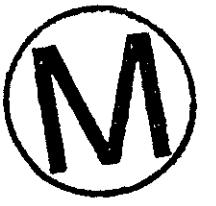

APPENDIX A
DERIVATION OF RELATIONSHIPS FOR THE AIR-FLOW MODELS

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A1.0 Introduction

This appendix shows the unrestricted and restricted air-flow models used to determine the performance of the panel closure system alternatives. These analyses are order-of-magnitude estimates of the volume of gas that might flow through the panel seal systems at the Waste Isolation Pilot Plant (WIPP).

A2.0 Model for Unrestricted Flow of VOCs

A model for the unrestricted flow of volatile organic compounds (VOC) was developed to predict the mass flow rates of VOCs and to compare this mass flow rate to the design migration limit for VOCs. As gas generation and panel volumetric creep closure proceed, a mixture of gases containing the VOC concentrations flows from each waste container. It is assumed for the unrestricted flow model that the headspace concentrations serve as a constant source of VOCs. This assumption is highly conservative, because most containers only have trace quantities of VOCs either trapped in the headspace or adsorbed on the surfaces of the various waste forms. It is believed that only a small number of waste containers have significantly greater sources of VOCs, such as a solvent-soaked rag or a can containing residual partially dried paint. Only these waste containers have a likelihood of maintaining a constant headspace VOC concentration as gas generation proceeds. However, the exact proportion of waste containers with higher VOC concentrations versus those with trace quantities is currently unknown. These data are based on results of the characterization of approximately 500 transuranic (TRU) mixed waste drums at the Idaho National Engineering Laboratory (INEL) and Rocky Flats.

The VOCs migrate due to advection from volumetric closure of the panel void space at a rate of about 28,250 ft^3 (800 m^3) per year. Gas generation for the waste inventory at a rate of 0.1 mole per drum per year (8,200 moles per panel per year) results in a volumetric flow rate of 7,060 ft^3 (200 m^3) per year. Because flow is unrestricted, the VOCs migrate under a pressure of one atmosphere. Other assumptions in the unrestricted model are as follows:

- Any gases released into the mine atmosphere would be reduced in concentration by 460,000[1] cfm of uncontaminated air. The mass flow rate of individual VOCs from individual panels following their closure is summed to determine the mass flow rate of VOCs through the exhaust shaft.

- This calculation considers the schedule for closure of individual panels as illustrated in Figure A-1 during the operational life of the WIPP. The VOC mass flow rate changes with time, with the maximum mass flow release occurring after 10 panel equivalents have been closed, about 25 years.

- Each VOC is analyzed in the calculations. Carbon tetrachloride is the most restrictive VOC in terms of satisfying the health-based levels for individual VOCs.

- Open panels of waste will not be considered as a source contributing to the emissions for a no-migration demonstration.

Considering only advection to result in the migration of VOCs, the mass-balance relationship is:

$$C_p * Q_p = C_{es} * Q_{es}$$

where

C_p = Head space concentration for an individual VOC
Q_p = Flow rate of VOCs from the panel that may vary with time
C_{es} = Concentration of VOCs at the exhaust shaft.
Q_{es} = Underground ventilation flow rate for the exhaust shaft

Air dispersion modeling is used for evaluating the receptor concentrations at the WIPP site boundary based upon the exhaust shaft source term. The air dispersion modeling considers such factors as meteorological data, release velocity, release temperature, and proximity of the WIPP site boundary to the exhaust shaft. The results of the modeling are expressed as a ratio R of the concentration at the exhaust shaft to the concentration at at the WIPP site boundary:

$$C_{es} \leq RC_{hbl}$$

This inequality can be expressed in terms of mass flow rate:

[1]The design ventilation rate for the WIPP underground is 425,000 standard cfm (12,000 standard m^3 per minute) under standard temperature and pressure conditions of 25 degrees Celsius and 1 atmosphere. The ventilation flow rate of 460,000 cfm (13,025 m^3 per minute) is the observed ventilation rate at the repository horizon under actual temperature and pressure conditions.

