

This report was not issued as shown, but was incorporated into a larger Chambers Works report under the consent order

Section 1

Chambers Works

ISC3 Modeling Methodology and Results

Emission Source Information

The ISC3 model was used to calculate ambient ground-level air concentrations for emissions of C8 from the Chambers Works site. Table 1 shows the stack parameters and emission rates used in the model for each emission point. Section 3 of this report contains the basis for the emission estimates of C8.

Modeling Methodology

Dispersion and deposition modeling was performed using the U.S. EPA's Industrial Source Complex 3 Model (ISC3), version 00101, provided by Trinity Consultants. All modeling was done in accordance with the procedures in EPA's Guideline on Air Quality Models (40 CFR Part 51, Appendix W). The EPA regulatory default options and rural dispersion coefficients were used in the model.

The C8 emission sources were evaluated for downwash effects from surrounding buildings. The Building Profile and Input Program (BPIP) provided by Trinity consultants was used to provide wind direction specific building parameters. All buildings on the site were evaluated to determine if they could potentially impact the stack by causing building downwash effects. Table 2 lists the buildings included in the model and their heights.

A 100-meter receptor grid extending out 600 meters from the plant fenceline was used. In addition, discrete receptors with 50-meter spacing were placed on the plant property line. Since the area surrounding the plant site is flat, no terrain elevations were used. A plot of the receptor grid used is shown in Figure 1.

Five years of meteorological data (1989-1993) were analyzed. The surface data is from New Castle County Airport (Wilmington, DE) and the upper air data is from Washington Dulles Airport (Sterling, VA). An anemometer height of 6.1 meters was used for the modeling.

Modeling Results

An averaging time of one year was used to determine the annual average ground-level concentrations over the entire receptor grid. The modeling results for each year are shown in Table 3. A contour plot of the annual average concentrations for the year 1990 is shown in Figure 2. The maximum off-site value predicted by the model was $0.00364 \mu\text{g}/\text{m}^3$ for the year 1990. This value was located at a receptor on the plant property line along highway US130.

Table 1
Stack Parameters and Emission Rates

Process Area	Source	Emission Rate (lb/hr)	Stack Height	Stack Diameter	Flowrate or Velocity	Temperature
DDE	Building 1163 Stack	0.033	25 ft	31"	92 ft/s	194°F
Telomer A	DMA Roof #1	6.06E-06	70 ft	2"	17 acfm	150°F
ZFAN Crude	1156 Building Hotwell	4.45E-05	12 ft	2"	0.033 acfm	65°C
185 Alcohol Drying	185 Building Hotwell	2.94E-06	0 ft	6"	0 acfm*	40°C
185 Alcohol Drying	TS-45 Tank Vent	1.62E-06	25 ft	3"	10 ft/s	70°C
D Building	D Building Roof	1.87E-05	55 ft	2"	1 acfm	ambient
D Building	D Building Jets	2.04E-06	88 ft	36"	10,000 acfm	ambient
EO Center	Hotwell and Stack	2.19E-05	85 ft	4"	80 acfm	ambient

*185 building hotwell stack points at the ground

Table 2
Building Heights

Building Name	Height (ft)	Building Name	Height (ft)
1	60	43	16
J26	38	1050	22
1089	15.5	1163	13.5
1094	30	115 East	45
T3	45	115 West	30
589	15	656	30
745	50	1402	25
888	60	185	68
1183	60	1156	45
1182	60	234	30
669	40	788	40
1205	31		

Table 3
Modeling Results

Year	Annual Average Concentration ($\mu\text{g}/\text{m}^3$)	Location
1989	0.00309	plant fenceline along US130
1990	0.00364	" "
1991	0.00305	" "
1992	0.00267	" "
1993	0.00300	plant fenceline along DE River

