MARTIN MARIETTA

Calculational Methods for Analysis of Postulated UF$_6$ Releases

W. R. Williams

OPERATED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

NRC FORM 335 (11-81)	U.S. NUCLEAR REGULATORY COMMISSION **BIBLIOGRAPHIC DATA SHEET**	1. REPORT NUMBER *(Assigned by DDC)* NUREG/CR-4360, Vol. 1 ORNL/ENG/TM-31/V1

4. TITLE AND SUBTITLE *(Add Volume No., if appropriate)* Calculational Methods for Analysis of Postulated UF$_6$ Releases	2. *(Leave blank)*
	3. RECIPIENT'S ACCESSION NO.

7. AUTHOR(S) W. R. Williams	5. DATE REPORT COMPLETED MONTH August YEAR 1984

9. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS *(Include Zip Code)* Oak Ridge National Laboratory Post Office Box X Oak Ridge, TN 37831	DATE REPORT ISSUED MONTH September YEAR 1985
	6. *(Leave blank)*
	8. *(Leave blank)*

12. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS *(Include Zip Code)* Division of Risk Analysis and Operations Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission Washington, DC 20555	10. PROJECT/TASK/WORK UNIT NO.
	11. FIN NO. B0495

13. TYPE OF REPORT Topical	PERIOD COVERED *(Inclusive dates)*

15. SUPPLEMENTARY NOTES	14. *(Leave blank)*

16. ABSTRACT *(200 words or less)*

Calculational methods and computer programs for the analysis of source terms for postulated releases of UF$_6$ are presented. Required thermophysical properties of UF$_6$, HF, and H$_2$O are described in detail. UF$_6$ reacts with moisture in the ambient environment to form HF and H$_2$O. The coexistence of HF and H$_2$O significantly alters their pure component properties, and HF vapor polymerizes. A release rate model of UF$_6$ is presented that considers the transient conditions inside containment and the flashing, multiphase flow of UF$_6$ along the release pathway. Transient compartment models for simulating UF$_6$ releases inside rooms ventilated by forced- and induced-draft systems are also described. The basic compartment model mass and energy balances are supported by simple heat transfer, ventilation system, and deposition models. A model that can simulate either a closed compartment or a steady-state ventilation system is also discussed. Listings of all main programs (including two plotting routines) and subroutines are included. Example problems illustrate the analysis of postulated releases using the described programs.

17. KEY WORDS AND DOCUMENT ANALYSIS   17a. DESCRIPTORS

uranium hexafluoride (UF$_6$)	cylinder	computer codes
accidents	cold trap	compartment models
scenarios	pigtail	release rate models
releases	fuel cycle	physical and thermodynamic properties
analysis	modeling	

17b. IDENTIFIERS/OPEN-ENDED TERMS

18. AVAILABILITY STATEMENT unlimited	19. SECURITY CLASS *(This report)* unclassified	21 NO. OF PAGES 134
	20. SECURITY CLASS *(This page)* unclassified	22 PRICE s 16.95

NRC FORM 335 (11-81)

Martin Marietta Energy Systems, Inc., Engineering
Process Engineering

Calculational Methods for Analysis of Postulated UF$_6$ Releases

W. R. Williams

CONTENTS

Volume 1

Volume 2

ACKNOWLEDGEMENT
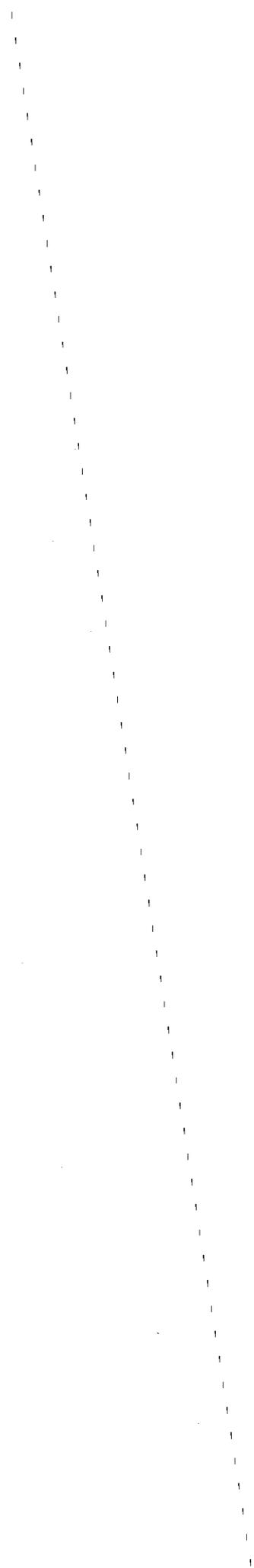
EXECUTIVE SUMMARY

The Nuclear Regulatory Commission (NRC), Office of Nuclear Regulatory Research has for several years been conducting the Fuel Cycle Facility Safety Research Program (FCFSRP) to develop methods for analyzing postulated accidents at NRC-licensed facilities. One objective of FCFSRP being carried out by the NRC Division of Risk Analysis was to develop an Accident Analysis Handbook (AAH) for use by both NRC and NRC licensees. This report provides a detailed description of calculational methods for the analysis of postulated uranium hexafluoride (UF_6) releases that were developed for inclusion in the AAH.

In an earlier report (M. Siman-Tov et al. 1984) various accident scenarios involving postulated releases of UF_6 were identified as were a number of calculational methods that would be useful for analyzing such postulated accidents. From among the calculational methods identified, several methods were selected as necessary for a first-order approximation of accident consequences. This report describes the implementation of most of those selected methods into a series of computer programs that can be used for analysis of postulated UF_6 releases.

When UF_6 is released from containment into moist air, it will react with the water vapor in the air to form hydrogen fluoride (HF) and uranyl fluoride (UO_2F_2). In modeling postulated releases, UF_6 is encountered in solid, liquid, and vapor phases. HF and H_2O can exist in liquid and vapor phases, and their coexistence significantly affects their vapor pressures and liquid-phase enthalpies. Self-association (polymerization) of HF vapor also occurs. Correlations for various physical and thermodynamic properties are presented in Chap. 2. The solid-vapor composition to be expected from the flashing of UF_6 liquid is also discussed.

Chapter 3 discusses simulating releases of UF_6 from cylinders through either a breach or a broken (or misvalved) piping system. Because of the equilibrium phase behavior of UF_6, multiphase flow frequently occurs. A major complicating factor is the existence of the UF_6 triple point at about 22 psia, a pressure frequently lying between the pressure of UF_6 in containment and the pressure of the surroundings. The description of analysis methods for determining release rates is generalized for a multicomponent system; however, the implementation of these methods into computer models is limited to UF_6. The simulation of the phase behavior of UF_6 within containment as a function of initial conditions, mass flow rates into and out of containment, and heating rate is also discussed.

Although the methods discussed in Chap. 3 can be used for developing source terms for outdoor releases of UF_6, additional methods are needed for analyzing releases postulated to occur indoors. These methods, which are incorporated into compartment models, are discussed in Chap. 4. A number of simple models has been developed to simulate heat transfer, flow-through ventilation system components, and deposition. Mass and energy balances within a compartment are also presented.

Four main programs that use an extensive set of common subroutines have been developed for simulating postulated accident releases of UF_6.

- CYLIND simulates the transient release of UF_6 from containment through a breach or piping system.

- FODRFT and INDRFT are used to simulate transient behavior resulting from the release of UF_6 inside compartments ventilated by forced-draft and induced-draft ventilation systems, respectively.

- BATCH is a closed compartment model (no ventilation) with an "open-compartment" option that allows it to be used to simulate a steady-state release directly into a forced-draft ventilation system exhausting to a known pressure.

Preceding page blank

Input requirements for CYLIND are given in Chap. 3, and input requirements for FODRFT, INDRFT, and BATCH are given in Chap. 4. Two plotting programs have also been written using DISSPLA version 9.0 subroutines. CYLPLT plots output from CYLIND, and COMPLT plots output from FODRFT and INDRFT. Listings of the main programs are provided in Appendix A. Appendix B lists all subroutines required by CYLIND, FODRFT, INDRFT, and BATCH.

Six example problems encompassing a total of 16 cases are provided to illustrate the use of CYLIND, FODRFT, INDRFT, and BATCH. These examples include: (1) releases from cylinders (a) through a breach in the cylinder wall and (b) through a ruptured piping system, (2) releases occurring in compartments ventilated by (a) forced draft and (b) induced draft, and (3) a release into a ventilation system. Problem statements, input descriptions, and a summary of results for each example are provided in Chap. 5; complete output generally appears in Appendix C, although for two cases the output is provided in Chap. 5. Plots generated by CYLPLT and COMPLT are used to illustrate results of the example problems.

The approach used in developing the various compartment model programs lends itself to future refinement of the models used as well as to the development of more elaborate models involving multiple compartments. By virtue of its necessary inclusion in the described models as a reaction product of UF_6, the models FODRFT, INDRFT, and BATCH can also be used to simulate releases of HF.

ABSTRACT

Calculational methods and computer programs for the analysis of source terms for postulated releases of UF_6 are presented. Required thermophysical properties of UF_6, HF, and H_2O are described in detail. UF_6 reacts with moisture in the ambient environment to form HF and H_2O. The coexistence of HF and H_2O significantly alters their pure component properties, and HF vapor polymerizes. A release rate model of UF_6 is presented that considers the transient conditions inside containment and the flashing, multiphase flow of UF_6 along the release pathway. Transient compartment models for simulating UF_6 releases inside rooms ventilated by forced- and induced-draft systems are also described. The basic compartment model mass and energy balances are supported by simple heat transfer, ventilation system, and deposition models. A model that can simulate either a closed compartment or a steady-state ventilation system is also discussed. Listings of all main programs (including two plotting routines) and subroutines are included. Example problems illustrate the analysis of postulated releases using the described programs.

1. INTRODUCTION AND SUMMARY

The Nuclear Regulatory Commission (NRC), Office of Nuclear Regulatory Research (NRR), initiated the Fuel Cycle Facility Safety Research Program (FCFSRP) to develop predictive methods for analyzing postulated accidents at NRC-licensed facilities. In mid-1982, FCFSRP was expanded to include the development of accident scenarios and analytical methods pertaining to the release of uranium hexafluoride (UF_6). Union Carbide Corporation, Nuclear Division (UCC-ND), the operating contractor for the Oak Ridge National Laboratory (ORNL) and two of the three gaseous diffusion plants located in the United States,* was selected to develop the UF_6-related material. One objective of FCFSRP being carried out by the NRC Division of Risk Analysis (DRA) was to develop an Accident Analysis Handbook (AAH) to be used for NRC licensing and by NRC licensees. This report provides a more detailed description of material planned for inclusion in the AAH.

In an earlier report (Siman-Tov 1984), various accident scenarios involving postulated releases of UF_6 were identified, as were a number of calculational methods which would be useful for analyzing such postulated accidents. From among the calculational methods identified, several methods were selected as necessary for a first-order approximation of accident consequences. This report describes the implementation of most of those selected methods into a series of computer programs that can be used for analysis of postulated UF_6 releases.

When UF_6 is released from containment into moist air, it will react with the water (H_2O) vapor in the air to form hydrogen fluoride (HF) and uraynl fluoride (UO_2F_2). In modeling postulated releases, UF_6 is encountered in solid, liquid, and vapor phases, whereas both HF and H_2O can exist in liquid and vapor phases. Self-association (polymerization) of HF also occurs. Correlations for various physical and thermodynamic properties are presented in Chap. 2, along with information on subroutines in which the correlations have been implemented.

Chapter 3 discusses simulating releases of UF_6 from cylinders through either a breach in containment or a broken (or misvalved) piping system. Because of the equilibrium phase behavior of UF_6, multiphase flow frequently occurs. A major complicating factor is the existence of the UF_6 triple point at about 22 psia, a pressure frequently lying between the pressure of UF_6 in containment and the pressure of the surroundings. In addition to subroutines for flow rate analysis, subroutines for modeling UF_6 phase behavior inside containment are also included in Chap. 3.

Although the methods discussed in Chap. 3 can be used for developing source terms for outdoor releases of UF_6, additional methods are needed for analyzing releases postulated to occur indoors. Such methods are discussed in Chap. 4. A number of subroutines based on simple models have been developed to simulate heat transfer, flow through ventilation system components, and deposition. A subroutine has also been written to perform mass and energy balances within a compartment given initial compartment conditions and inlet and outlet stream conditions. Two main programs have been written to model the transient behavior in compartments ventilated by either forced draft or induced draft. Another main program has been written to model a release into a closed compartment or a steady release of UF_6 into a ventilation system supplied by a constant volume blower. These main programs are described in Sect. 4.6.

In Chap. 5, several example problems are given to demonstrate the use and input required for the various main programs described. These examples include: (1) releases from cylinders through

---

*On April 1, 1984, Martin Marietta Energy Systems, Inc., took over responsibility as operating contractor of these facilities.

a breach in the cylinder wall and through a ruptured piping system, (2) releases occurring in compartments ventilated by forced draft and induced draft, and (3) a release into a ventilation system.

Two plotting programs have also been developed using DISSPLA version 9.0. One program, described in Chap. 3, is used to plot selected output from the main cylinder release program. The other program, described in Chap. 4, is used to plot output from either of the transient-compartment model main programs. Plots generated by these programs are used to illustrate the results of example problems in Chap. 5.

Listings of all main programs are provided in Appendix A. All subroutines are listed in Appendix B. Program output for most of the example problems presented in Chap. 5 are provided in Appendix C.

2. PHYSICAL AND THERMODYNAMIC PROPERTIES MODELS

The modeling of UF_6 releases requires consideration of various physical and thermodynamic properties for UF_6, HF, H_2O, UO_2F_2, and air. The moisture in the air reacts with UF_6 to form HF and UO_2F_2. Section 2.1 presents properties for solid, liquid, and vapor UF_6. Because of the strong interaction between HF and H_2O, properties for these compounds in both the liquid and vapor phase are discussed together in Sect. 2.2. Subroutines for the properties discussed in Sects. 2.1 and 2.2 are discussed at the end of each section, respectively. Properties of air and UO_2F_2, which occur as a vapor and solid, respectively, are given in Sect. 2.3. In Sect. 2.4, the method and subroutine used for calculating mixture enthalpies are described.

2.1 URANIUM HEXAFLUORIDE

At room temperature uranium hexafluoride (UF_6) is a colorless volatile solid that forms transparent crystals of high refractive index. The crystals sublime without melting under atmospheric pressure; when heated at pressures greater than about 22 psia, they melt to form a clear, colorless, liquid of high density. The sublimation point (at atmospheric pressure) is about 133.8°F. Despite the high molecular weight of UF_6, the properties of its vapor closely approximate those of an ideal gas. A phase diagram for UF_6 is given in Fig. 1, and some commonly used properties of UF_6 are presented in Table 1. The physical properties correlations given in this

ORNL-DWG-85c-15258

LIQUID

SOLID

TRIPLE POINT
147.3 °F, 22.04 psia

VAPOR

PRESSURE (psia)

TEMPERATURE (°F)
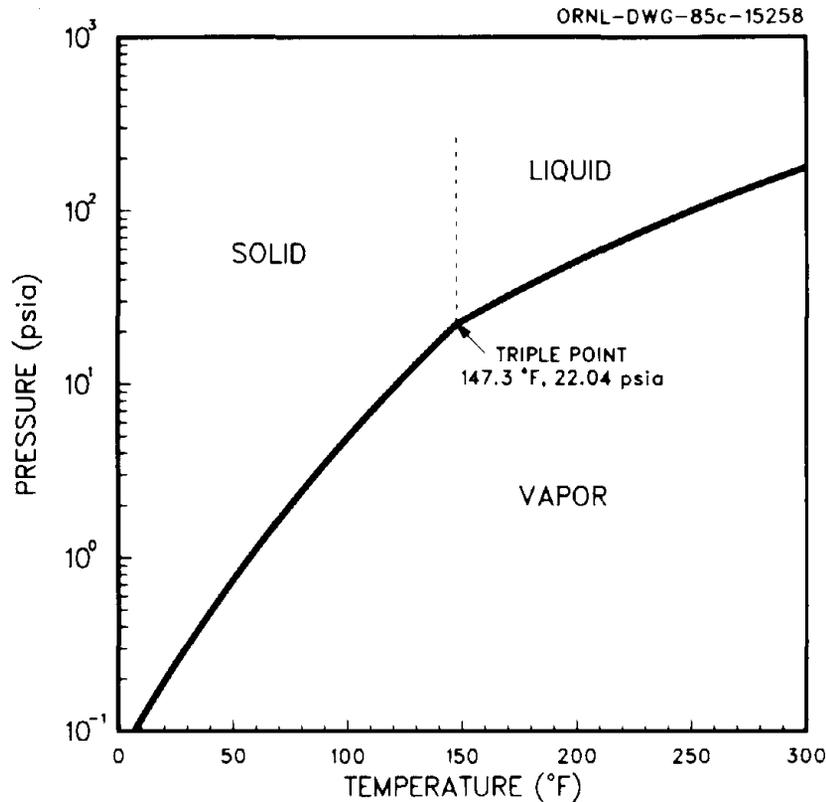
Fig. 1. Phase diagram for uranium hexafluoride. The curve separating the vapor region from the condensed regions corresponds to the vapor pressure of UF_6.

