 10H_2O$ (s) in water

[1] Standard cubic feet of gas measured at 70 °F and atmospheric pressure.

From a hazard screening standpoint, a screening based on the chemicals listed in column 2 will provide a bounding chemical screening assessment. The composite list and the assumed quantities that could be spilled in an accident are shown in Table 3.

Table 3. Chemicals Used in the Analytical Laboratory

Chemical	Formula	CAS Registry No.	Amount Per Delivery
Acetone	C_3H_6O	67-64-1	16 L
Aluminum Nitrate	$Al(NO_3)_3$	13473-90-0	1 kg
Ascorbic acid	$C_6H_8O_6$	50-81-7	1 kg
Barium chloride	$BaCl_2$	10361-37-2	1 kg
Collodion (Pyroxylin) Solution	$C_{12}H_{16}O_6(NO_3)_4$	9004-70-0	1 liter
Diphenyl Carbazide	$C_{13}H_{14}N_4O$	140-22-7	1 kg
Ethanol	C_2H_6O	64-17-5	16 L
Ferrous Sulfamate	$Fe(SO_3NH_2)_2$	14017-39-1	5 kg
Ferrous Sulfate	$FeSO_4$	7720-78-7	1 kg
Hydrochloric Acid (36 weight percent)	HCl	7647-01-0	16 L
Hydrofluoric Acid (49 weight percent)	HF	7664-39-3	16 L
Hydrogen Peroxide (30 weight percent)	H_2O_2	7722-84-1	16 L
Isopropanol	$(CH_3)_2CHOH$	67-63-0	16 L
Magnesium Perchlorate	$MgCl_2O_8$	10034-81-3	1 kg
Methanol	CH_3OH	67-56-1	16 L
Nitric Acid (68 weight percent)	HNO_3	7697-37-2	16 L
Oxalic Acid	$HO(CO)_2OH$	122-62-7	1 kg
Potassium Chloride	KCl	7447-40-7	16 L
Potassium Dichromate	$K_2Cr_2O_7$	231-906-6	1 kg
Potassium Oxalate	$K_2(CO)_2$	583-52-8	1 kg
Scintillation cocktail		9016-45-9	1 kg
Sodium Carbonate	Na_2CO_3	497-19-8	1 kg
Sodium Hydroxide	NaOH	1310-73-2	16 L
Sodium Nitrite	Na_2SO_3	7632-00-0	1 kg
Sodium Pyrophosphate	$Na_4P_2O_7$	7722-88-5	1 kg
Sulfuric Acid (95 weight percent)	H_2SO_4	7664-93-9	55 gallons

Last, gases used in the Analytical Laboratory, the Process Gas Supply System, the Argon and Helium Supply System, and the Nitrogen Supply System are listed in Table 4.

Table 4. Liquefied and Pressurized Gases Used in Processes

Gas	System	Quantity Present (volume)	Quantity Present (mass) (kg)
Argon	Argon and Helium Supply	900 gallons of refrigerated liquid	4750
Nitrogen	Nitrogen Supply	1500 gallons as refrigerated liquid	5150
Nitrogen	Nitrogen Supply	1 70-liter and 2 25-liter dewars	108.8
Oxygen	Analytical Laboratory	Gas cylinder, 291 SCF	10.927
P-10 (90%Ar/10% Methane)	Analytical Laboratory	Gas cylinder, 291 SCF	12.36
6% Hydrogen/94% Argon	Process Gas Supply	Gas cylinder, 291 SCF	12.88
6% Hydrogen/94% Helium	Process Gas Supply	Gas cylinder, 291 SCF	1.326
1% Hydrogen/99% Argon	Process Gas Supply	Gas cylinder, 291 SCF	13.53
Hydrogen	Process Gas Supply	Gas cylinder, 291 SCF	0.688
Helium	Process Gas Supply	2 skids of 16 gas cylinders, (291 SCF each cylinder)	21.87
1% Oxygen/99% Argon	Process Gas Supply	Gas cylinder, 291 SCF	13.63
25% Helium/75% Oxygen	Process Gas Supply	Gas cylinder, 291 SCF	8.537
Propane	Analytical Laboratory	Pressurized liquid -20 pounds	9.072

A standard cubic foot (SCF) of each gas listed in Table 4 is measured at 70 °F and atmospheric pressure. The cylinders that hold this quantity of gas have a volume of approximately 50 liters and are filled to a pressure of around 2650 psig. The helium inventory is on a skid containing 16 standard gas bottles. While two skids might be present at the facility, one would be close to empty when the second arrived; therefore, the release from only one skid is modeled. Based on the definition of a SCF, and assuming ideal gas behavior, the gram moles present in a gas cylinder can be calculated using the following formula:

$$gm \cdot moles = 291 \cdot ft^3 \cdot \left(\frac{294.26 \cdot °K}{273.15 \cdot °K} \right) \cdot \left(\frac{28.31685 \cdot liters/ft^3}{22.4 \cdot liters/gm \cdot mole} \right) = 341.5:$$

Expressed in terms of pounds, each bottle will hold 0.753 pound moles of the gases. To get the last column in Table 4, the number of gram moles, 341.5, has been multiplied by the molecular weight of the gases and divided by 1000.

The density of the cryogenic liquids was taken at their normal boiling point at atmospheric pressure. The densities for liquid nitrogen, liquid argon, and propane were taken from the Hazardous Material Handbook (Reference 3). They were 807 kg/m^3 for nitrogen and 1394 kg/m^3 for argon. For propane, the specific gravity of the liquid propane was listed as 0.58. All the chemicals listed in Tables 3 and 4 will be screened to determine which, when spilled, would result in an alert level.

3.0 Chemical Screening Analyses

The chemical screening analysis consisted of four steps:

1. The amount of a chemical that would be supplied in a single delivery was estimated.