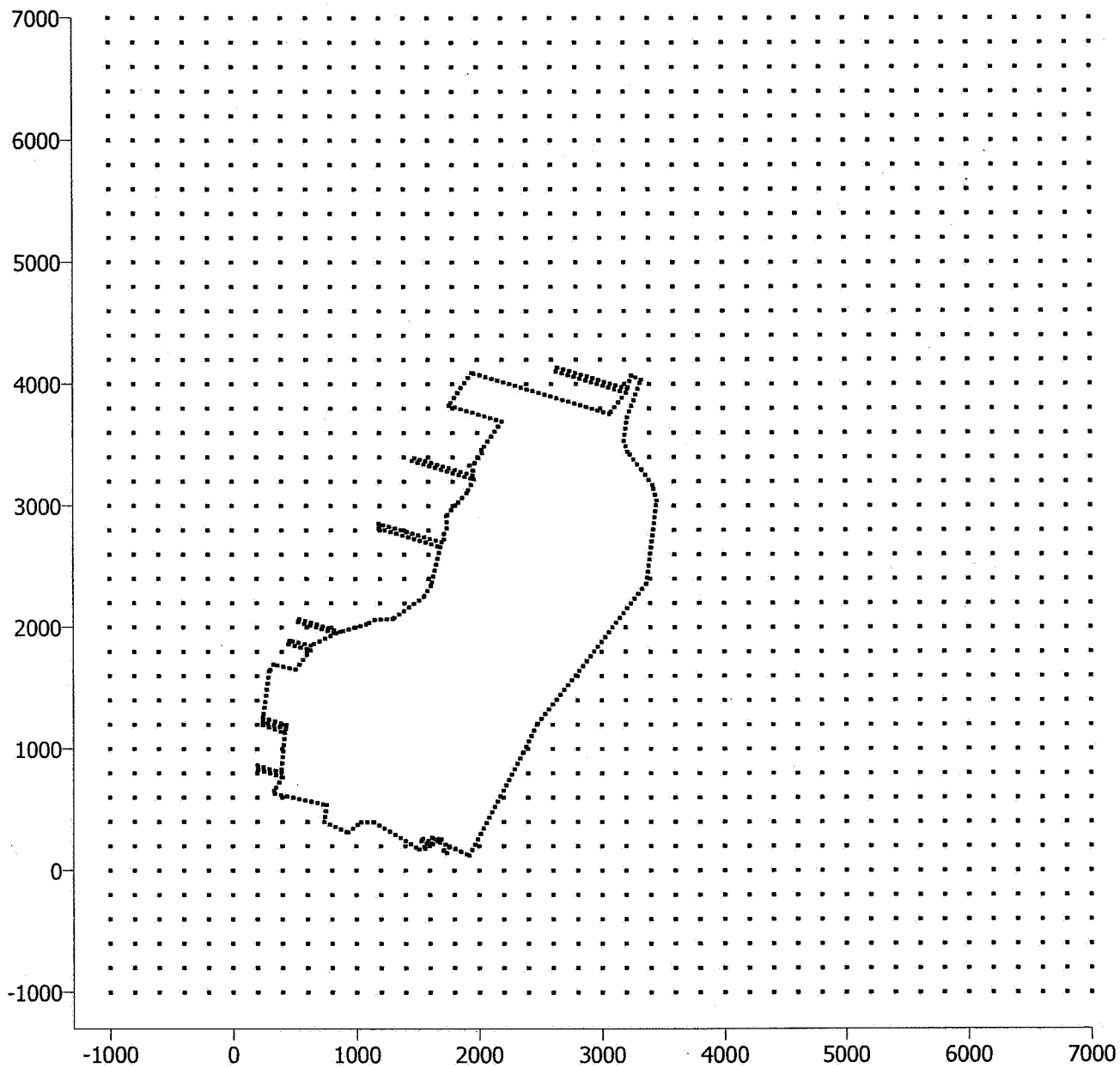


Figure 1
Receptor Grid

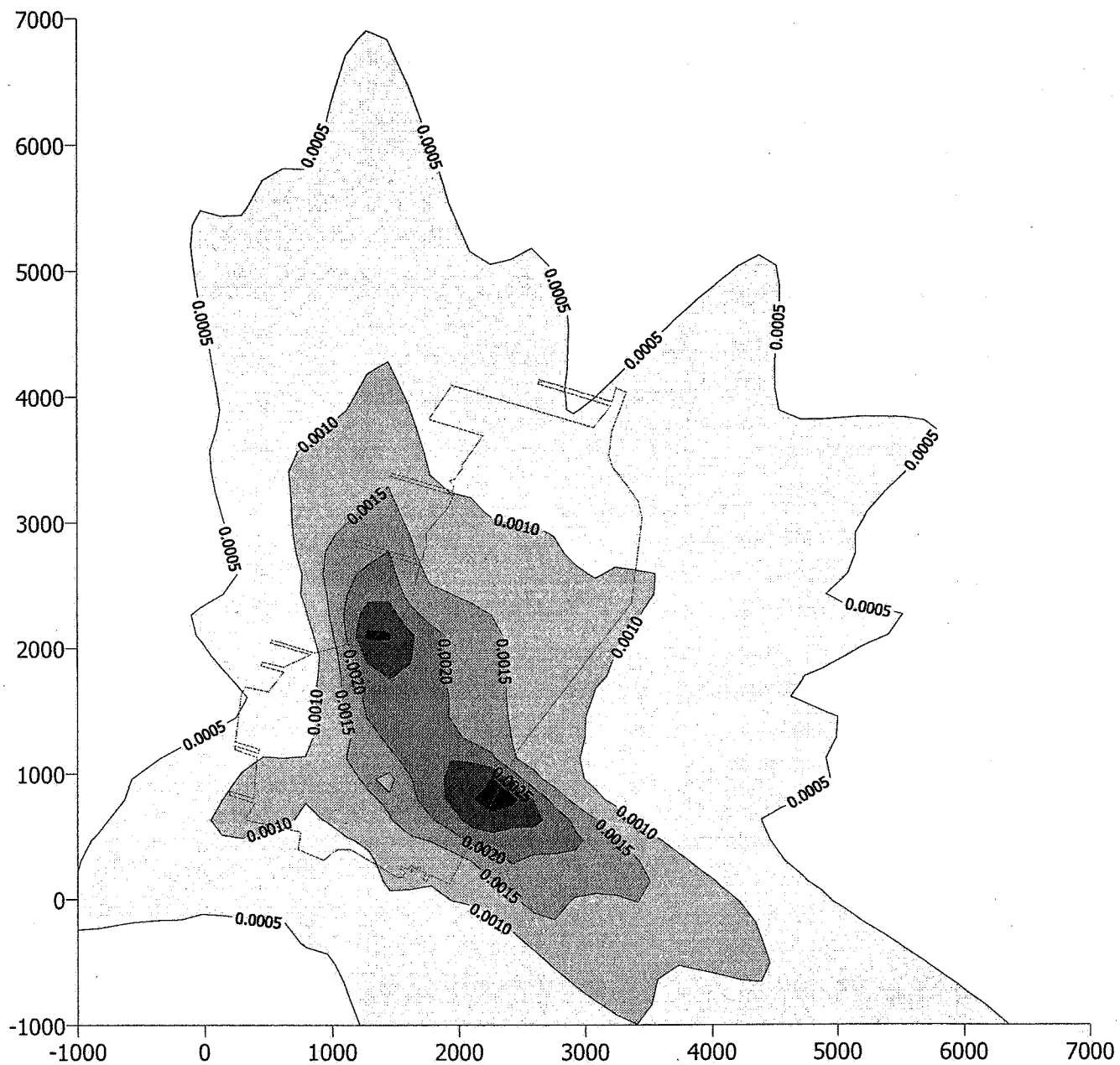


Figure 1
Annual Average Concentrations – 1990 Meteorological Data

Section 2
Washington Works
Screen3 Modeling Methodology and Results

Data and Modeling Procedures

Dispersion modeling was performed using the U.S. EPA's Screen3 model. This model is a screening tool which gives predictions of ambient ground level concentrations for a single stack. Due to the assumptions made in the model, particularly those regarding meteorological conditions, these predictions will always be more conservative than predictions made by the ISC3 model.