3

Table 1. Properties of uranium hexafluoride

Characteristics	Value
Chemical formula	UF_6
Molecular weight	
$^{235}UF_6$	349
$^{238}UF_6$	352
Sublimation point at 14.7 psia	133.8°F
Density of solid at 68°F	318 lb/ft³
Critical temperature	446°F
Critical pressure	669 psia
Triple point data	
Vapor pressure	22.04 psia
Temperature	147.3°F
Density of solid	303 lb/ft³
Density of liquid	227 lb/ft³
Density of vapor	1.25 lb/ft³
Heat of sublimation	59.5 Btu/lb
Heat of fusion	23.5 Btu/lb
Heat of vaporization	36.0 Btu/lb
Thermal conductivity	
−53 to −28°F (solid) (average)	0.234 Btu/(hr-ft-°F)
95 to 133°F (solid) (average)	0.328 Btu/(hr-ft-°F)
162°F (liquid)	9.27×10^{-2} Btu/(hr-ft-°F)

section in engineering units are based on correlations or data reported by DeWitt (1960) unless otherwise referenced.

Sections 2.1.1 through 2.1.8 cover correlations for evaluating vapor pressure, the vapor phase compressibility factor, densities, viscosities, thermal conductivities, heat capacities, enthalpies, and entropies, respectively. Section 2.1.9 discusses other useful properties of UF_6. Not all UF_6 properties described herein are required for the cylinder and compartment models discussed subsequently. The heat of reaction of UF_6 with water is discussed in Sect. 2.1.10. Methods for performing flashing and vapor phase expansion calculations are described in Sect. 2.1.11. Subroutines for evaluating the properties of UF_6, based on correlations described in Sects. 2.1.1 through 2.1.8, are presented in Sect. 2.1.12, along with a subroutine for evaluating the saturation temperature corresponding to a given UF_6 pressure. A subroutine for performing flashing and vapor phase expansion calculations is also presented in Sect. 2.1.12.

2.1.1 Vapor Pressure

These vapor pressure correlations were recommended by DeWitt (1960, p. 81). The vapor pressure over the solid from 32°F to the triple point is given by

$$\ln P^\circ = 10.4443 + 9.64233 \times 10^{-3} T_F \tag{1}$$

$$- [3907.41/(T_F + 298.149)] \ ,$$

where

$P°$ = vapor pressure, psia,

T_F = temperature, °F.

The vapor pressure over the liquid from the triple point to 241°F is given by

$$\ln P° = 12.1600 - [4668.07/(T_F + 367.533)] \ , \tag{2}$$

and from 241°F to the critical point by

$$\ln P° = 13.7627 - [6976.11/(T_F + 511.866)] \ . \tag{3}$$

Estimated uncertainties reported by DeWitt (1960) for the three equations, based on a 95% confidence level, are ±0.05%, ±0.03%, and ±0.3%, respectively. Equations 1 and 2 intersect at a temperature of 147.3°F and a pressure of 22.04 psia, which agrees with the reported triple point (DeWitt 1960, p. 89). Equations 2 and 3 do not intersect, but it was observed that Eq. 3 overestimated vapor pressure from 240 to 276°F, whereas Eq. 2 underestimated the reported data of Oliver et al. over the same range (DeWitt, 1960, p. 85). To obtain a continuous function for vapor pressure, a weighted function combining Eqs. 2 and 3 was developed which yielded better agreement with the reported data than either equation individually, as shown in Table 2. The new equation, used in the computer subroutine VPRUF6 for the estimation of vapor pressure between 240 and 276°F is

$$P° = [(276 - T_F)P_2 + (T_F - 240)P_3]/36 \ , \tag{4}$$

where

P_2 = vapor pressure evaluated at T_F using Eq. 2,

P_3 = vapor pressure evaluated at T_F using Eq. 3.

Table 2. Comparison of predicted UF$_6$ vapor pressure, using Eqs. 2, 3, and 4 to the data of Oliver et al.[5]

Temperature (°F)	Vapor pressures (psia)			
	Oliver et al.	Eq. 2	Eq. 3	Eq. 4
240.85	88.888	88.862	89.549	88.878
255.51	106.59	106.44	106.89	106.64
271.74	128.97	128.75	129.04	129.01

A plot of vapor pressure vs temperature, based on the preceeding equations, is shown in Fig. 1, the phase diagram for UF_6.

2.1.2 Equation of State and Vapor Compressibility Factor

Magnuson (DeWitt, 1960 pp. 24, 97-101) proposed an equation of state for UF_6 which may be expressed as

$$PV/RT_R = 1/(1 + aT_R^{-3}P) \ , \tag{5}$$

where

P = pressure, psia,
V = molar volume, ft^3/lb mole,
R = ideal gas constant = 10.73 psia-ft^3/lb mole-°R,
T_R = absolute temperature, °R = T_F + 459.67,
a = nonideality parameter = 4.8923 × 10^5.

The stated range over which the nonideality parameter was evaluated is 127 to 270°F.
The compressibility factor, Z, is defined by

$$Z = PV/RT_R \ . \tag{6}$$

Thus, by comparison with Eq. 5,

$$Z = 1/(1 + aT_R^{-3}P) = T_R^3/(T_R^3 + aP) \ . \tag{7}$$

Other quantities required for sonic velocity and constant volume heat capacity calculations are,

$$Z_p = Z - P(\partial Z/\partial P)|_{T_R} = 2Z - Z^2 \ , \tag{8}$$

and

$$Z_t = Z + T_R(\partial Z/\partial T_R)|_P = 4Z - 3Z^2 \ . \tag{9}$$

2.1.3 Density

The following data on the density of solid UF_6 were reported by DeWitt (1960, p. 17).

Temperature (°C)	Density (g/cm^3)
20.7	5.09 ± 0.06
25	5.06 ± 0.005
62.5	4.87

The above densities can be correlated within the reported experimental error by

$$\rho_s = 330.0 - 0.1800\,T_F \quad , \tag{10}$$

where

$$\rho_s = \text{density, lb/ft}^3 \quad .$$

The liquid density correlation is modified from the correlation of Hoge and Wechsler (DeWitt 1960, p. 19, Eq. 5). Based on data reported in DeWitt (1960, p. 20), the predicted saturated liquid density is within 0.1% of experimental data between 65 and 131°C (149 and 268°F) and within 0.22% at 162°C (324°F). Unit conversion of the Hoge and Weshsler equation, which assumed a triple point temperature of 64.052°C, yields

$$\rho_l = 250.6 - 0.1241\,T_F - 2.620 \times 10^{-4}\,T_F^2 \quad . \tag{11}$$

where

$$\rho_l = \text{density, lb/ft}^3 \quad .$$

At subatmospheric pressure, UF_6 vapor is nearly ideal. As pressure increases, the density of UF_6 vapor based on the Magnuson equation of state derived for temperatures from 127 to 270°F, which correspond to pressures from 12 to 130 psia, is given by

$$\rho_v = (MW/10.73)(P/T_R)Z \quad , \tag{12}$$

where

$$\rho_v = \text{density, lb/ft}^3,$$
$$MW = \text{molecular weight, lb/lb mole,}$$
$$P = \text{pressure, psia.}$$

This equation, which differs by about 2.5% from ideal behavior at 122°F and 10.2 psia, is used for all vapor density calculations in the computer routines discussed subsequently. Deviation from ideal behavior decreases as temperature and pressure decrease.

The densities of solid and liquid UF_6 are plotted as functions of temperature in Fig. 2. The density of UF_6 vapor as a function of temperature and pressure assuming a molecular weight of 352 lb/lb mole is plotted in Fig. 3.

2.1.4 Viscosity

The viscosity correlation of Blatt for liquid UF_6 between 158 and 410°F (DeWitt 1960, p. 44) yields

$$\mu_l = 0.404\exp[(997 + 0.041\,P)/T_R] \quad , \tag{13}$$
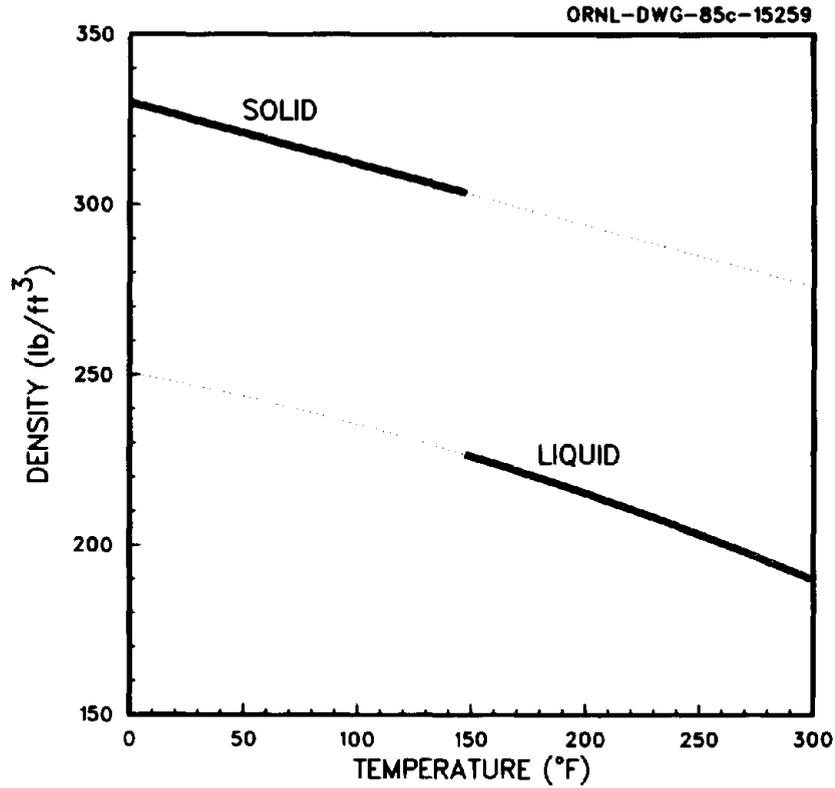
Fig. 2. Density of solid and saturated liquid uranium hexafluoride. The dotted lines represent extrapolated density values used when converging the mass/energy/volume balance for UF_6 inside a cylinder (see Sect. 3.1.1).
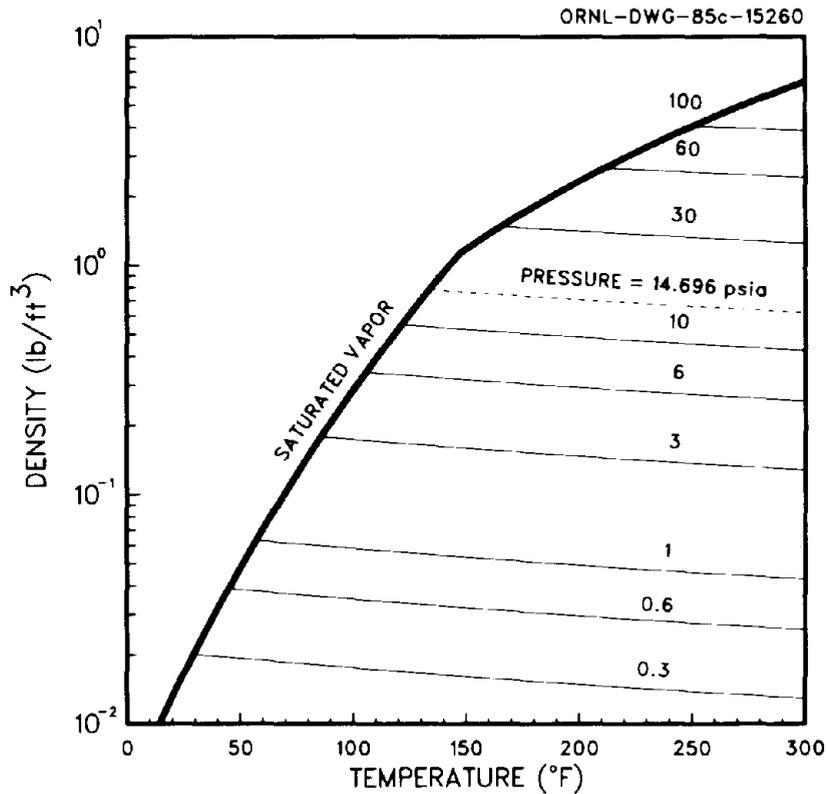
Fig. 3. Density of uranium hexafluoride vapor.

where

μ_l = viscosity, lb_m/ft-hr.

Note that the sum of the terms in the numerator of the exponential function agrees with Blatt's data reported by DeWitt (1960, Table 25, p. 42) rather than the difference. An expression reported by DeWitt (1960, p. 39, Eq. 18) for vapor viscosity was found to be in error when compared to reported experimental data (DeWitt 1960, p. 41). New coefficients were evaluated yielding the expression,

$$\mu_v{}^* = 0.8516\ T_K^{0.9305}\ ,\tag{14}$$

where

$\mu_v{}^*$ = viscosity, micropoise,

T_K = absolute temperature, K.

The data of Myerson and Eicher (DeWitt 1960, p. 41) are shown below along with predicted values obtained using Eq. 14. After conversion of units, vapor viscosity is given by

$$\mu_v = 1.192 \times 10^{-4}\ T_R^{0.9305}\ ,\tag{15}$$

where

μ_v = viscosity, lb_m/ft-hr.

Temperature (°C)	Viscosity (micropoise)	
	Myerson & Eicher	Eq. 14
40	178.7	178.8
60	189.0	189.4
80	199.9	200.0
110	216.1	215.7
140	231.9	231.4
170	248.0	247.1
200	261.1	262.5

The viscosity of liquid UF_6 as a function of temperature and pressure is plotted in Fig. 4 and of UF_6 vapor as a function of temperature in Fig. 5.

2.1.5 Thermal Conductivity

The average thermal conductivity of solid UF_6 between -53 and $-28°F$ is 0.234 Btu/hr-ft-°F and between 95 and 133°F is 0.328 Btu/hr-ft-°F (Barber 1983). Assuming a linear relationship between thermal conductivity and temperature,

$$k_s = 0.2586 + 0.0006084\ T_F\ ,\tag{16}$$
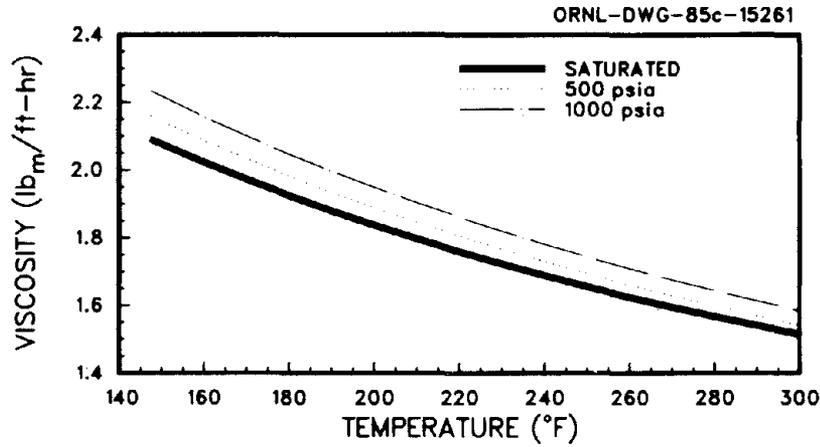
Fig. 4. Viscosity of liquid uranium hexafluoride.
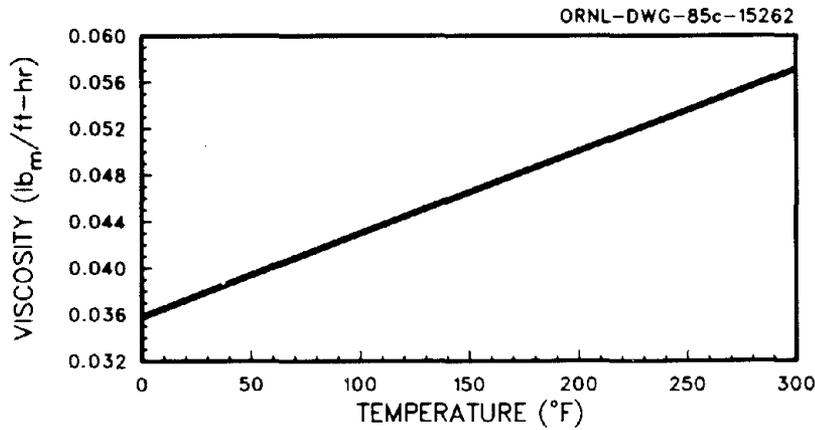
Fig. 5. Viscosity of uranium hexafluoride vapor.

where

k_s = thermal conductivity, Btu/hr-ft-°F.