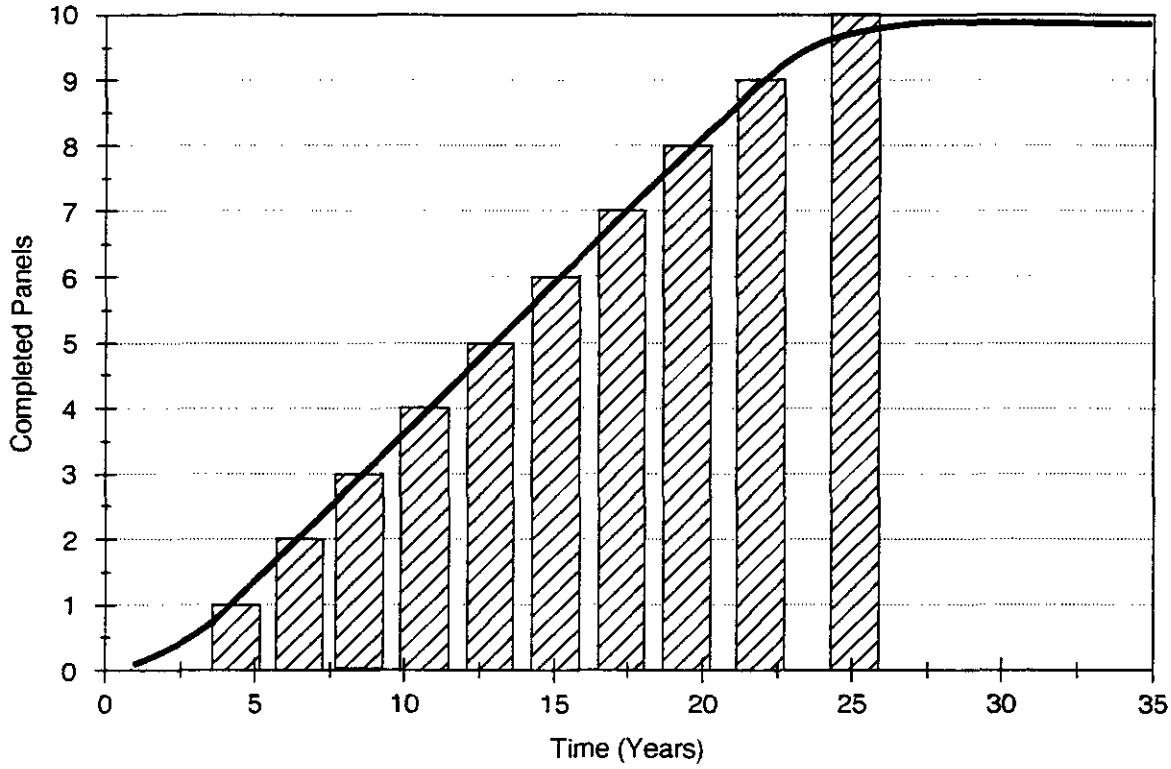

Figure A-1
Schedule for Panel Completion

$$\frac{C_p * Q_p}{Q_{es}} * \frac{1}{R} \leq C_{hbl}$$

where

R = Ratio of the concentrations at the exhaust shaft to the concentrations at the WIPP site boundary

C_{hbl} = Concentration to satisfy the health-based level for the individual VOC.

The ratio of the concentrations at the WIPP site boundary, R equals 10,753, reflecting the substantial atmospheric dispersion in reducing the concentration of VOCs.

The flow rates of VOCs from the panels are calculated for two mechanisms, gas generation and volumetric closure, using the following:

$$Q_p = Q_{gr} + Q_c$$

where

Q_{gr} = Volumetric flow rate due to gas generation[2] (200 m^3 per year per panel)

Q_c = Volumetric flow rate due to panel volumetric closure (800 m^3 per year per panel).

Table A-1 presents the closed panel release limits (migration limits) for VOCs based upon the health-based concentrations of individual VOCs. This inequality can be rewritten as:

$$C_p \cdot Q_p \leq C_{hbl} \cdot Q_{es} \cdot R$$

Table A-2 presents for a single closed panel and ten equivalent closed panels, the release rate for individual VOCs at the end of the 35-year operating period.

For the WIPP site boundary, the VOC concentrations are reduced substantially in the atmosphere. The above analysis shows that the concentration at the WIPP site boundary would be approximately 4 orders of magnitude lower than the concentration at the exhaust shaft. The predicted VOC mass flow rates due to unrestricted flow suffice to comply with the

[2]The volumetric flow due to gas generation is calculated as the gas generation rate (0.1 moles per drum per year) times the number of drums within a panel times the specific volume under atmospheric pressure.

Table A-1
Closed Panel Release Limits for VOCs

Compound	WIPP Site Boundary Health-Based Exposure Level[a] (micrograms per cubic meter)	Exhaust Shaft Concentration Migration Limit (micrograms per cubic meter)	Closed Ten Panel Migration Limit (grams per minute)
Carbon disulfide	10.00	107,530	1,400
Carbon tetrachloride	0.13	1,398	18
Chlorobenzene	20.00	215,060	2,801
Chloroform	0.09	968	13
1,1-dichloroethylene	0.40	4,301	56
Methyl ethyl ketone	1000.00	10,753,000	140,045
Methylene chloride	4.26	45,808	597
1,1,2,2-tetrachoroethane	0.35	3,764	49
Toluene	400.00	4,301,200	56,018