Although there are several different sources of C8 emissions in the Telomers area at the Washington Works site, these emission points are all headered together into a common stack. The following parameters for this stack were used in the model:

Stack Height: 85 feet
Diameter: 1.5 feet
Temperature: 68°F
Velocity: 47 ft/s
C8 Emission Rate: 0.16 lb/yr (1.83×10^{-5} lb/hr)

The C8 emission rate is based on the maximum production rate for the Telomers area. The basis for the emission calculations is shown in the attached document titled "Calculation of Emissions from the Telomers Process."

To determine the impacts of building downwash on dispersion from the stack, the Screen3 model uses only the dominant downwash structure as an input to the model. The dominant downwash structure can be found by first locating all buildings which have an area of influence encompassing the stack. The area of influence is defined by EPA as a distance of five times the lesser of the height or the maximum projected width of the building. Once all of the potential downwash structures are located, the dominant downwash structure is determined by calculating the GEP (Good Engineering Practice) stack height for each building. The building with the greatest GEP stack height is the building that should be included in the Screen3 model. The GEP stack height is calculated according to the following formula:

$$H = h + 1.5L$$

where H = GEP stack height

h = building height

L = lesser of the building height or maximum projected width

The following table shows the buildings that were included in the downwash analysis and their respective GEP's:

Building	Height (ft)	Length (ft)	Width (ft)	Max Projected Width (ft)	GEP (ft)
164	44	90	90	125	110
180	64	70	25	75	160
184*	96	195	120	230	240

*This building has the highest GEP and was used in the model.

Modeling Results

Using the above data the Screen3 model predicted a maximum off-site ground level concentration of $0.0023 \mu\text{g}/\text{m}^3$ at a distance of 289 feet from the source. This concentration is based on a 1-hour averaging time. To convert a Screen3 model result to an annual average, EPA guidance directs the user to multiply the predicted Screen3 concentration by a value of 0.05. This gives an annual average concentration of $1.15 \times 10^{-4} \mu\text{g}/\text{m}^3$. This concentration is four orders of magnitude below the recommended ambient air concentration level in the community.

A copy of the Screen3 model output is attached.

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*** SCREEN3r MODEL RUN ***
 *** VERSION DATED 96043 ***

WASHINGTON WORKS TELOMERS EMISSIONS ** 0

SIMPLE TERRAIN INPUTS:

SOURCE TYPE	=	POINT
EMISSION RATE (G/S)	=	.230576E-05
STACK HEIGHT (M)	=	25.9080
STK INSIDE DIAM (M)	=	.4572
STK EXIT VELOCITY (M/S)	=	14.3256
STK GAS EXIT TEMP (K)	=	293.1500
AMBIENT AIR TEMP (K)	=	293.0000
RECEPTOR HEIGHT (M)	=	.0000
URBAN/RURAL OPTION	=	RURAL
BUILDING HEIGHT (M)	=	29.2608
MIN HORIZ BLDG DIM (M)	=	36.5760
MAX HORIZ BLDG DIM (M)	=	59.4360

THE REGULATORY (DEFAULT) MIXING HEIGHT OPTION WAS SELECTED.
 THE REGULATORY (DEFAULT) ANEMOMETER HEIGHT OF 10.0 METERS WAS ENTERED.

BUOY. FLUX = .004 M**4/S**3; MOM. FLUX = 10.719 M**4/S**2.