A single value of thermal conductivity having a reported accuracy of ±3% for liquid UF_6 at 162°F is reported by DeWitt (1960, p. 46). Review of several sources showed the following general form for expressing thermal conductivity of a liquid:

$$k_l = (BC_{p,l}\rho_l^{4/3})/T_R \ ,$$ (17)

where B is an empirical constant. Using the reported value of thermal conductivity along with estimated values of heat capacity and density, B was evaluated yielding the following correlation for the thermal conductivity of liquid UF_6:

$$k_l = (0.3247 \ C_{p,l}\rho_l^{4/3})/T_R \ ,$$ (18)

where

k_l = thermal conductivity, Btu/hr-ft-°F,

$C_{p,1}$ = liquid heat capacity, Btu/lb-°F.

The thermal conductivity of UF$_6$ vapor based on DeWitt (1960; p. 44, Eq. 25) is given by

$$k_v = 3.27 \times 10^{-3}(1 + 0.0025\, T_F) \ ,$$ (19)

where

k_v = thermal conductivity, Btu/hr-ft-°F.

Equation 19 was reported by DeWitt (1960) as representing the most reliable thermal conductivity values between 32 and 212°F.

The thermal conductivities of UF$_6$ solid, liquid, and vapor are plotted in Fig. 6.

2.1.6 Heat Capacity

DeWitt presented a series of heat capacity, enthalpy, and entropy correlations for solid, liquid, and vapor UF$_6$ (1960, pp. 56-70). Several of these correlations contained typographical errors;
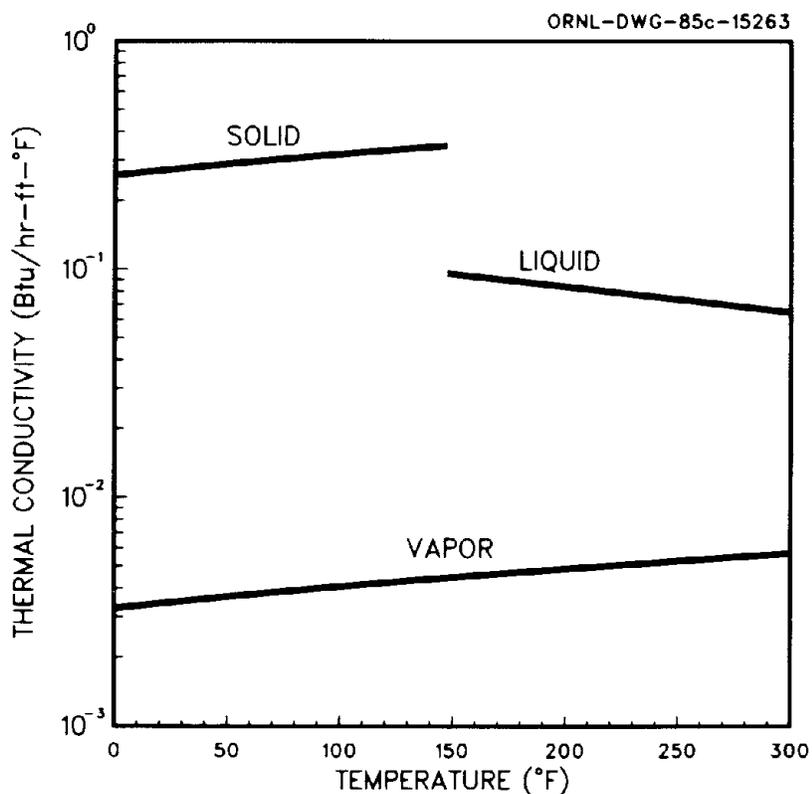
Fig. 6. Thermal conductivity of solid, liquid, and vapor uranium hexafluoride.

however, since enthalpy is the integral of the heat capacity and entropy is the integral of the quotient of heat capacity and temperature, errors were identified and corrected prior to converting the correlations to engineering units. Tabular data reported by DeWitt (1960, p. 59) beyond the range of applicability of the equations presented below imply the reference state for these correlations is solid UF_6 at 0 K for which the heat capacity, enthalpy, and entropy values are zero.

The heat capacity of solid UF_6 between $-10°F$ and the triple point is given within 1% by

$$C_{p,s} = -5.70531 \times 10^{-2} + 2.55091 \times 10^{-4} T_R + (9645.63/T_R^2) \ , \tag{20}$$

where

$C_{p,s}$ = heat capacity, Btu/lb-°R.

The heat capacity of saturated liquid UF_6 from the triple point to 206°F is given within 0.6% by

$$C_{p,l} = 5.10057 \times 10^{-2} + 1.02633 \times 10^{-4} T_R + (6139.34/T_R^2) \ , \tag{21}$$

where

$C_{p,l}$ = heat capacity, Btu/lb-°R.

The correlation for the heat capacity of UF_6 vapor is reported by DeWitt (1960) to be accurate to within 1% between -10 and 440°F at atmospheric pressure. To obtain enthalpies at pressures other than 1 atm (14.696 psia), a heat capacity departure function was calculated based on taking the derivative of the enthalpy departure function given in Reid et al. (1977) after incorporating the compressibility factor obtained from the Magnuson equation of state (see Sect. 2.2). The resulting expression for the constant pressure heat capacity of UF_6 vapor is

$$C_{p,v} = [9.21307 \times 10^{-2} + 1.25253 \times 10^{-5} T_R - (2951.71/T_R^2)] \tag{22}$$

$$+ 3.0939 \times 10^{-3} [(4Z - 3Z^2)|_{P,T} - (4Z - 3Z^2)|_{14.7,T}] \ ,$$

where

$C_{p,v}$ = heat capacity, Btu/lb-°R.

Heat capacities of solid, liquid, and vapor UF_6 are plotted in Fig. 7.

The heat capacity ratio for UF_6 vapor may be estimated using the constant pressure vapor heat capacity (Reid et al. 1977, p. 134),

$$\gamma = \frac{C_{p,v}}{C_{v,v}} = \frac{MW \, C_{p,v}}{MW \, C_{p,v} - 1.9872 \, Z_t^2/Z_p} \tag{23}$$

where

γ = heat capacity ratio,
$C_{v,v}$ = constant volume heat capacity, Btu/lb-°R,
MW = molecular weight, lb/lb mole.
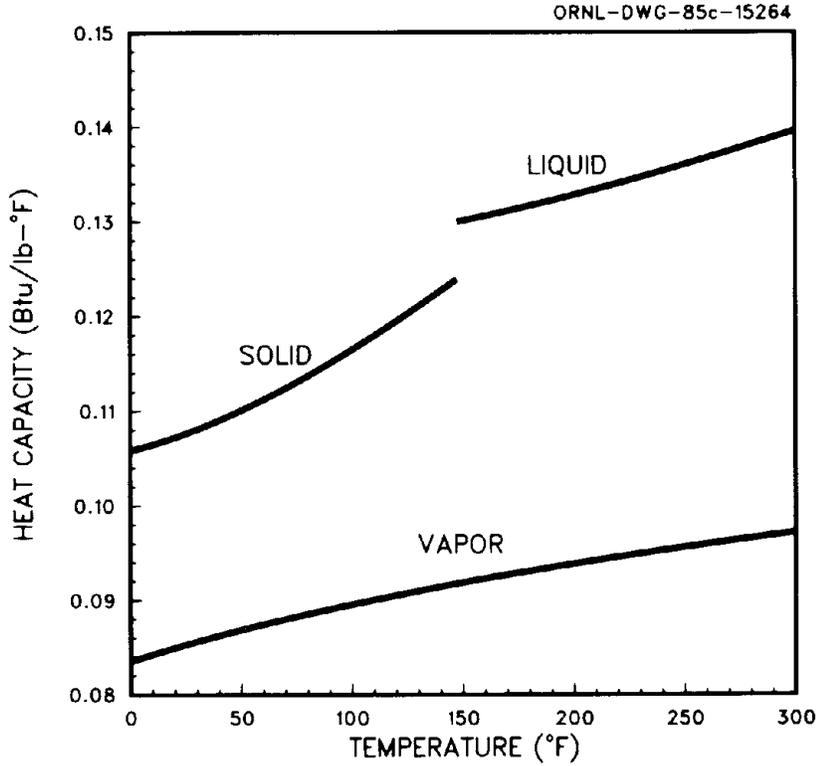
Fig. 7. Heat capacity of solid, liquid, and vapor uranium hexafluoride.

Rearrangement of Eq. 23 yields an expression for the constant volume heat capacity of UF_6 vapor,

$$C_{v,v} = C_{p,v} - (1.9872 Z_t^2 / MW Z_p) \; . \tag{24}$$

2.1.7 Enthalpy

Based on integration of the preceding heat capacity equations, the following correlations for the enthalpy of UF_6 solid, liquid, and vapor are obtained.

$$H_s = 50.4460 - 5.70531 \times 10^{-2} T_R + 1.27509 \times 10^{-4} T_R^2 \tag{25}$$

$$- (9645.63/T_R) \; ,$$

$$H_l = [30.6133 + 5.10057 \times 10^{-2} T_R + 5.13165 \times 10^{-5} T_R^2 \tag{26}$$

$$- (6139.34/T_R)] + [0.18268(P - P°)(1/\rho_l) \; ,$$

$$H_v = [43.2614 + 9.21307 \times 10^{-2} T_R + 6.26265 \times 10^{-6} T_R^2 \tag{27}$$

$$+ (2951.71/T_R)] + [3.0939 \times 10^{-3} T_R(Z|_{P,T} - Z|_{14.7,T})] \; ,$$

where

H = enthalpy, Btu/lb,

s,l,v = subscripts denoting solid, liquid, and vapor, respectively.

Equation 25 deviates from experimental values by less than 0.01% between 17°F and the triple point (147.3°F) and by less than 1% between −55 and 17°F. Equation 26, excluding the last term, is stated (DeWitt 1960, p. 59) to deviate from experimental values by less than 0.01%; however, a temperature range of applicability was not given (a range of 147.3 to 206°F might be assumed based on heat capacity correlations). The last term in Eq. 26 is a correction for supersaturated liquids, assuming an incompressible fluid. No estimate of deviation from experimental values is available for the vapor enthalpy. Heats of vaporization, sublimation, and fusion may be obtained by using these equations. Enthalpies of saturated UF_6 solid, liquid, and vapor are plotted in Fig. 8.

2.1.8 Entropy

Use of the preceding heat capacity equations in integrating $dS = (C_p/\text{T})dT$ leads to the following entropy equations for UF_6 solid, liquid, and vapor.
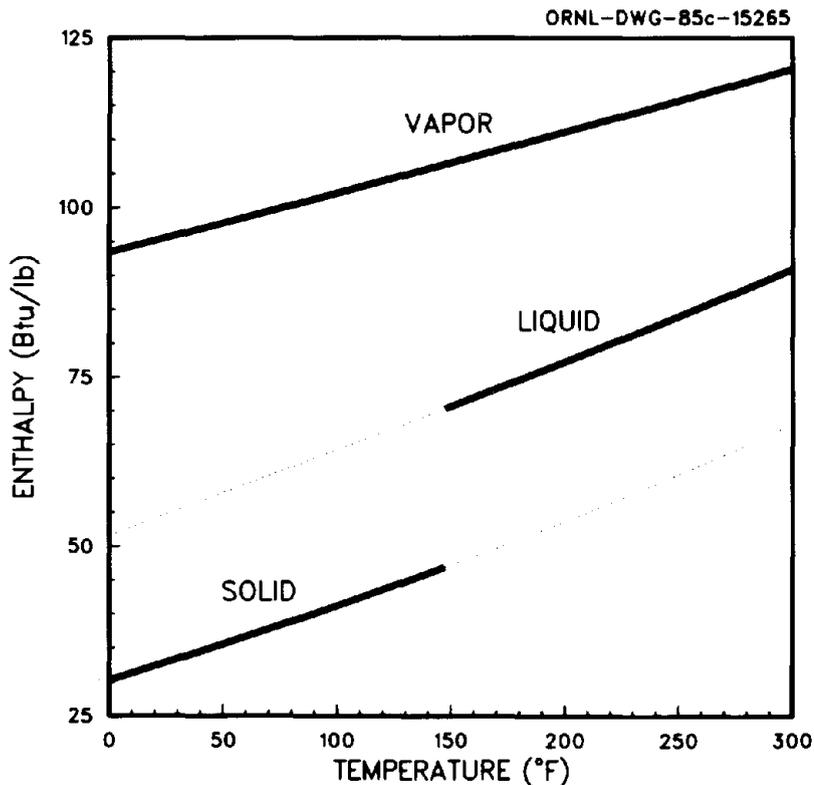
Fig. 8. Enthalpy of solid, liquid, and vapor uranium hexafluoride. The dotted lines represent extrapolated enthalpy values used when converging the mass/energy/volume balances for UF_6 inside a cylinder.

$$S_s = 0.393535 - 5.70531 \times 10^{-2} \ln T_R \tag{28}$$

$$+ 2.55019 \times 10^{-4} T_R - (4822.82/T_R^2) \ ,$$

$$S_l = -0.172963 + 5.10057 \times 10^{-2} \ln T_R \tag{29}$$

$$+ 1.02633 \times 10^{-4} T_R - (3069.67/T_R^2) \ ,$$

$$S_v = -0.332704 + 9.21307 \times 10^{-2} \ln T_R + 1.25237 \times 10^{-5} T_R + (1475.86/T_R^2) \ , \tag{30}$$

$$+ 3.0939 \times 10^{-3} (Z|_{P,T} - Z|_{14.7,T}) + 1.0313 \times 10^{-3} \ln[(1 - Z|_{14.7,T})/(1 - Z|_{P,T})] \ ,$$

where

S = entropy, Btu/lb-°R.

Equation 28 deviates from experimental values by less than 0.01% from 32°F to the triple point. Equation 29 is stated to deviate by less than 0.01% from experimental values, but no temperature range of applicability is given. DeWitt (1960, p. 70) reports that entropy values obtained using Eq. 30 are in reasonable agreement with those obtained from other sources. Entropies of UF_6 solid, liquid, and vapor are plotted in Fig. 9.
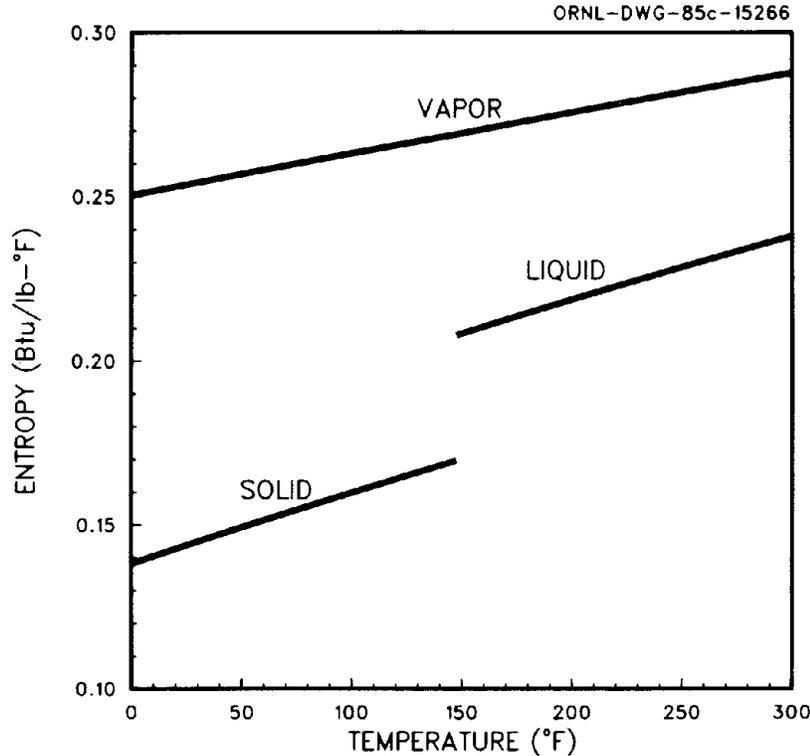
Fig. 9. Entropy of solid, liquid, and vapor uranium hexafluoride.

2.1.9 Other properties

Liquid coefficient of compressibility

The liquid coefficient of compressibility is needed for sonic velocity calculations. Data reported by Barber (1979) between the triple point and 320°F were found to be represented reasonably by

$$\ln \beta = 4.4264 - (17542/T_R) + (4917700/T_R^2) \ , \tag{31}$$

where

β = coefficient of compressibility, psia^{-1}.

Sublimation point and triple point

UF_6 does not have a normal boiling point but reaches a sublimation point at 133.8°F when the vapor pressure over the solid is 14.7 psia. The triple point for UF_6 at which solid, liquid, and vapor phases coexist is about 147.3°F, which yields a vapor pressure of about 22.04 psia based on the preceding vapor pressure equations.

Critical properties

At the critical point, UF_6 has a critical temperature of 906°R, a critical pressure of 669 psia, and a critical specific volume of 4.10 ft^3/lb-mole. Based on a molecular weight of 352, the critical density is 85.84 lb/ft^3.