Table A-2
Closed Panel Release Rates for VOCs

Compound	Average Headspace Concentration (milligrams per cubic meter)[a]	Single-Panel Volumetric-Release Rate (cubic meters per minute)	Ten-Panel Volumetric-Release Rate (cubic meters per minute)	Single-Panel Mass-Release Rate (grams per minute)	Ten-Panel Mass-Release Rate (grams per minute)
Carbon disulfide	0.41	0.0019	0.019	7.80×10^{-7}	7.80×10^{-6}
Carbon tetrachloride	3625.77	0.0019	0.019	6.90×10^{-3}	6.90×10^{-2}
Chlorobenzene	63.99	0.0019	0.019	1.22×10^{-4}	1.22×10^{-3}
Chloroform	76.79	0.0019	0.019	1.46×10^{-4}	1.46×10^{-3}
1,1-dichloroethylene	48.68	0.0019	0.019	9.26×10^{-5}	9.26×10^{-4}
Methyl ethyl ketone	241.73	0.0019	0.019	4.60×10^{-4}	4.60×10^{-3}
Methylene chloride	3387.03	0.0019	0.019	6.45×10^{-3}	6.45×10^{-2}
1,1,2,2-tetrachloroethane	69.65	0.0019	0.019	1.33×10^{-4}	1.33×10^{-3}
Toluene	105.51	0.0019	0.019	2.01×10^{-4}	2.01×10^{-3}

[a]Westinghouse Electric Corporation, 1995, "Underground Hazardous Waste Management Unit Closure Criteria for the Waste Isolation Pilot Plant Operational Phase," *WID/WIPP-2038*, Westinghouse Electric Corporation, Waste Isolation Division, Carlsbad, New Mexico.

closed ten-panel migration limit based upon the health-based levels at the WIPP site boundary over the operational life of the repository.

A3.0 Air Model

The modeling assumptions for the restricted air-flow model are as follows:

- The gases are generated at a specified rate (0.10 moles per drum per year).
- The gases flow out of the panel entries according to Darcy's law under quasi-steady state conditions.
- The gases within the pore space obey the ideal gas law
- The rates of gas generation, gas outflow, and change in compressive storage must balance.
- Hydrodynamic dispersion is neglected in the analysis.

After panel closure, the volume, moles of gas, and pressure are changing as functions of time. The ideal gas law (Hiller and Herber, 1960) is written as:

$$p = \frac{n * R * T}{V}$$

where

p = Pressure
n = Moles of gas in the panel
R = Universal gas constant
T = Absolute temperature
V = Volume

Differentiating with respect to t and using the chain rule, we obtain the following relationship:

$$\frac{dp}{dt} = R * T * \frac{\frac{dn}{dt} * V - n * \frac{dV}{dt}}{V^2}$$

The volumetric closure rate is negative and constant as discussed below. The rate at which gas enters the panel minus the rate that gas leaves the panel must equal the change in moles stored. We obtain the mass-balance relationship:

$$\frac{dn}{dt} = g_r - \frac{p}{R*T} * K_s * \frac{A}{L} * \frac{p - p_{atm}}{\gamma}$$

where

g_r	=	Panel gas generation rate
p_{atm}	=	Atmospheric pressure
γ	=	Air density
K_s	=	Effective panel closure system conductivity
A	=	Cross-sectional area
L	=	Length of flow path

We define the conductance (C) as:

$$C = K_s * \frac{A}{L}$$

and substituting into the ordinary differential equations (ODE), we obtain

$$\frac{dp}{dt} = R*T* \frac{g_r - \frac{p}{R*T} * C * \frac{p - p_{atm}}{\gamma} * V - n * \frac{dV}{dt}}{V^2}$$

$$\frac{dn}{dt} = g_r - \frac{p}{R*T} * C * \frac{p - p_{atm}}{\gamma}$$

These two first-order coupled ODEs can be solved by a simple explicit finite difference technique:

$$p_j = p_{j-1} + R * T * \frac{g_r - \frac{p_{j-1}}{R*T} * C * \frac{p_{j-1} - p_{atm}}{\gamma} * V - n_{j-1} * \frac{dV}{dt}}{V^2} * \Delta t$$

$$n_j = n_{j-1} + g_r - \frac{p_{j-1}}{R*T} * C*\frac{p_{j-1} - p_{atm}}{\gamma}\Delta t$$

where

p_j, n_j = the pressure and moles of gas at the current time step
P_{j-1}, n_{j-1} = the pressure and moles of gas at the previous time step

subject to the boundary condition that the initial pressure equals atmospheric pressure, and the initial moles of gas can be determined by the ideal gas law at initial volume and pressure. Further note that the volume can be expressed as the linear function:

$$V(t) = \alpha * t + \beta$$

where

α = slope of the volume-time relationship
β = intercept of volume-time relationship
t = time

These expressions can be substituted into the above explicit finite difference relationships, and the pressure and molar air flow rates determined as functions of time.

$$\frac{dV}{dt} = \alpha$$