*** FULL METEOROLOGY ***

 *** SCREEN AUTOMATED DISTANCES ***

*** TERRAIN HEIGHT OF 0. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES

DIST (M)	CONC (UG/M**3)	STAB	U10M (M/S)	USTK (M/S)	MIX HT (M)	PLUME HT (M)	SIGMA Y (M)	SIGMA Z (M)	DWASH
10.	.0000	0	.0	.0	.0	.00	.00	.00	NA
100.	.2091E-02	6	1.0	1.7	10000.0	26.21	4.07	18.28	SS
200.	.1291E-02	6	1.0	1.7	10000.0	26.21	7.73	24.04	SS
300.	.8797E-03	6	1.0	1.7	10000.0	26.21	11.23	30.17	SS
400.	.6730E-03	6	1.0	1.7	10000.0	26.21	14.64	30.53	SS
500.	.5466E-03	6	1.0	1.7	10000.0	26.21	17.97	30.89	SS
600.	.4609E-03	6	1.0	1.7	10000.0	26.21	21.24	31.25	SS
700.	.3988E-03	6	1.0	1.7	10000.0	26.21	24.46	31.60	SS
800.	.3517E-03	6	1.0	1.7	10000.0	26.21	27.63	31.95	SS
900.	.3147E-03	6	1.0	1.7	10000.0	26.21	30.78	32.29	SS
1000.	.2848E-03	6	1.0	1.7	10000.0	26.21	33.88	32.63	SS
1100.	.2601E-03	6	1.0	1.7	10000.0	26.21	36.96	32.96	SS
1200.	.2394E-03	6	1.0	1.7	10000.0	26.21	40.01	33.29	SS
1300.	.2217E-03	6	1.0	1.7	10000.0	26.21	43.04	33.62	SS
1400.	.2065E-03	6	1.0	1.7	10000.0	26.21	46.05	33.94	SS
1500.	.1932E-03	6	1.0	1.7	10000.0	26.21	49.03	34.26	SS
1600.	.1815E-03	6	1.0	1.7	10000.0	26.21	51.99	34.57	SS
1700.	.1711E-03	6	1.0	1.7	10000.0	26.21	54.94	34.89	SS

1800.	.1618E-03	6	1.0	1.7	10000.0	26.21	57.87	35.20	SS
1900.	.1534E-03	6	1.0	1.7	10000.0	26.21	60.78	35.50	SS
2000.	.1459E-03	6	1.0	1.7	10000.0	26.21	63.68	35.80	SS

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND 10. M:									
88.	.2254E-02	6	1.0	1.7	10000.0	26.21	3.65	17.65	SS

DWASH= MEANS NO CALC MADE (CONC = 0.0)
 DWASH=NO MEANS NO BUILDING DOWNWASH USED
 DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
 DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
 DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

 *** REGULATORY (Default) ***
 PERFORMING CAVITY CALCULATIONS
 WITH ORIGINAL SCREEN CAVITY MODEL
 (BRODE, 1988)

*** CAVITY CALCULATION - 1 ***		*** CAVITY CALCULATION - 2 ***	
CONC (UG/M**3)	= .8839E-03	CONC (UG/M**3)	= .1001E-02
CRIT WS @10M (M/S)	= 1.27	CRIT WS @10M (M/S)	= 2.37
CRIT WS @ HS (M/S)	= 1.54	CRIT WS @ HS (M/S)	= 2.87
DILUTION WS (M/S)	= 1.00	DILUTION WS (M/S)	= 1.44
CAVITY HT (M)	= 38.48	CAVITY HT (M)	= 32.60
CAVITY LENGTH (M)	= 67.12	CAVITY LENGTH (M)	= 48.77
ALONGWIND DIM (M)	= 36.58	ALONGWIND DIM (M)	= 59.44

 END OF CAVITY CALCULATIONS

 *** SUMMARY OF SCREEN MODEL RESULTS ***

CALCULATION PROCEDURE	MAX CONC (UG/M**3)	DIST TO MAX (M)	TERRAIN HT (M)
SIMPLE TERRAIN	.2254E-02	88.	0.
BLDG. CAVITY-1	.8839E-03	67.	-- (DIST = CAVITY LENGTH)
BLDG. CAVITY-2	.1001E-02	49.	-- (DIST = CAVITY LENGTH)

 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

Note: The off-site concentration referenced in the report is the concentration shown for simple terrain. This concentration is valid for receptor locations near the fenceline since this area is relatively flat. Although the model predicted a building cavity concentration which is higher than the predicted value for simple terrain, this concentration will occur on site and is not applicable for this analysis.

Section 3

Calculation of Emissions from the Telomers Process

Emissions of perfluoro-octanoic acid (PFOA) from processes on the Chambers Works and Washington Works sites were calculated based on analytical data which suggests that this compound is present in the telomers mixture. Analytical data was provided to me at various points in processing of telomer products and this data was used to determine vapor phase emissions from a variety of vessels during process steps that include filling, evacuating, distilling, reacting, homogenizing and packing out. This document is to serve as an explanation of the basis for such calculations, the assumptions made and areas of uncertainty.