Molecular weight

The molecular weight of UF_6 varies with the enrichment of the uranium and is given by,

$$MW = 352.04 - 0.03\,E \ , \tag{32}$$

where

E = enrichment in ^{235}U, %.

The small variation in molecular weight (less than 1% between 0 and 100% enrichment) is negligible, and a molecular weight of 352 can generally be used. Most of the properties subroutines include correction factors for molecular weight, and the main programs allow a molecular weight to be read as input. The default molecular weight provided is 352.025.

2.1.10 UF₆ Reaction with H₂O

UF_6 reacts with water, including moisture in the air, to form uranyl fluoride (UO_2F_2) and hydrogen fluoride (HF). The equation for the chemical reaction is

$$UF_6(v) + 2\,H_2O(v) \rightarrow UO_2F_2(s) + 4\,HF(v) + \Delta H_{rxn} \ . \tag{33}$$

A review of material related to this reaction led to an article by Popov et al. (1957, pp. 9-12) from which the heat of reaction (a positive heat of reaction implies an exothermic reaction) of

$$UF_6(s) + 2 H_2O(l) \rightarrow UO_2F_2(s) + 4 HF(v) \tag{34}$$

was found to be -7416 Btu/lb-mole of UF_6 reacted at 89.6°F. Using enthalpy correlations reported herein, a heat of reaction at 77°F for Eq. 33 was calculated to be 25,199 Btu/lb-mole of H_2O reacted. Note that, in making the conversion from one reference condition to the other, HF vapor is treated as a monomer.

2.1.11 Flashing

The estimation of UF_6 release rates, as described in Chap. 3, is complex because of the phase behavior of UF_6. Two or perhaps three phases of UF_6 will generally be present inside containment; if liquid UF_6 or a multiphase mixture of UF_6 is released from containment, the phase composition of UF_6 flowing from containment through the release pathway to the ambient surroundings will be constantly changing. Methods for evaluating the phase composition of UF_6 as a function of pressure along a release pathway are discussed in this section. Phase behavior inside containment and the evaluation of release rates are discussed in Chap. 3.

Upper and lower bounds on the vapor mass fraction at the point of release to the environment as well as at a given pressure in a piping system can be estimated from thermodynamic considerations. If the expansion process is assumed to be reversible (i.e., isentropic), a lower bound on the vapor fraction can be estimated. An upper bound on the vapor mass fraction can be estimated by assuming an adiabatic, isenthalpic process. Both assumptions are in error because heat would be transferred to the piping system and because the expansion would be irreversible; however, the error is relatively small.

If an isentropic process is assumed for the release of UF_6, then

$$\overline{S}_i = X S_{v,f} + (1 - X) S_{c,f} \ , \tag{35}$$

where

$\quad X = $ vapor mass fraction,
$\quad S = $ entropy, Btu/lb-°F,
$\quad v,c = $ subscripts for vapor and condensed phases,
$\quad i,f = $ subscripts for initial and final conditions, and
$\quad \bar{\ } = $ superscript indicating average.

Rearranging yields,

$$X = (\overline{S}_i - S_{c,f})/(S_{v,f} - S_{c,f}) \ . \tag{36}$$

The quantity $\overline{S}_i$ is the entropy of the UF_6 as it enters the release pathway and the average entropy along the release pathway. To evaluate X based on the preceding equation, the temperature that would yield a vapor pressure equal to the outlet pressure (or intermediate pressure along the release

pathway) is determined, then that temperature is used to evaluate $S_{v,f}$ and $S_{c,f}$ assuming saturation. If S_i is based on a multiphase mixture of UF_6 being released from containment into the release pathway, then X based on Eq. 36 may be greater than 1. In this latter case, as well as when UF_6 vapor is released, a superheated vapor is released; therefore, no condensed phase occurs and Eq. 36 is not applicable. The final temperature may be determined by iteration using the equation for entropy of the vapor at unsaturated conditions (Eq. 30) and the criterion that the final entropy equals the average entropy. If a subcooled liquid (i.e., $P > P_{sat}$) enters the release pathway, $X = 0$ in the pathway until $P = P_{sat}$. From that point on, Eq. 36 is applicable.

For an adiabatic, isenthalpic process,

$$\overline{H}_i = XH_{v,f} + (1 - X)H_{c,f} \ , \tag{37}$$

where

H = enthalpy, Btu/lb.

Rearranging yields,

$$X = (\overline{H}_i - H_{c,f})/(H_{v,f} - H_{c,f}) \ , \tag{38}$$

where the enthalpies are determined in a manner analogous to the entropies. Again, if X is found to be greater than 1 by Eq. 38, a superheated vapor is released, and the enthalpy equation for the vapor (Eq. 27) is used to determine the final release temperature. If a subcooled liquid enters the release pathway, $X = 0$ in the pathway and Eq. 26 is used to determine the temperature in the pathway until $P = P_{sat}$.

For the special case of the release of saturated liquid UF_6 at a given temperature to a final pressure of 14.7 psia, Eq. 36 for an isentropic release becomes

$$X = -3.383935 + 0.507936 \ln T_R + 1.02206 \times 10^{-3} T_R \tag{39}$$

$$- (3.05691 \times 10^4)/(T_R{}^2) \ ,$$

and Eq. 38 for an isenthalpic release becomes

$$X = -0.244302 + 8.51871 \times 10^{-4} T_R + 8.57062 \times 10^{-7} T_R{}^2 \tag{40}$$

$$- (1.02536 \times 10^2)/T_R \ .$$

These expressions for the lower and upper bounds on the vapor mass fraction resulting from a release of saturated liquid UF_6 to a final pressure of 14.7 psia are plotted in Fig. 10. If the final pressure is other than 1 atm, Eqs. 36 and 38 should be used to bound the vapor mass fraction. Also, if the final pressure exceeds the triple point pressure, the condensed phase will be liquid rather than solid.
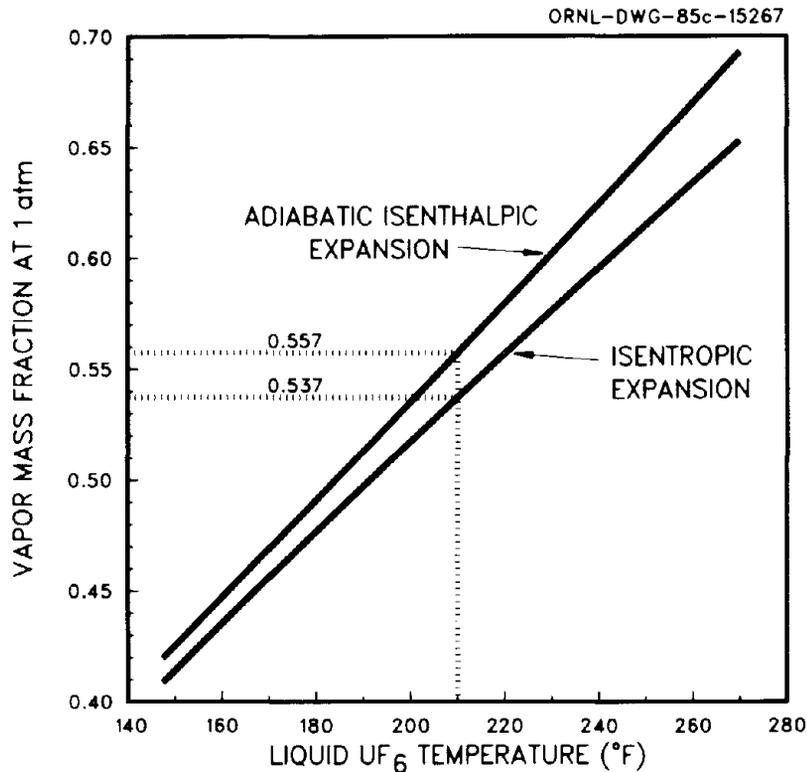
Fig. 10. Initial vapor mass fraction resulting from a release of saturated UF₆ liquid to a pressure of 1 atm. (Example: For saturated UF₆ liquid at 210°F, the initial vapor mass fraction will be between 0.537 and 0.557 when a release to a pressure of 1 atm occurs.)

2.1.12 Subroutines

Nine subroutines have been developed to predict UF₆ physical and thermodynamic properties. These subroutines and the purpose of each are listed in Table 3. Seven of the subroutines require temperature, pressure, and molecular weight as input; molecular weight is not used in VISUF6, which evaluates viscosities. VPRUF6 requires temperature as input and gives vapor pressure as output; EQTUF6 gives the saturation temperature corresponding to a given UF₆ pressure supplied as input. In many cases, properties reported by DeWitt (1960) were given using moles as the unit of mass. A molecular weight of 352 was used in converting equations to engineering units, so the computer routines include molecular weight as input to adjust for other molecular weights resulting from uranium enrichment operations. Appendix B contains listings of all properties subroutines.

The subroutine FLASH has been developed to estimate the vapor mass fraction at a final pressure given the initial temperature, pressure, UF₆ molecular weight, vapor mass fraction, and liquid mass fraction of the nonvapor fraction, the final pressure, and whether the release is to be considered isentropic or isenthalpic. Output includes the final temperature, vapor mass fraction, and liquid mass fraction of the nonvapor fraction. If the vapor mass fraction would be greater than 1 according to Eq. 36 or 38, the subroutine sets the final vapor mass fraction equal to 1 and determines the final temperature of the superheated vapor. At the triple point, the condensed phase is assumed to be liquid. Appendix B contains a listing of the subroutine FLASH.

Table 3. UF$_6$ physical and thermodynamic properties subroutines

Subroutine	Properties calculated
VPRUF$_6$	Vapor pressure for a given temperature
EQTUF$_6$	Equilibrium temperature for a given pressure
ZUF$_6$	Vapor compressibility factor and related terms given temperature and pressure
DENUF$_6$	Solid, liquid, and vapor densities given temperature, pressure, and molecular weight
VISUF$_6$	Liquid and vapor viscosities given temperature and pressure
THCUF$_6$	Solid, liquid, and vapor thermal conductivities given temperature, pressure, and molecular weight
CPUF$_6$	Solid, liquid, and vapor (constant pressure) heat capacities, vapor heat capacity ratio, and vapor constant volume heat capacity given temperature, pressure, and molecular weight.
HUF$_6$	Solid, liquid, and vapor enthalpies given temperature, pressure, and molecular weight
SUF$_6$	Solid, liquid, and vapor entropies given temperature, pressure, and molecular weight

2.2 HF-H$_2$O SYSTEM

Two sets of physical properties for the HF-H$_2$O system are of particular interest in current modeling efforts. These properties are vapor pressure and enthalpy. This section discusses the estimation of (1) partial vapor pressures of HF and H$_2$O as functions of temperature and the composition of the condensed phase in equilibrium with the vapor and (2) liquid and vapor phase enthalpies. Estimation of the effective molecular weight of HF and the enthalpy effects of HF self-association in the vapor phase are incorporated into vapor pressure and enthalpy calculations.

2.2.1 Self-Association of HF Vapor

HF does not exist in a purely monomeric form but is linked into short polymers by hydrogen bonding. Beckerdite et al. (1983, pp. 287-93) report that a monomer-trimer-hexamer (1-3-6) model reasonably represents the self-association of HF. Using the data of Strohmeier and Briegleb,* which was reported by Beckerdite et al. (1983, p. 292) and which is shown in Table 4, the following equations were derived for the 1-3 and 1-6 equilibrium coefficients:

*The data of Fredenhagen were also used initially in deriving expressions for K_3 and K_6. Subsequently, it was observed that, on extrapolation to lower temperatures potentially encountered in simulating atmospheric dispersion, use of the combined data sets would result in vapor enthalpies that were less than liquid enthalpies for high HF-to-H$_2$O ratios.

**Table 4. HF monomer-to-trimer and monomer-to-hexamer
equilibrium coefficients**

Temperature (K)	Equilibrium coefficient data of Strohmeier and Briegleb[a]		Predicted equilibrium coefficients[b]	
	$K_3 \times 10^3$ (atm^{-2})	$K_6 \times 10^3$ (atm^{-5})	$K_3 \times 10^3$ (atm^{-2})	$K_6 \times 10^3$ (atm^{-5})
299.15	210 ± 10	1620 ± 50	221	1688
305.15	120 ± 8	450 ± 30	92	387
311.15	48 ± 6	84 ± 4	40	94
317.15	9.0 ± 0.7	23 ± 0.4	18	24
329.15	5.2 ± 0.1	1.9 ± 0.3	3.9	1.8

[a]Taken from Table III of Beckerdite, J. M., Powell, D. R., and Adams, E. T., Jr. 1983. "Self-Association of Gases. 2. The Association of Hydrogen Fluoride," *J. Chem. Eng. Data* 28, 287–93.
[b]Predicted using Eqs. 41 and 42.

$$\ln K_3 = (23884.0/T_R) - 51.2393 \ , \tag{41}$$

$$\ln K_6 = (40319.6/T_R) - 87.7927 \ , \tag{42}$$

where

K_3 = equilibrium coefficient for the monomer-to-trimer association, psia^{-2},

K_6 = equilibrium coefficient for the monomer-to-hexamer association, psia^{-5}.

Note that K_n is based on the following association model:

$$n(\text{HF})_1 \rightleftharpoons (\text{HF})_n \tag{43}$$

and

$$K_n = [P_{(\text{HF})_n}]/[P_{(\text{HF})_1}]^n \ , \tag{44}$$

where

P = pressure, psia,

$(\text{HF})_n$ = an n-mer of HF.

K-values calculated from Eqs. 41 and 42 are shown in Table 4 for comparison with the data of Strohmeier and Briegleb.

The partial vapor pressure of HF as obtained by the methods described in the next section, or the partial pressure of HF, is the sum of the partial pressures of the monomer, trimer, and hexamer; therefore,

$$P_{HF} = P_{(HF)_1} + P_{(HF)_3} + P_{(HF)_6} \; , \tag{45}$$

where

P_{HF} = vapor pressure or partial pressure of HF.

Rearranging Eq. 44 and substituting into Eq. 45 yields

$$P_{HF} = P_{(HF)_1} + K_3 P_{(HF)_1}^3 + K_6 P_{(HF)_1}^6 \; . \tag{46}$$

To find the effective molecular weight, it is necessary to recognize that, in the vapor phase,

$$\rho_i = (P_i MW_i)/RT \tag{47}$$

and

$$\rho_T = \sum \rho_i \; . \tag{48}$$

By using these relationships,

$$\rho_{HF} = \frac{P_{HF} MW_{HF}}{RT} = \frac{P_{(HF)_1} MW_{(HF)_1}}{RT} + \frac{P_{(HF)_3} MW_{(HF)_3}}{RT} + \frac{P_{(HF)_6} MW_{(HF)_3}}{RT} \; , \tag{49}$$

which yields

$$MW_{HF} = [P_{(HF)_1} MW_{(HF)_1} + P_{(HF)_3} MW_{(HF)_3} + P_{(HF)_6} MW_{(HF)_6}]/P_{HF} \; , \tag{50}$$

where MW is molecular weight. The quantity, MW_{HF}, is the effective molecular weight to be used in determining vapor phase densities of HF and in converting between vapor weight fraction and vapor mole fraction. It also follows from Eq. 47 that the weight fraction of an n-mer of HF to the total HF in the vapor phase is given by

$$W_{(HF)_n} = [P_{(HF)_n} MW_{(HF)_n}]/(P_{HF} MW_{HF}) \; , \tag{51}$$

The partial vapor pressure of HF obtained as a function of temperature and weight fraction of HF in the condensate (see Sect. 2.2.2) appears to be the effective pressure of the associated HF. Thus, the partial vapor pressure of HF is predicted and then the effective molecular weight is determined. If no condensed phase occurs, the partial pressure of HF is determined iteratively along with the effective molecular weight of HF by assuming a partial pressure, calculating the effective molecular weight, and applying the ideal gas law to get a new partial pressure.

2.2.2 Partial Vapor Pressure of HF

The partial vapor pressure of HF is based on Fig. 11, which shows the partial vapor pressure of HF as a function of temperature for constant weight fractions of HF in the condensed HF-H_2O liquid mixture. These curves can be approximated by an equation of the form

$$\ln P_{HF} = (A/T_R) + B \ , \tag{52}$$

where

P_{HF} = partial vapor pressure of HF, mm,
T_R = absolute temperature, °R.

The empirical coefficients A and B and the maximum error for each curve based on data extracted from Fig. 11 are given in Table 5.

Attempts were made to correlate A and B as functions of weight fraction; however, all such attempts led to greater errors in predicted partial vapor pressure for the given lines. It was finally decided that pressures over condensate compositions other than those given in Table 1 would be best obtained by interpolation. Since pressure was presented on a log scale and since consecutive concentration lines are roughly equally spaced, the following interpolation method is used (except for condensate compositions below 5 wt % HF):

$$\ln P_{HF} = \ln P_{HF,1} + \frac{\ln P_{HF,2} - \ln P_{HF,1}}{0.05}(W_{HF,l} - W_{HF,l,1}) \quad \text{for } W_{HF,l} > 0.05 \ , \tag{53}$$

where

1, 2 = subscripts defining conditions for the known curves immediately above and below the concentration of interest and
$W_{HF,l}$ = weight fraction of HF in the condensate.

Note that $P_{HF,1}$ and $P_{HF,2}$ are evaluated at the temperature of interest for P_{HF}. Below 5 wt % HF, the partial vapor pressure of HF is calculated from

$$P_{HF} = P_{HF,5\,wt\,\%}(W_{HF,l}/0.05) \quad \text{for } W_{HF,l} < 0.05 \ . \tag{54}$$

ORNL–DWG 85-15583
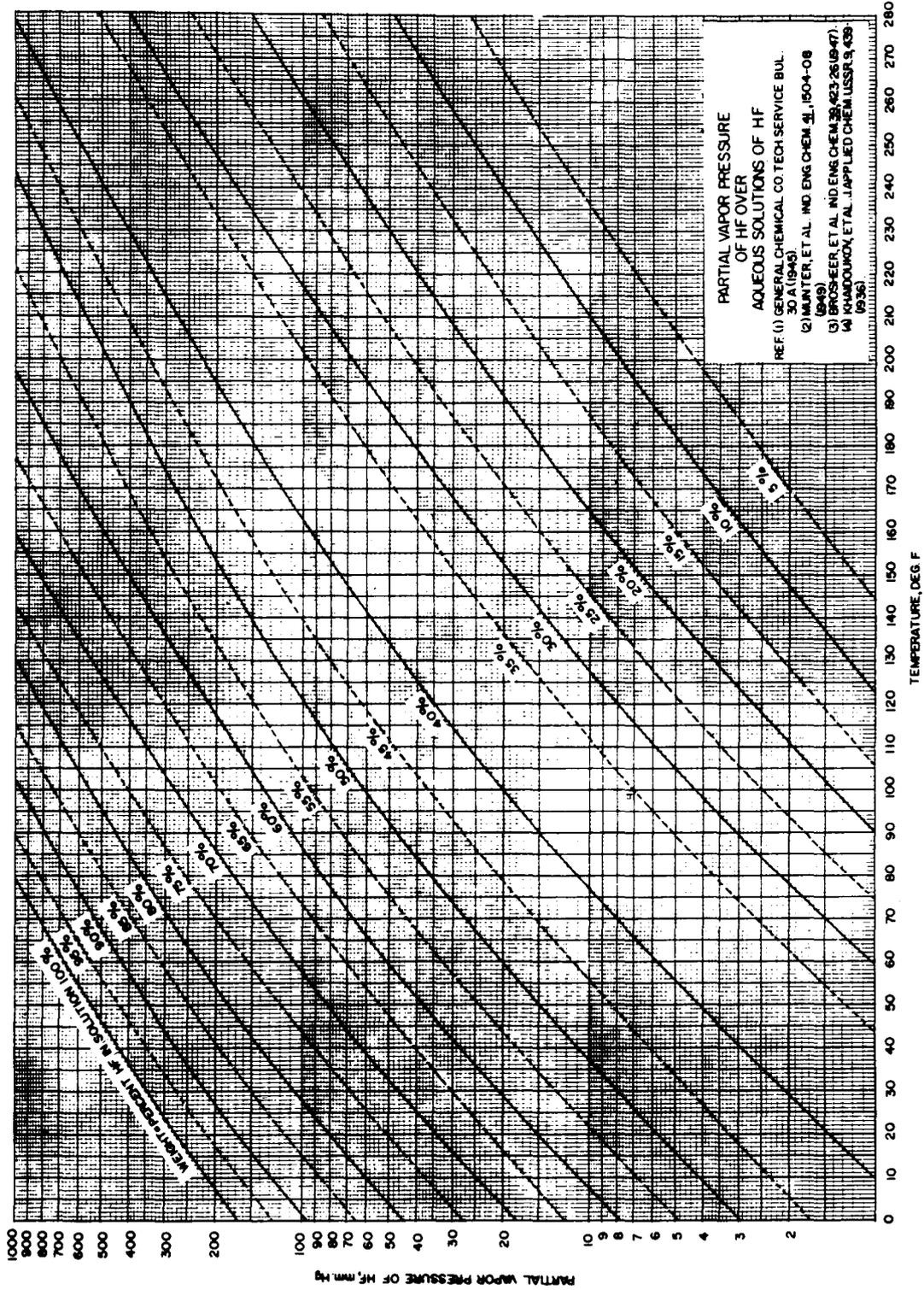
Fig. 11. Partial vapor pressure of HF over aqueous solutions of HF. (Source: Brian C. Rogers, Allied Chemical, personal communication to W. R. Williams, July 26, 1983.)

Table 5. Coefficients for estimating the partial vapor
pressure of HF by Eq. 52 over various liquid
mixtures of HF and H$_2$

Weight fraction of HF in liquid	A	B	Maximum error in estimate[a] (%)
0.05	−10689	17.680	3
0.10	−10536	18.069	4
0.15	−10647	18.793	5
0.20	−10675	19.409	2
0.25	−10460	19.595	3
0.30	−10362	19.951	4
0.35	−9779.5	19.429	4
0.40	−8917.7	18.948	5
0.45	−8188.2	18.256	5
0.50	−7770.0	17.975	3
0.55	−7575.0	18.054	3
0.60	−7411.4	18.178	3
0.65	−7315.7	18.365	3
0.70	−7163.4	18.457	3
0.75	−6984.3	18.492	2
0.80	−6459.7	17.857	2
0.85	−6269.7	17.812	1
0.90	−5891.7	17.391	2
0.95	−5849.8	17.555	1
1.00	−5641.0	17.364	1

[a]Error is estimated relative to Fig. 11. The accuracy of
Fig. 11 is not known.

2.2.3 Partial Vapor Pressure of H$_2$O

In an azeotropic system, the minimum total vapor pressure of the system (assuming constant temperature) is expected to occur at the azeotropic composition as shown in Fig. 12. When correlations for the partial vapor pressure of H$_2$O were derived directly from data on the partial vapor pressure of H$_2$O as a function of condensate composition and temperature and then summed together with the corresponding partial vapor pressure of HF, the minimum total vapor pressure of the HF-H$_2$O system did not occur at the azeotrope. Since the available data on HF partial vapor pressures were more extensive than those on H$_2$O partial vapor pressures, a decision was made to accept that HF data and to force-fit an H$_2$O partial vapor pressure model to yield a minimum total pressure at the azeotrope.

Figure 13 is a plot of some available partial vapor pressure data for the HF-H$_2$O system. The curve for HF partial vapor pressure is primarily based on data from Fig. 11 and agrees fairly well with the data of Brosheer et al. (1947, pp. 423–27), which is limited to a maximum of 30 wt % HF.
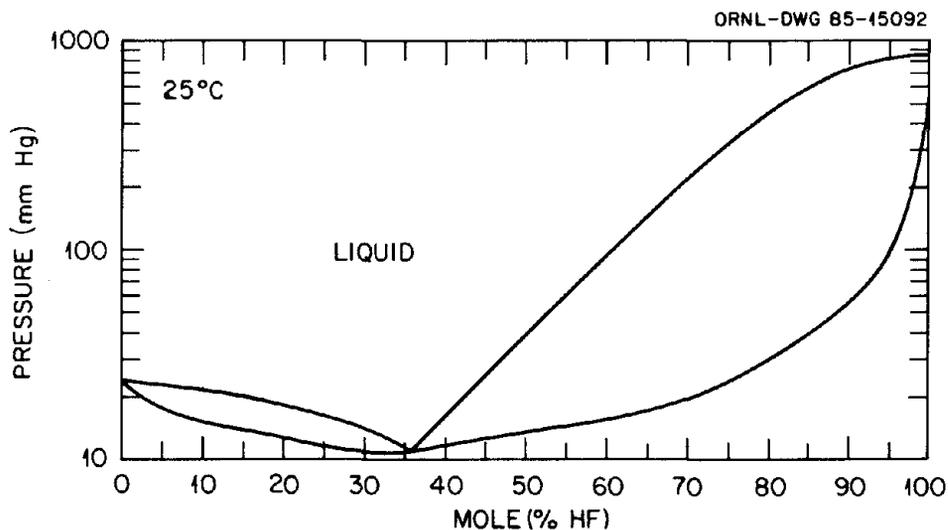
Fig. 12. An approximate pressure-composition diagram for the HF-H₂O system at 25°C.
Two-phase mixtures occur for pressure-composition combinations that fall within the two "wings"
lying between those regions labeled liquid and vapor. (Source: W. H. McCulla, *Determinations of
the Rate of HF Hydration and the Effects of Moisture Condensation*, K/PS-155, April 30, 1982.)
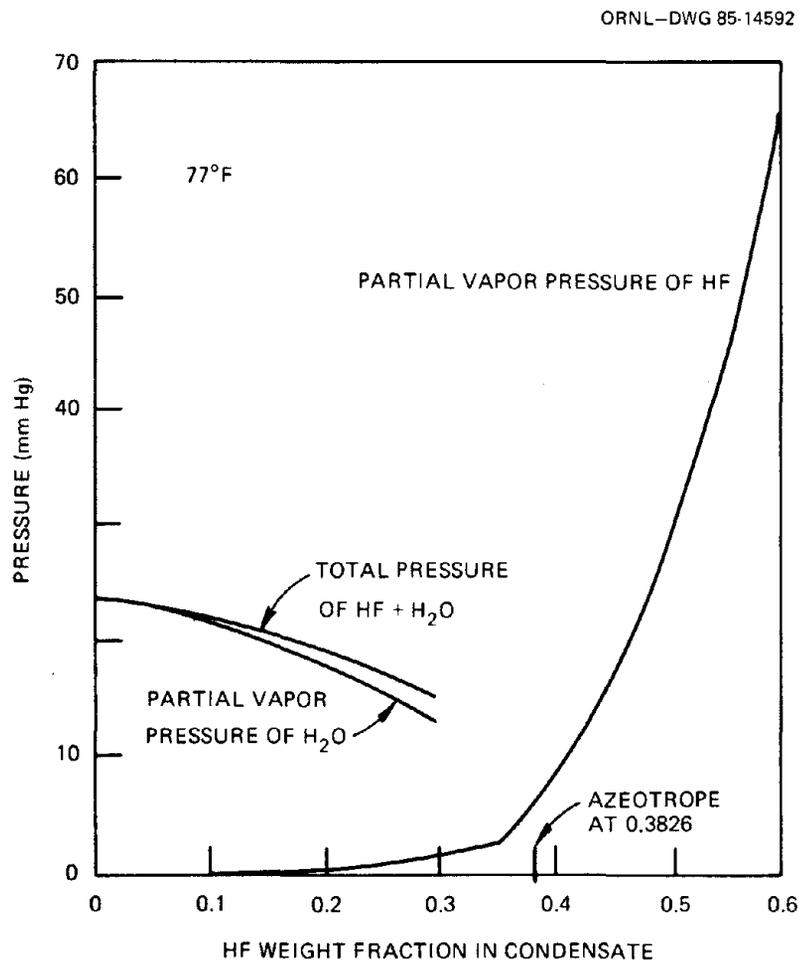
Fig. 13. Available data on the partial vapor pressures of HF and H₂O at 77°F.

The curves corresponding to H₂O partial pressure and total pressure are based on the data of Brosheer et al. Also identified on Fig. 13 is the azeotrope for the HF-H₂O system.

Figure 14(a) illustrates the inconsistency in data that led to the decision to force-fit an H₂O partial vapor pressure model. The solid curves in Fig. 14 are those shown in Fig. 13. Point 1 corresponds to the partial vapor pressure of HF calculated from the correlations of Sect. 2.2.2. By using the effective molecular weight of HF and the azeotropic composition, the partial vapor pressure of H₂O (point 2) can be determined. The total pressure, point 3, is the sum of the partial vapor pressures. Obviously, a minimum total pressure would occur at a condensate composition between 30 wt % HF and the azeotrope, which is not consistent with the expected behavior of an azeotropic system.

Since the plot of HF partial vapor pressures (see Fig. 11) appears to represent a more extensive data base than that available for H₂O, the HF data were subsequently used and H₂O partial vapor pressure data were ignored. Thus, the current method for calculating the partial vapor pressure of H₂O proceeds as follows. First, calculate the partial vapor pressure of HF for the desired temperature at the azeotropic composition (38.26 wt % HF) and the effective molecular weight of HF using the correlations given in Sect. 2.2.1 (note point 1 in Fig. 13). Next, evaluate the vapor mole fraction of HF corresponding to the azeotropic weight fraction and the given temperature using the following equation:

$$Y_{HF} = \frac{(W_{HF,v}/MW_{HF})}{(W_{HF,v}/MW_{HF}) + [(1 - W_{HF,v})/MW_{H_2O}]} \tag{55}$$

ORNL-DWG 85-14591
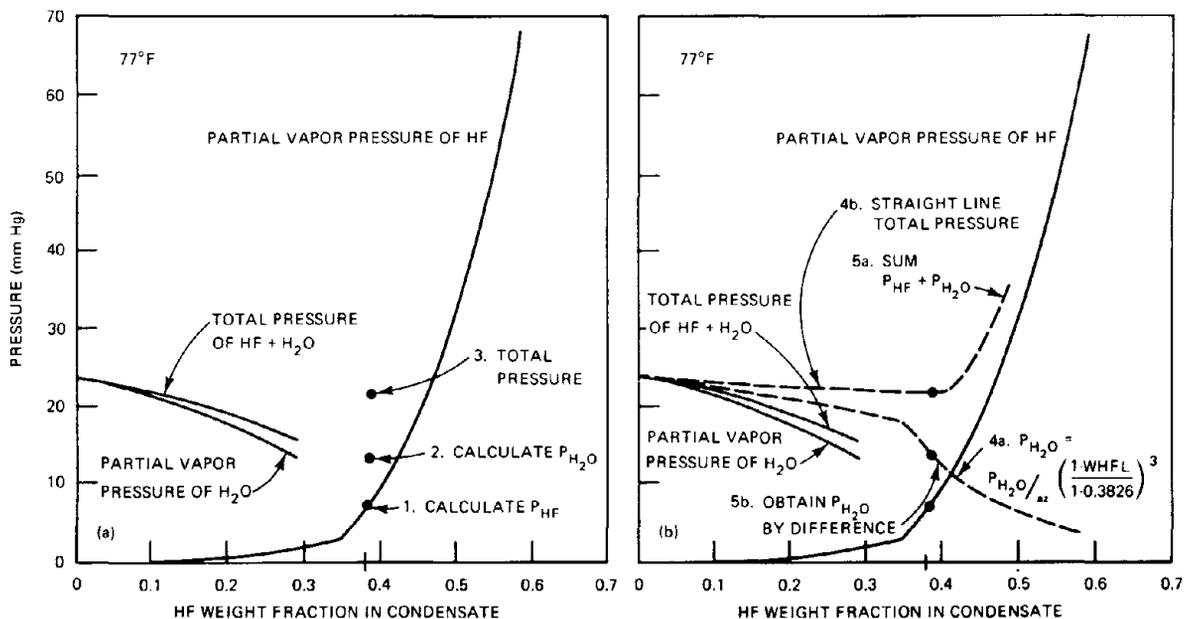
Fig. 14. Procedure for obtaining the partial vapor pressure of H₂O. Figure 14(a) shows the first three steps superimposed on the curves shown in Fig. 13 and demonstrates data inconsistency. Figure 14(b) shows the final two steps, which differ depending on condensate composition. Steps 4a and 5a go together above the azeotrope, while steps 4b and 5b go together below the azeotrope.

where

Y_{HF} = vapor mole fraction of HF,

$W_{HF,v}$ = weight fraction of HF in the vapor,

MW_{H_2O} = molecular weight of H_2O.

The azeotropic partial vapor pressure of H_2O [point 2 in Fig. 14(a)] is given by

$$P_{H_2O,azeotrope} = P_{HF,azeotrope}[(1 - Y_{HF})/(Y_{HF})] \ . \tag{56}$$

Next, calculate the vapor pressure of pure H_2O (Reid 1977, pp. 629–32) from

$$\ln P^{\circ}_{H_2O} = 18.3034 - [6869.59/(T_F - 376.64)] \ , \tag{57}$$

where

$P^{\circ}_{H_2O}$ = vapor pressure for pure H_2O,(mm),

T_F = temperature (°F).