Basic Physical Property Data

The primary property determining vapor phase composition above a mixture containing PFOA is the vapor pressure. Recent measurements of the vapor pressure (2003) were used in all the emission calculations and is best described by the following equation:

$$\ln (\text{VP}) \text{ in psia} = 12.7965 - 3388.046 / (T \text{ oK} - 130.441)$$

The vapor pressure of PFOA is quite low, and when combined with the extremely low levels of PFOA in the telomers the emission rates will typically be quite low.

All other physical property data used were from estimates of the various telomer products and/or intermediates that are normally processed at the two sites.

Vapor Phase Composition Calculations

The composition of the vapor phase during all processing steps was determined by calculating the partial pressure of the PFOA above the organic solution using Raolt's law and the ideal gas law.

The use of Raolt's law implies that the liquid solution is ideal and that the activity coefficient of PFOA out of telomers is 1.0. For similar compounds this would normally be a reasonable first pass assumption, however there is no measured vapor-liquid equilibrium data to verify that this is indeed the case. As a result the partial pressure could be greater (positive deviation systems) or less (negative deviation systems) than calculated by Raolt's law.

The use of the ideal gas law implies that all processing steps are at low to medium pressures (below 100 psig). This is indeed the case, as the highest pressure encountered in processing is 55 psig.

The calculation of vapor composition also assumes that the vapor is primarily nitrogen such that the molecular weight of the vapor is approximately 28 lb/lbmole. Based on processing temperatures and available vapor pressure data this is a reasonable assumption.

The mole fraction of PFOA in the vapor is therefore calculated as follows:

$$y = x (\text{VP}) / P_{\text{tot}}$$

where y and x represent mole fractions of PFOA in the vapor and liquid phases respectively. Total pressure of the system is represented as P_{tot} and VP represents the vapor pressure of PFOA at the liquid temperature.

Liquid Phase Composition Calculations

The liquid phase composition was determined by analysis and is altered only when additions are made to the vessel contents. To be conservative, during a distillation or evacuation step (low boiler removal) it was assumed that the composition of any vapor leaving the condenser was based on the partial pressure above the vessel contents at the condenser temperature. Since the PFOA content in the condenser liquid will be lower than in the vessel this assumption may be quite conservative in estimating the emissions.

During processing steps in which other materials are added to the vessel the vapor displaced is assumed to be at the partial pressure prior to dilution. Subsequent process steps take credit for any dilution effects provided by addition of other materials.

When two liquid phases are present (water additions) there is no credit taken for dilution and the liquid phase composition is assumed to remain unchanged. This results in a conservative estimate for the emissions estimates.

During processing steps if there was analytical data for PFOA content at that step, it was this value which was provided as input to the calculations.

Vapor Flow Rate Calculations

During any filling step it was assumed that the vapor displaced was equal in volume to the liquid charged to the vessel and in equilibrium with the liquid. During steps in which the vessel pressure was changed, such as in pressurization and venting or evacuation, the mass of vapor discharged was calculated using the ideal gas law and the vapor space of the particular vessel as follows:

$$\text{Total Mass of Vapor Discharged} = V \Delta P MW / (RT)$$

The mole fraction of PFOA in the vapor was determined at the initial pressure and instantaneous equilibrium assumed. Pressure let-downs were assumed to occur much faster than the mass transfer rate to the vapor during venting and/or evacuations.

Total Annual Emission Calculations

Emissions were calculated based on the operating procedures for each step of the typical area processes. These total emissions were then divided by the total batch time to arrive at an hourly rate of emission and multiplied by 8760 hours/year to arrive at an annual rate. For those processes that operated on a continuous basis the emission rate calculated was multiplied by 8760 hours/year to arrive at the annual emission rate. The following represents the total emissions calculated for the telomers area of Chambers Works and Washington Works.

Chambers Works	0.9 lbs/yr
Washington Works	0.16 lbs/yr