To find the partial vapor pressure of H_2O over a condensate having a weight fraction of HF less than the azeotropic composition (0.3826), use

$$P_{H_2O} = P^{\circ}_{H_2O} + (P_{HF,azeotrope} + P_{H_2O,azeotrope} - P^{\circ}_{H_2O}) \tag{58}$$

$$\times (W_{HF,l}/W_{HF,azeotrope}) - P_{HF} \quad \text{for } W_{HF,l} \leqslant W_{HF,zeotrope} \ ,$$

where P_{HF} is calculated at the condensate composition of interest. Equation 58 [which corresponds to the dashed line 5b in Fig. 14(b)] assumes a linear relationship between the total pressure of the HF-H_2O system [represented by the first two terms to the right of the equals sign and line 4b on Fig. 14(b)] and the weight fraction of HF in the condensate below the azeotropic composition. To find the partial vapor pressure of H_2O over a condensate having a weight fraction of HF greater than the azeotropic composition [see line 4a on Fig. 14(b)], use

$$P_{H_2O} = P_{H_2O,axeotrope}[(1 - W_{HF,l})/(1 - W_{HF,azeotrope})]^3 \quad \text{for } W_{HF,l} \geqslant W_{HF,azeotrope} \ . \tag{59}$$

The choice of the exponent 3 in Eq. 59 is somewhat arbitrary; nevertheless, it permits a less-sharp discontinuity in the slope of P_{H_2O} versus $W_{HF,l}$ than would exponents less than 3. Higher exponents would allow P_{H_2O} to decrease too rapidly such that a total pressure minimum would occur above the azeotrope, causing numerical problems.

In analyses subsequent to development of the methods described in this section for predicting the partial vapor pressure of H_2O, it has been determined that predicted total vapor pressures for the HF-H_2O system at the azeotrope correspond to temperatures about 10°F above those specified. It is anticipated that, if the available data on H_2O partial vapor pressures were retained and the

partial vapor pressures of HF were modified between 35 wt % and about 50 wt % (see Fig. 13), a better set of correlations for the partial vapor pressure of H_2O could be derived.

2.2.4 Enthalpy of HF-H₂O Vapor Mixtures

Figure 15 is an enthalpy concentration diagram for the HF-H_2O system at 1 atm. At temperatures above 250°F, HF polymerization is negligible and the interaction between HF and H_2O in the vapor phase appears to be ideal, as evidenced by the straight-line relationship between the enthalpy of the vapor mixture and the weight percent of HF in the mixture. At lower temperatures, however, association of HF into polymers significantly reduces the enthalpy of the vapor mixture as the weight percent of HF approaches 100 wt %. This latter trend may be observed by noting the intersections of the equilibrium tie lines for various temperatures with the saturated vapor curve. These intersections, particularly above 90 wt % HF, are much lower than would be predicted by extrapolation of data above 250°F.

The enthalpy model for an HF-H_2O vapor mixture is composed of two parts: (1) a base enthalpy, assuming no polymerization, which is based on extrapolation of data above 250°F to lower temperatures, and (2) a correction term based on the polymerization of HF. The base enthalpy is given by

$$H_{base} = (1051.0 + 0.472\,T_F) - (376.0 + 0.136\,T_F)W_{HF,v} \quad , \tag{60}$$

where

H_{base} = uncorrected enthalpy for an HF-H_2O vapor mixture, Btu/lb,

$W_{HF,v}$ = weight fraction of HF in the vapor phase, $lb_{HF\ vapor}/lb_{HF-H_2O\ vapor}$.

The correction term is obtained from Eqs. 41 and 42 using the following basic thermodynamic relationship:

$$\Delta G_i = -RT \ln K_i = \Delta H_i - T\Delta S_i \quad , \tag{61}$$

where

ΔG_i = Gibbs free energy,

R = ideal gas constant,

T = absolute temperature,

K_i = equilibrium coefficient,

ΔH_i = heat of reaction,

ΔS_i = entropy.

Recognizing that Eqs. 41 and 42 are in the form

$$\ln K_n = (A_n/T) + B_n \quad , \tag{62}$$

ORNL–DWG 85-15584

Fig. 15. Enthalpy-concentration diagram for liquid and vapor mixtures of HF and H₂O showing equilibrium tie lines at 1 atm. (Source: Brian C. Rogers, Allied Chemical, personal communication to W. R. Williams, July 26, 1983).

and that Eq. 61 can be rearranged to a similar form, then it is found that

$$\Delta H_n = -RA_n \quad . \tag{63}$$

Using the relationship of Eq. 63, the heat of association for $(HF)_3$ is -790.642 Btu/lb $(HF)_3$ formed and for $(HF)_6$ is -667.358 Btu/lb $(HF)_6$ formed. These heats of association are applied as correction factors to Eq. 60 to obtain the following expression for enthalpy:

$$H_v = (1051.0 + 0.472\, T_F) - [376.0 + 0.136 T_F \tag{64}$$

$$+ \ 790.642 \ W_{(HF)_3} + 667.358 \ W_{(HF)_6}] W_{HF,v} \quad ,$$

where

$\quad H_v \ = $ enthalpy of a vapor mixture of HF and H_2O, Btu/lb,

$W_{(HF)_n} = $ weight fraction of an n-mer of HF as defined by Eq. 51, $lb_{n\text{-mer}}/lb_{HF\ vapor}$.

2.2.5 Enthalpy of HF-H₂O Liquid Mixtures

The lower portion of Fig. 15, which corresponds to liquid mixtures of HF and H_2O, is shown in expanded scale on Fig. 16. Significant nonideal behavior is exhibited that would normally be modeled as a heat of mixing. In this modeling effort, empirical correlations have been derived to give enthalpy as a function of temperature and composition. The left side of the figure (dilute HF solutions) was used to develop the correlations required to proceed to the right side (high-concentration HF solutions). The correlations are of the form

$$H_l = A_i + B_i W_{HF,l} + C_i W_{HF,l}^2 \quad , \tag{65}$$

where

$\quad H_l \ = $ enthalpy of the HF-H₂O liquid mixture, Btu/lb

$\quad W_{HF,l} = $ weight fraction of HF in the HF-H₂O liquid mixture lb HF/lb mixture.

Values for the coefficients A_i, B_i, and C_i are given in Table 6 along with the range of applicability and boundary conditions. Note that coefficients for lower intervals than the desired weight fraction of HF must be calculated to obtain cofficients for the needed interval. The preceding set of equations (Eq. 65 and Table 6) for liquid enthalpy are fairly accurate except above 90 wt % HF. Below 20 wt %, deviations between predicted and expected values are negligible. From 20 to 90 wt %, deviations up to 2 Btu/lb have been observed. Above 90 wt %, deviations of 7 Btu/lb have been observed; however, it may be worth noting that enthalpy can change that much with a 0.5% change in HF concentration.

2.2.6 HF-H₂O Vapor-Liquid Equilibrium

Preceding sections have presented methods for calculating the vapor phase composition given the liquid composition. This section describes how to obtain the phase splits for HF and H_2O in a
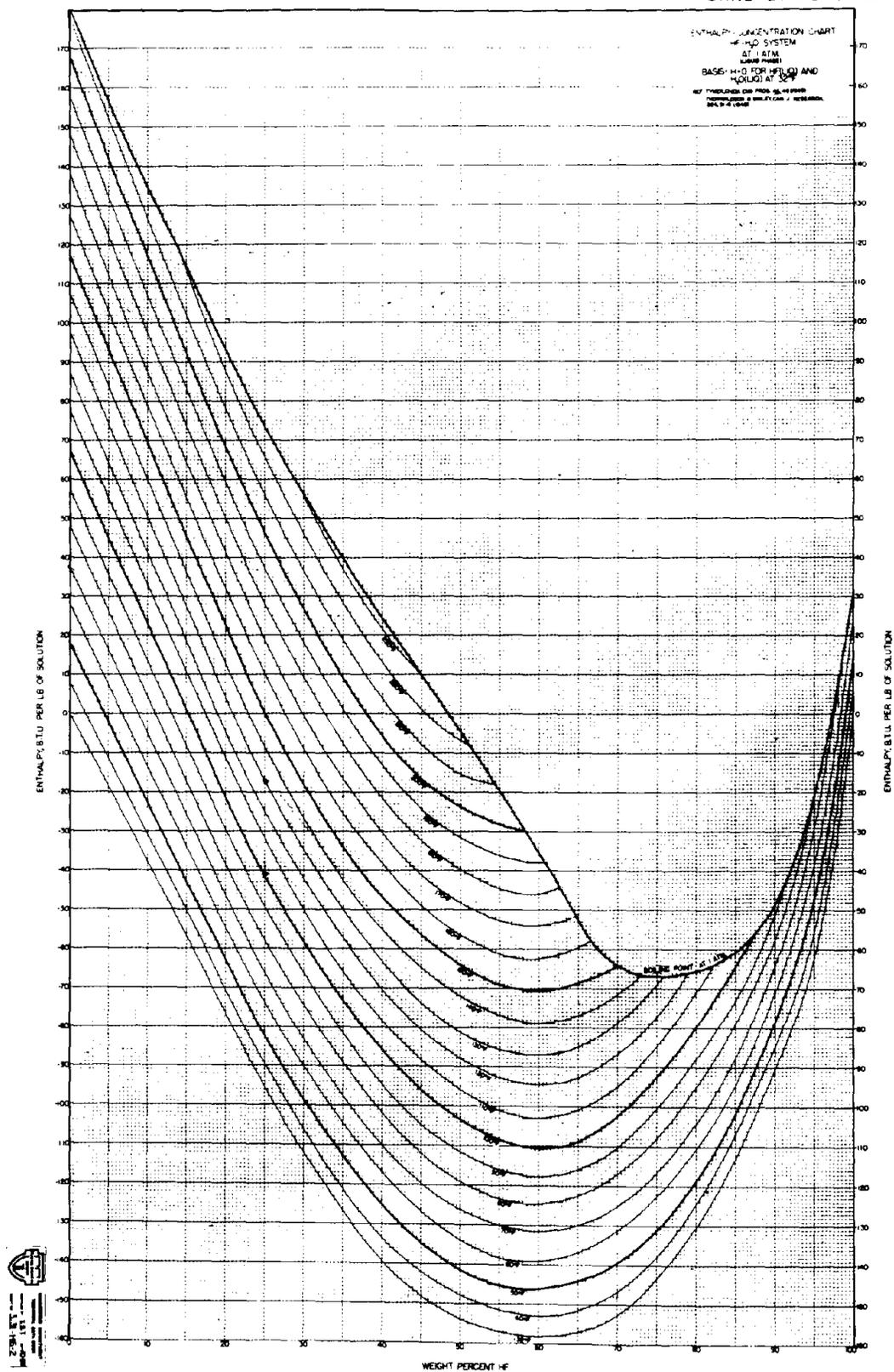
Fig. 16. Enthalpy-concentration diagram for liquid HF-H$_2$O mixtures. (Source: Brian C. Rogers, Allied Chemical, personal communication to W. R. Williams, July 26, 1983.)

Table 6. Correlations for coefficient of Eq. 65

(T = temperature, °F; H = enthalpy, Btu/lb)

Interval	Limits of $W_{HF,l}$	Coefficients	Boundary conditions
1	0.0–0.2	$A_1 = -32.252 + 0.99783\ T$ $B_1 = -357.75 - 0.969\ T + 0.0013\ T^2$ $C_1 = 0$	
2	0.2–0.6	$C_2 = (H_{20} - H_{60} + 0.4\ M_{20})/-0.16$ $B_2 = M_{20} - 0.4\ C_2$ $A_2 = H_{20} - 0.2\ B_2 - 0.04\ C_2$	$H_{20} = A_1 + 0.2\ B_1$ $H_{60} = -179.68 + 0.63569\ T + 5.8429 \times 10^{-4}\ T^2$ $M_{20} = B_1$
3	0.6–0.8	$C_3 = (H_{60} - H_{80} + 0.2\ M_{60})/-0.04$ $B_3 = M_{60} - 1.2\ C_3$ $A_3 = H_{60} - 0.6\ B_3 - 0.36\ C_3$	$H_{80} = -159.26 + 0.7985\ T$ $M_{60} = B_2 + 1.2\ C_2$
4	0.8–0.9	$C_4 = (H_{80} - H_{90} + 0.1\ M_{80})/-0.01$ $B_4 = M_{80} - 1.6\ C_4$ $A_4 = H_{80} - 0.8\ B_4 - 0.64\ C_4$	$H_{90} = -111.54 + 0.67057\ T$ $M_{80} = B_3 + 1.6\ C_3$
5	0.9–1.0	$C_5 = (H_{90} - H_{100} + 0.1\ M_{90})/-0.01$ $B_5 = M_{90} - 1.8\ C_5$ $A_5 = H_{90} - 0.9\ B_5 - 0.81\ C_5$	$H_{100} = -23.3142 + 0.870283\ T$ $M_{90} = B_4 + 1.8\ C_4$

multicomponent system. For the multicomponent systems of interest, the overall composition and the total enthalpy are known. For compartment models, these quantities are known with respect to the total mass of material in the compartment. The total volume of the compartment is also known. Given this information, it is possible to obtain the individual phase compositions and temperature as well as the total pressure.

The procedure for evaluating phase composition in the compartment model is to assume a temperature, evaluate the phase compositions and total pressure at that temperature given the overall composition, and then calculate the total enthalpy at these conditions. The calculated total enthalpy is then compared to the known total enthalpy of the system. Temperature is used as the variable on which to iterate until the calculated enthalpy matches the known enthalpy.

In evaluating phase compositions, the vapor phase is assumed to be ideal. As was outlined in Sect. 2.2.1, an effective molecular weight for HF can be calculated; this effective molecular weight is used to obtain the number of moles of HF vapor present. Generally, condensation is assumed to proceed independently for all components except HF and H_2O. Thus, the maximum partial pressure a component can exert is generally limited by the vapor pressure of that component. In the case of HF and H_2O, when both components are present the effective vapor pressures are reduced (i.e., the partial vapor pressure of the individual component is less than the vapor pressure of the pure component).

The first step in evaluating the phase composition of the HF-H_2O subsystem is to evaluate the maximum partial pressure of each component in the given volume at the given temperature based on the total mass of each component, assuming no condensation but including the effect of HF polymerization. Next, the weight fraction of HF in a liquid phase that would give the maximum partial pressure of HF is calculated. If a weight fraction greater than 1 is calculated, condensation will occur and the next step is skipped. If a weight fraction less than 1 is calculated, the sum of the partial vapor pressure of HF and H_2O at the given temperature and calculated weight fraction of HF in the liquid is calculated and compared to the sum of the maximum partial pressures,

assuming no condensation. If the sum of the maximum partial pressures is less than or equal to the sum of the partial vapor pressures, no condensation will occur; thus, all HF and H_2O is in the vapor phase.

If condensation occurs, two special cases are to be considered: condensation of a pure component and condensation at the azeotrope. These cases occur when the weight fraction of HF in the HF-H_2O subsystem is found to be 0 (pure H_2O), 0.3826 (azeotropic mixture of HF and H_2O, implying the same composition in the liquid and vapor phases), or 1 (pure HF). For these specific cases, the partial vapor pressures are calculated for HF and H_2O along with the appropriate effective molecular weight for HF vapor; then, the mass of each component that can exist in the vapor phase at its partial vapor pressure in the given volume at the given temperature is calculated, assuming that the ideal gas law applies. The mass of each component in the liquid phase is determined by subtracting the mass in the vapor phase from the total mass for each component.

When condensation is predicted at compositions other than those discussed in the preceding paragraph, an iterative procedure is required to evaluate the phase composition. Initial and lower limits for the iteration are the azeotropic weight fraction and the weight fraction of HF in the HF-H_2O subsystem. The correct liquid weight fraction will always be between these two limits. Note that the azeotropic weight fraction is an upper limit for subsystem compositions less than the azeotropic composition and a lower limit for subsystem compositions greater than the azeotropic composition. The closure criterion for the iterative procedure is that the partial pressures of HF and H_2O must approximately equal their partial vapor pressures.

The principle relationship required, besides the partial vapor pressure and polymerization correlations, is

$$m_{\text{vap}} = \frac{[m_{H_2O}W_{\text{HF},l} - m_{\text{HF}}(1 - W_{\text{HF},l})]}{W_{\text{HF},l} - W_{\text{HF},v}} \tag{66}$$

where

m_{vap} = mass of HF and H_2O in the vapor phase,

m_{H_2O}, m_{HF} = total mass of H_2O and HF, respectively,

$W_{\text{HF},l}, W_{\text{HF},v}$ = weight fractions of HF in the liquid and vapor phases, respectively.

As $W_{\text{HF},l}$ approaches the azeotrope, m_{vap} approaches infinity (provided the subsystem composition is other than azeotropic); as $W_{\text{HF},l}$ approaches the subsystem composition, m_{vap} approaches 0. Given the total amount of vapor in the HF-H_2O subsystem, the partial pressures exerted by HF and H_2O can be calculated and compared to the sum of the partial vapor pressures. Once the closure criterion is met, the individual vapor phase masses are calculated and, by calculatng the difference, the liquid phase masses are obtained.

2.2.7 Subroutines

Three computer subroutines have been developed for evaluating thermodynamic properties of the HF-H_2O system. The subroutine PHFH2O gives the individual partial vapor pressures of HF and H_2O as well as their sum along with the vapor mole fraction of HF in the HF-H_2O system given the temperature and weight fraction of HF in the HF-H_2O condensate. The enthalpies of

liquid and vapor mixtures are calculated by HHFH2O given the weight fraction of HF in the liquid and vapor phases, respectively, and the temperature. The weight fractions of HF trimer and hexamer in the vapor phase (with respect to total HF in the vapor phase) are also required. The subroutine HFPOLY calculates the effective molecular weight of HF in the vapor phase as well as the trimer and hexamer fractions required by HHFH2O given the temperature and partial pressure of HF. A logical variable has been included in the call to HFPOLY to specify whether the n-mer weight fractions should be calculated. Listings of these three routines are given in Appendix B.

The subroutine PHASE requires as input the compartment temperature and volume as well as the total masses of HF and H_2O present. The masses of HF and H_2O found in each phase are calculated and returned. PHASE is listed in Appendix B.

2.3 OTHER COMPONENTS

In addition to the properties already discussed for UF_6, HF, and H_2O, several properties are needed for UO_2F_2 and air. UO_2F_2 is a solid, while air is a vapor over the temperature range of interest for the current models. UO_2F_2 has a density of 398 lb/ft^3 and has a heat capacity of 0.0821 Btu/lb-°F. The density of air is obtained by applying the ideal gas law. The heat capacity of air is 0.24073 Btu/lb-°F.

2.4 MIXTURE ENTHALPIES

In modeling a release of UF_6 within a compartment, total enthalpy becomes an important criterion for determining the final temperature and pressure in the compartment at the end of a time interval. Total enthalpy is the sum of the differences in enthalpy for each component between the current conditions and reference conditions. Reference temperature for all components is 77°F. A reference pressure of 14.696 psia is used for UF_6 because departure functions are included in UF_6 enthalpy correlations (see Sect. 2.1.7). The reference state for air, H_2O, and UF_6 is vapor, while that of UO_2F_2 is solid. The reference state of HF is a monomeric vapor.

Total enthalpy is expressed mathematically by

$$\Delta H_{total} = \Delta H_{air} + \Delta H_{HF-H_2O} + \Delta H_{UF_6} + \Delta H_{UO_2F_2} \, , \tag{67}$$

where the component ΔH values are determined as follows. For air,

$$\Delta H_{air} = 0.24037 \, m_{air}(T - 77) \, , \tag{68}$$

where m_i is mass of component i in the compartment, lb. For the HF-H_2O system, the weight fractions of HF in both liquid and vapor phases, as well as in the total HF-H_2O subsystem, are determined from

$$W_{HF,l} = m_{HF,l}/(m_{HF,l} + m_{H_2O,v}) \, , \tag{69}$$

$$W_{HF,v} = m_{HF,v}/(m_{HF,v} + m_{H_2O,v}) \, , \tag{70}$$

and

$$W_{HF} = \frac{m_{HF,l} + m_{HF,v}}{m_{HF,l} + m_{HF,v} + m_{H_2O,l} + m_{H_2O,v}} \quad . \tag{71}$$

Also, the weight fractions of HF monomer, trimer, and hexamer must be known at the temperature of interest. The value of ΔH_{HF-H_2O} is given by

$$\Delta H_{HF-H_2O} = (m_{HF,l} + m_{H_2O,l})H_l(T,w_{HF,l} \tag{72}$$

$$+ (m_{HF,v} + m_{H_2O,v})H_v(T,w_{(HF)_3},w_{(HF)_6},w_{HF,v})$$

$$- (m_{HF,l} + m_{HF,v} + m_{H_2O,l} + m_{H_2O,v})H_v(77,0,0,w_{HF}) \quad ,$$

where H_l is found from methods given in Sect. 2.2.5. H_v is given by Eq. 64. For UF$_6$,

$$\Delta H_{UF_6} = (m_{UF_6,s}H_{UF_6,s}(T) + m_{UF_6,l}H_{UF_6,l}(T,P) \tag{73}$$

$$+ (m_{UF_6,v}H_{UF_6,v}(T,P)$$

$$- (m_{UF_6,s} + m_{UF_6,l} + m_{UF_6,v})H_{UF_6,v}(77,14.696) \quad .$$

For UO$_2$F$_2$,

$$H_{UO_2F_2} = 0.0821 m_{UO_2F_2}(T - 77) \quad . \tag{74}$$

These equations are used in the subroutine DENTHL, which makes use of the previously mentioned subroutines HUF6 and HHFH2O. The temperature, pressure, and mass of each component in each phase must be known (or assumed) before the total enthalpy can be calculated. DENTHL can also be used for flow streams by assuming that m_i refers to mass flow rate (lb/Δt) rather than mass (lb).

3. RELEASE RATE MODELS

This chapter describes methods for calculating mass flow rates of UF_6 released from containment to the environment through a postulated breach in containment or break in a piping system. The estimation of such release rates is complicated by UF_6 phase behavior. Two or possibly three phases of UF_6 will usually be present inside containment; the phase composition of UF_6 will usually be constantly changing along the length of the release pathway; and, if liquid UF_6 alone enters the release pathway, two-phase flow may be induced at any point in the pathway where pressure drops below the liquid saturation pressure. Special considerations must be made when flow at any point in the pathway approaches the UF_6 triple point, the temperature and associated saturation vapor pressure at which three phases—solid, liquid, and vapor—may coexist in thermodynamic equilibrium.

Section 3.1 describes methods for estimating the phase interface level within containment and the expected phase composition of UF_6 leaving containment (Sect. 3.1.2) as well as the phase composition within containment (Sect. 3.1.1). The first two items have been incorporated into the subroutine LEVEL, whereas the latter method is incorporated into INTMEB. Section 3.2 describes release rate methods. Flow through a breach can be assessed according to methods described in Sect. 3.2.2, whereas methods for evaluating flow through a broken (or misvalved) piping system are presented in Sect. 3.2.1. These flow rate methods are incorporated into BREACH and PIPSYS, respectively. The four subroutines, LEVEL, INTMEB, BREACH, and PIPSYS, are listed in Appendix B.

Section 3.3 describes the integration of the various methods presented in Sects. 3.1 and 3.2 into a method for determining the release rate of UF_6 from containment following a postulated accident. The main program, CYLIND, uses the four subroutines listed in the preceding paragraph to implement this method for a transient release. A plotting program, CYLPLT, which plots output from CYLIND, is described in Sect. 3.4.

3.1 CONTAINMENT (CYLINDER) SUBROUTINES

The conditions of UF_6 inside containment (e.g., a cylinder) must be known to perform flow rate analyses. These conditions include the temperature, pressure, and phase composition, the determination of which are discussed in Sect. 3.1.1. It is also necessary to know whether a single or multiphase mixture enters the release pathway (a breach or piping system). The determination of the phase interface level inside containment and, subsequently, the conditions of UF_6 entering the release pathway are discussed in Sect. 3.1.2.

3.1.1 Internal Mass and Energy Balance

During the release of UF_6, the phase composition within containment may pass through three basic phase regimes. Although it is recognized that there are probably temperature gradients within containment that could, for example, permit UF_6 to solidify on cool surfaces while liquid is present at other than the triple point temperature, it is assumed herein that the UF_6 within containment exists at a uniform temperature at any specific point in time. It is further assumed that phases are in thermodynamic equilibrium; that is, the pressure of the vapor is the vapor pressure over the condensed phase(s) existing at the current temperature. The three phase regimes considered are

37

1. liquid-vapor, which exists from the time of initial release until the internal pressure has decreased to the triple point at 147.3°F and 22.04 psia;
2. solid-liquid-vapor, which exists until the system has lost sufficient heat to exist as a solid-vapor system; and
3. solid-vapor, which exists below the triple-point conditions.

The first step in determining the transient-phase composition is to determine the total mass and enthalpy of the UF_6 in the cylinder at the end of a time step as functions of the initial masses and enthalpies of the individual phases and the mass flow rates and heat gains and losses over the time step. The required mass and energy balances are

$$m_f = m_{v,i} + m_{l,i} + m_{s,i} + (\dot{m}_{in} - \dot{m}_{out})\Delta t \ , \tag{75}$$

$$m_f\overline{H}_f = m_{v,i}H_{v,i} + m_{l,i}H_{l,i} + m_{s,i}H_{s,i} + (\dot{m}_{in}\overline{H}_{in} - \dot{m}_{out}\overline{H}_{out} + Q)\Delta t \ , \tag{76}$$

where

$$m = \text{mass, lb,}$$
$$\text{f,i} = \text{denote final and initial conditions,}$$
$$\text{v,l,s} = \text{denote vapor, liquid, and solid phase,}$$
$$\dot{m} = \text{mass fow rate, lb/sec,}$$
$$\text{in,out} = \text{denote flow into or out of containment,}$$
$$\Delta t = \text{time step, sec,}$$
$$H = \text{enthalpy, Btu/lb,}$$
$$^- = \text{denotes average value,}$$
$$Q = \text{heat input per unit time, Btu/sec.}$$

The only unknowns in the above equations, if the $\dot{m}$ and H inlet and outlet terms are based on conditions at the beginning of the time step, are $\dot{m}$ and $\overline{H}_f$. Equation 75 yields m_f directly, and $\overline{H}_f$ is then readily determined from Eq. 76.

Once m_f and $\overline{H}_f$ are known, mass, energy, and volume balances for the end of the time step are written

$$m_f = m_{v,f} + m_{l,f} + m_{s,f} \ , \tag{77}$$

$$m_f\overline{H}_f = m_{v,f}H_{v,f} + m_{l,f}H_{l,f} + m_{s,f}H_{s,f} \ , \tag{78}$$

and

$$V_T = (m_{v,f}/\rho_{v,f}) + (m_{l,f}/\rho_{l,f}) + (m_{s,f}/\rho_{s,f}) \ , \tag{79}$$

where

$$V_T = \text{volume of containment, ft}^3,$$
$$\rho = \text{density, lb/ft}^3.$$

These equations may be solved for the individual phase masses to obtain the following expressions in which m_f and $\overline{H}_f$ are known from the preceding set of equations (75 and 76), V_T is given, and the densities and enthalpies are functions of temperature only because the phases are assumed to be in equilibrium.

$$m_{v,f} = \frac{\rho_{v,f}[V_T \rho_{s,f} \rho_{l,f}(H_{l,f} - H_{s,f}) + m_f \rho_{l,f}(\overline{H}_f - H_{l,f}) - m_f \rho_{s,f}(\overline{H}_f - H_{s,f})]}{\rho_{l,f} \rho_{s,f}(H_{l,f} - H_{s,f}) + \rho_{v,f} \rho_{l,f}(H_{v,f} - H_{l,f}) - \rho_{v,f} \rho_{s,f}(H_{v,f} - H_{s,f})} , \tag{80}$$

$$m_{l,f} = [(\overline{H}_f - H_{s,f})/(H_{l,f} - H_{s,f})]m_f - [(H_{v,f} - H_{s,f})/(H_{l,f} - H_{s,f})]m_{v,f} , \tag{81}$$

and

$$m_{s,f} = m_f - m_{l,f} - m_{v,f} . \tag{82}$$

These equations may be used for any temperature; however, certain conditions must be met in determining (by trial and error) the temperature at the end time step.

1. At the triple point all masses must be equal to or greater than zero. If $m_{s,f}$ is negative at the triple-point temperature, the final temperature is greater than the triple-point temperature; and, if $m_{l,f}$ is negative, the final temperature is less than the triple-point temperature.

2. When the final temperature is known to be greater than the triple-point temperature, $m_{s,f}$ must equal zero. If $m_{s,f}$ is positive, the final temperature is less than the estimated temperature; and, if $m_{s,f}$ is negative, the final temperature is greater than the estimated temperature.

3. When the final temperature is known to be less than the triple point temperature, $m_{l,f}$ must equal zero. If $m_{l,f}$ is positive, the final temperature is greater than the estimated temperature; and, if $m_{l,f}$ is negative, the final temperature is less than the estimated temperature.

These criteria are summarized in Table 7. Note that use of the above equations for evaluating individual phase masses requires extrapolating solid-phase density and enthalpy above the triple-point temperature and liquid-phase density and enthalpy below the triple-point temperature. The correlations given in Sects. 2.1.3 and 2.1.7 for these physical properties are sufficiently well-behaved over the temperature range of interest to be extrapolated, as is illustrated by the dotted lines in Figs. 2 and 8.

After flow rates into or out of containment have been calculated by methods to be discussed in Sect. 3.2, the methods described previously in this section can be used to determine conditions at the end of a time step. The subroutine INTMEB has been developed to perform the mass and energy balances inside containment, given the mass of UF_6 in each phase and the saturation temperature at the beginning of the time step as well as the flow rates into or out of containment and the heat flow into containment.* Initial conditions are replaced by final conditions which have been determined iteratively by applying the guidelines summarized in Table 7. A listing of INTMEB is included in Appendix B.

At the beginning of a simulation, initial conditions must be specified to begin calculations. Specification of total UF_6 mass within containment, containment volume, and initial temperature

---

*Heat transfer to the cylinder is not discussed in this report and has been assumed to be negligible in example problems.

Table 7. Criteria for determining the
temperature at the end of a time step based on
Eqs. 80–82

Estimated final temperature[a]	Sign of estimated final mass for each phase			Conclusion
	$m_{v,f}$	$m_{l,f}$	$m_{s,f}$	
$T = T_{tp}$	+	+,0	+,0	$T_f = T$
	+	+,0	−	$T_f > T$
	+	−	+,0	$T_f < T$
$T > T_{tp}$	+	+	0	$T_f = T$
	+	+	+	$T_f < T$
	+	+	−	$T_f > T$
$T < T_{tp}$	+	0	+	$T_f = T$
	+	+	+	$T_f > T$
	+	−	+	$T_f < T$

[a]T = estimated temperaure for end of time step; T_{tp} = triple-point temperaure; and T_f = temperature at end of time step.

are sufficient to define the phase split within containment unless the specified temperature corresponds to the triple-point temperature. At temperatures other than the triple point,

$$X = [(V_T/m) - (1/\rho_c)]/[(1/\rho_v) - (1/\rho_c)] \ , \tag{83}$$

where

X = vapor mass fraction,
c = subscript implying condensed phase (solid or liquid).

Other variables are defined earlier in this section. Therefore, the mass of UF_6 in the vapor and condensed phases are given by

$$m_v = Xm \tag{84}$$

and

$$m_c = (1 - X)m \ , \tag{85}$$

respectively. If the triple point temperature is specified, the liquid mass fraction of the nonvapor fraction, X_l, must also be specified. Then,

$$1/\rho_c = (X_l/\rho_l) + [(1 - X_l)/\rho_s] \ . \tag{86}$$

Substituting the value of ρ_c obtained from Eq. 86 into Eq. 83, one obtains X and, subsequently, the mass of vapor present by Eq. 84. The mass of liquid and solid UF_6 present are given by,

$$m_l = (1 - X)X_l m \tag{87}$$

and

$$m_s = (1 - X)(l - X_l)m \ . $$

These final calculations to obtain initial conditions, which are represented by Eqs. 83 through 88, are included in the main program CYLIND.

3.1.2 Liquid-Vapor Interface Level and Phase Composition of UF_6 Leaving Containment

The phase composition of the UF_6 entering the release pathway is a function of the location of the entrance of the pathway with respect to the level of the interface between the vapor and condensed phase. In this section correlations are presented for determining the height of the phase interface in containment, which is modeled as a right circular cylinder, as well as the position of the interface relative to the release pathway. Also considered are the pressure heads occurring when the pathway entrance is submerged and the phase composition of the stream entering the pathway as the phase interface crosses the pathway entrance.

A right circular cylinder was chosen as the geometry to be modeled because it corresponds well to most process vessels as well as to cylinders used to store UF_6. Given the containment volume, diameter, and length, and the volume of vapor present in containment, the phase interface for a horizontal cylinder is found from

$$H = \frac{D}{2}\left\langle 1 + \cos\left\{\frac{180L}{V_T}\left[\frac{V_v}{L} + \left(H - \frac{D}{2}\right)\sqrt{HD - H^2}\right]\right\}\right\rangle \tag{89}$$

where

$\quad H$ = height of the phase interface, in.,
$\quad D$ = cylinder diameter, in.,
$\quad L$ = cylinder length, in.,
$\quad V_T$ = cylinder volume, in.^{3},
$\quad V_v$ = volume of vapor in containment, in.^{3}.

The quantity H is found by iteratively substituting a value for H for the right-hand side of Eq. 89 until a calculated value of H is found within the desired accuracy. In the case of a vertical cylinder,

$$H = [1 - (V_v/V_T)]L \ . \tag{90}$$

Based on a simple model assuming no entrainment, if the interface level is above the entrance to the release pathway, a nonvapor release from containment into the release pathway occurs, and if the interface level is below the pathway entrance, a vapor release occurs. A multiphase mixture will enter the release pathway as the interface crosses the entrance to the pathway. To determine the mass fraction of the vapor in the mixture, first calculate the height of the interface level with respect to the bottom of the entrance. For a circular breach in the end of a cylinder oriented horizontally, such as one might have if a valve is sheared off (see Fig. 17),

$$h = H - [(D/2) + R \cos\alpha - (d/2)] \ , \tag{91}$$

where

$h =$ height of interface above bottom of breach, in.,

$R =$ distance from centerline of cylinder to breach, in.,

$\alpha =$ angle with respect to the vertical of line passing through the center of the cylinder and the breach, degrees,

$d =$ diameter of the breach, in.

For a circular breach in the side of a vertically oriented cylinder,

$$h = H - (Z - d/2) \ , \tag{92}$$

ORNL–DWG 85-14590
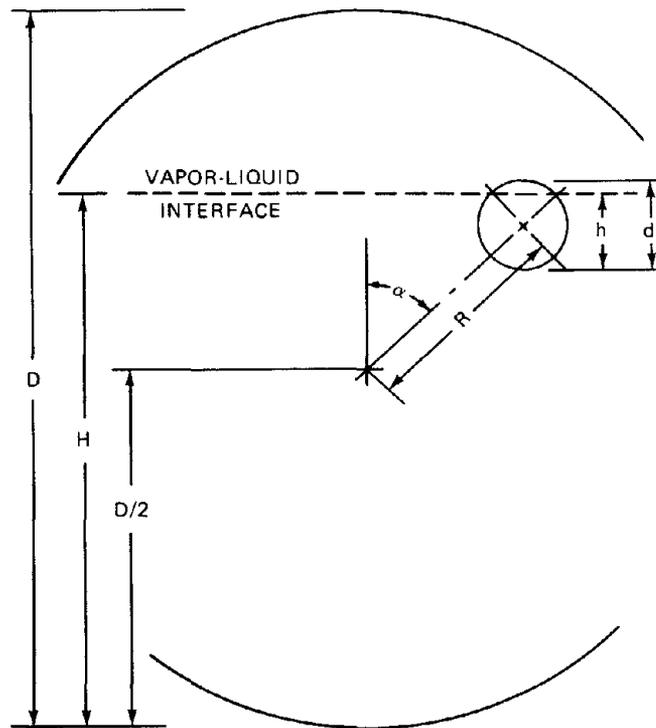
Fig. 17. Illustration of variable meanings used in determining the initial phase of a UF_6 release.

where

Z = height from bottom of cylinder to center of breach, in.,

For a breach in the bottom of a vertically oriented cylinder, $h = H$; whereas for a breach in the top, a vapor release occurs (also, $h = 0$).

If $h \geq d$, a nonvapor release occurs and the pressure of the condensed UF_6 entering the release pathway should be increased to

$$P = P^\circ + (\rho_c/1728)[h - (d/2)] , \qquad (93)$$

where

P = pressure of liquid UF_6 entering exhaust pathway, psia,
P° = vapor pressure of UF_6, psia,
ρ_c = condensed phase density, lb/ft^3.

If the breach is in the lower end of a vertically oriented cylinder, then $d = 0$ in Eq. 93. The density of the condensed phase is given by

$$\rho_c = m(1 - X)/(V_T - V_v) , \qquad (94)$$

where

m = total mass of UF_6 in containment, lb,
X = vapor mass fraction of UF_6 in containment.

If $h \leq 0$, a vapor release occurs.

For $0 < h < d$, the vapor volume fraction of the UF_6 entering the release pathway Y is given by,

$$Y = \frac{\arccos\left(\dfrac{2h - d}{d}\right)}{180} - \left(h - \frac{d}{2}\right)\sqrt{hd - h^2} \qquad (95)$$

and the vapor mass fraction is obtained from the following equations for mixture density which are equivalent,

$$\rho_m = Y\rho_v + (1 - Y)\rho_c , \qquad (96)$$

and

$$1/\rho_m = X/\rho_v + (1 - X)/\rho_c , \qquad (97)$$

where

ρ = density, lb/ft^3,

m,v,c = subscripts denoting mixture, vapor, and condensate, respectively,

X = vapor mass fraction.

Substituting for ρ_m yields

$$X = Y\rho_v/\rho_m \ . \tag{98}$$

The vapor mass fraction calculated in Eq. 98 is used for determining the enthalpy of the UF$_6$ exhausted from containment when the phase interface crosses the breach. Otherwise, $X = 0$ when the interface is above the breach and $X = 1$ when the interface is below the breach. The enthalpy of the UF exhausted is given by

$$H_{\text{out}} = XH_v + (1 - X)H_c \ . \tag{99}$$

where

H = enthalpy, Btu/lb.

Note that H_{out} does not include the effect of condensate head (Eq. 93), which effect is also not included in the internal mass and energy balance. In the subroutine LEVEL, however, the enthalpy calculated and passed to the flow rate subroutines to be discussed in Sect. 3.2 does include the enthalpy change resulting from the condensate head. The latter enthalpy is used for determining phase composition along the release pathway only, whereas the enthalpy calculated by Eq. 98 is used in Eq. 76.

A similar procedure can be followed for other containments and/or breach shapes and locations as a first-order approximation. Most of the above procedure has been implemented in the subroutine LEVEL. To characterize the cylinder, the user may specify the cylinder type through which default values are assigned for total internal volume, cylinder internal diameter, cylinder average internal length, the length of a ray from the center of the cylinder end to the center of a hole in the end, and the diameter of the hole. A user-defined cylinder type may also be specified, in which case values of the variables listed above must also be supplied. Default values of variables determined by the cylinder type are listed in Table 8. The user specifies separately the angle between an upward vertical ray and a ray from the cylinder center to the hole center. This angle α is the angle used in Eq. 91. Other input required by LEVEL includes the saturation temperature and/or saturation vapor pressure in the cylinder (the subroutine calculates or verifies the other) and total mass in the cylinder if different from the default value supplied in Table 8. If the cylinder temperature corresponds to the triple point temperature, the mass fraction of the nonvapor phase which is liquid must be specified. LEVEL returns the pressure at the release pathway entrance and the mass fractions of vapor, liquid, and solid UF$_6$ entering the pathway. Currently, LEVEL only applies to horizontal cylinders with breaches in the end. Of course, a horizontal cylinder with a breach in the side can be approximately modeled by defining an equivalent breach in the end (see Example 2, Sect. 5.1.1). A listing of LEVEL is provided in Appendix B.

Table 8. Cylinder types and default values
for use in the subroutine LEVEL^a

Cylinder type	Cylinder model	Maximum capacity^b (lb)	Internal volume (ft^3)	Internal diam. (in.)	Average length^c (in.)	Distance to valve^d (in.)	Valve inlet diameter (in.)	Maximum ^{235}U (%)
0	00			- - - - User specified - - - -				
1	5A	55	0.284	5	24.99	1.375	0.375	100
2	8A	255	1.319	8	45.34	1.375	0.375	12.5
3	12B	460	2.38	12	36.36	1.375	0.375	5
4	30B	5,020	26	29	68.02	9	0.875	52^e
5	48X	21,030	108.9	48	103.99	17	0.875	4.5^e
6	48Y	27,560	142.7	48	136.27	17	0.875	4.5^e

^{a}Table values are based on "Uranium Hexafluoride: Handling Procedures and Container Criteria," ORO-651, Rev. 4.

^{b}"Fill limits based on 250°F (121°C) maximum UF$_6$ temperature (203.3 lb UF$_6$/ft^3), certified minimum internal volumes [see above] for all cylinders, and a minimum safety factor of 5%. The operating limits apply to UF$_6$ with a minimum purity of 99.5%. More restrictive measures are required if additional impurities are present. The maximum UF$_6$ temperature must not be exceeded." (from ORO-651).

^{c}Based on cylinder volume divided by cross-sectional area based on internal diameter.

^{d}Measured from cylinder centerline to center of valve.

^{e}"Maximum enrichments indicated require moderation control equivalent to a UF$_6$ purity of 99.5%. Without moderation control, the maximum permissible enrichment is 1.0 wt% uranium-235" (from ORO-651).

3.2 FLOW RATE SUBROUTINES

This section discusses methods for evaluating fluid and mass velocities and criteria for determining when the flow is choked. The methods presented can be used for single or multiphase flow, including flashing and compressible flow. Section 3.2.1 addresses flow rate analysis in a piping system. Section 3.2.2 discusses analysis of flow through a breach in containment. The latter analysis is basically a simplified piping system where the pipe length goes to zero leaving only entrance and exit effects to be considered.

It is assumed that the exhaust pathway is sufficiently short such that the mass release rate is constant over the entire length at a given instant in time. Such an assumption appears valid because the change in the mass-release rate with time has been observed to be small, whereas the residence time is quite short. Given that the release rate over the entire length may be taken as constant at a given instant in time, the mass velocity can be determined at all points along the exhaust pathway from

$$\dot{m} = \rho A v / 144 = GA/144 \ , \tag{100}$$

where

$\dot{m}$ = mass release rate, lb/sec,

ρ = density, lb/ft^3,

A = flow area, in.^{2},

v = fluid velocity, ft/sec,

G = mass velocity, lb/ft^2-sec.

3.2.1 Flow through a ruptured piping system

The homogeneous flow model used in considering multiphase flow requires the following assumptions:

1. individual phase velocities are equal (i.e., no slip),
2. individual phases are in thermodynamic equilibrium with each other, and
3. a friction factor for two-phase flow can be suitably defined.

Based on these assumptions, Collier (1972) presented an equation for pressure drop that may be rearranged to give

$$\Delta L = -\left[\frac{4633.1\,\Delta P + G^2\,\Delta \bar{V}}{\dfrac{2f_{TP}\,G^2\bar{V}}{D} + \dfrac{g\sin\theta}{\bar{V}}} \right] \tag{101}$$

where

ΔL = incremental pipe length, ft,

ΔP = change in pressure, psi,

    = $P_2 - P_1$,

G = mass velocity, lb/ft^2-sec,

$\Delta \bar{V}$ = change in mixture specific volume, ft^3/lb

    = $\bar{V}_2 - \bar{V}_1$,

f_{TP} = Fanning friction factor for two-phase flow,

$\bar{V}$ = fluid specific volume, ft^3/lb,

    = $(\bar{V}_2 + \bar{V}_1)/2$,

D = pipe diameter, ft,

g = gravitation acceleration, ft/sec^2,

    = 32.174 ft/sec^2,

θ = angle of inclination of flow with respect to the horizontal, degrees,

1,2 = denote upstream and downstream conditions, respectively.

In accident analysis, the piping system is known, so increments of length calculated by the above equation must sum to the total length of the system. Depending on the assumed value of G and the values of ΔP and $\Delta \bar{V}$ (which is a function of ΔP since $\bar{V}$ is a function of P), ΔL may be positive, negative, or zero. If ΔL is found to be negative at any time before the total length has been used, the assumed G is too large. If ΔL is positive, but the total length calculated exceeds the available length, G is too small. The proper value for G is obtained when either (1) the value of ΔL calculated for the final ΔP brings the total calculated length to the total length or (2) when the next calculated ΔL is negative or zero, given that the previous ΔL had brought the calculated length to the total equivalent length. The latter condition (i.e., 2) corresponds to choked flow, which occurs when

$$G = [-4633.1(\Delta P/\Delta \bar{V})]^{0.5}\ , \tag{102}$$

which is obtained by setting the numerator of Eq. 101 to zero (i.e., $\Delta L = 0$). These conditions for finding G are summarized in Table 9.

To account for entrance and exit losses and the effect of fittings and valves, resistance coefficients are used. The general correlation for pressure drop across such a feature is

$$\Delta P = -(KG^2\overline{V}/9266.1) \ , \tag{103}$$

where K is the resistance coefficient and units for other variables are as defined for Eq. 101. Resistance coefficients are summarized in Table 10 for fittings and valves; these coefficients are functions of the nominal size of the fitting based on the following friction factor correlation (Crane Company 1980):

Table 9. Conditions for evaluating the mass velocity in a known piping system[a]

Sign of ΔL_i	Comparison of ΔL to L_T	Relationship of P to P_{surr}	Relationship of G to G_a	Remarks
$\Delta L_n = +$	$\sum_{j=1}^{n} \Delta L_j > L_T$	$P_{n,2} = P_{\text{surr}} - \Delta P_{\text{exit}}$	$G > G_a$	Repeat calculation using a larger G_a
$\Delta L_i = -$	$\sum_{j=1}^{i-1} \Delta L_j < L_T$	$P_{i,1} > P_{\text{surr}} - \Delta P_{\text{exit}}$	$G < G_a$	Repeat calculation using a smaller G_a
$\Delta L_i = -,0$	$\sum_{j=1}^{i-1} \Delta L_j > L_T$	$P_{i,1} > P_{\text{surr}} - \Delta P_{\text{exit}}$	$G = G_a$	Flow is choked[b]
$\Delta L_n = +$	$\sum_{j=1}^{n} \Delta L_j = L_T$	$P_{n,2} = P_{\text{surr}} - \Delta P_{\text{exit}}$	$G = G_a$	Flow is controlled by pressure

[a]Nomenclature:

ΔL = incremental length

i,n = subscripts denoting intermediate or final increment of length with respect to corresponding pressure drop. The final increment of pressure, ΔP_{exit}, brings $P_{n,2}$ to P_{surr}

j = subscript denoting summation

L_T = total length

$1,2$ = subscripts to P denoting pressure at the upstream and downstream ends of ΔL_i, respectively

P_{surr} = ambient pressure (add to ΔP for a sudden expansion to P_{surr} if L_T does not include equivalent lengths)

ΔP_{exit} = exit pressure loss

G = actual mass velocity which is being solved for

G_a = assumed mass velocity

[b]If ΔL_i is negative, a smaller ΔP_i may yield ΔL_i positive or zero. If positive, G would be slightly larger than G_a.

Table 10. Resistance coefficients for valves and fittings[a]

Description	K^b
Cylinder valves	
Nominal 1-in. valve	0.316
Nominal 3/4-in. valve	0.336
Gate valves, fully open	$8\,f_T$
Globe valves	$340\,f_T$
Butterfly valves	$(51.42 - 1.33\,\text{d})f_T$
Plug valves and cocks	
Straight way	$18\,f_T$
Three Way, straight through	$30\,f_T$
Three Way, through branch	$90\,f_T$
Standard elbows	
90°	$30\,f_T$
45°	$16\,f_T$
90° Pipe bends	
$0.5 \leqslant r/d < 1.25$	$[40 - 20(r/d)]f_T$
$1.25 \leqslant r/d < 2.29$	$[20 - 4(r/d)]f_T$
$2.29 \leqslant r/d < 6$	$[7 + 1.67(r/d)]f_T$
$6 \leqslant r/d < 10$	$[-2.5 + 3.25(r/d)]f_T$
$r/d \geqslant 10$	$[10 + 2(r/d)]f_T$
Standard tees	
Flow-through run	$20\,f_T$
Flow-through branch	$60\,f_T$

[a]Based on Crane Company 1980. *Flow of Fluids,* Technical Paper 410M.

[b]f_T is given by Eq. 104. Nominal pipe diameter d and pipe bend radius (based on pipe center line) r are given in inches.

$$f_T = 0.00574d^{-0.221}\ , \tag{104}$$

where

f_T = friction factor for fittings,

d = nominal pipe diameter for fitting or valve, in..

Resistance coefficients for sudden expansions and contractions are summarized in Table 11.

The friction factor and physical properties used in Eqs. 101 and 102 should be evaluated at average conditions over the ΔP interval. In Eq. 103, the mixture specific volume $\overline{V}$ for sudden contractions (entrances) should be evaluated at P_2 and for sudden expansions (exits), fittings, and valves at P_1, such that

Table 11. Resistance coefficients for sudden expansion and contractions[a]

Description	K[b]
Pipe exit (projecting, sharp-edged, or rounded)	1.0
Pipe enlargement	$(1 - \beta^2)^2$
Pipe entrance	
Projecting	0.78
Sharp edged	0.50
Rounded	$[2 + 77.78(r/d)]^{-1}$
Pipe contraction	$0.5(1 - \beta^2)$

[a]Based on Crane Company 1980, *Flow of Fluids*, Technical Paper 410M.

[b] $\beta = d_1/d_2$,

   d = pipe diameter. in.,

   1,2 = subscripts referring to the diameter of the smaller and larger pipes, respectively,

   r = radius of curvature of entrance rounding, in.

$$\Delta P = P_2 - P_1 \ , \tag{105}$$

where

P_2 = downstream pressure, psia,

P_1 = upstream pressure, psia.

The friction factor to be used is the Fanning friction factor based on an average value for the viscosity, which will be discussed subsequently. A suitable correlation for the friction factor has been derived by Churchill (1977)

$$f_{TP} = 2\{(8/Re)^{12} + [1/(A + B)^{3/2}]\}^{1/12} \ , \tag{106}$$

where

   $A = <2.457 \ln \{1/[(7/Re)^{0.9} + (0.27 \ \epsilon/D)]\}>^{16} \ ,$ (107)

   $B = (37,530/Re)^{16},$ (108)

   Re = Renolds number,

   ϵ/D = pipe roughness.

The Reynolds number is given by

$$Re = 3600DG/\mu_m \ , \tag{109}$$

where

μ_m = viscosity of the mixture, lb_m/ft-hr.

The average mixture specific volume and density of a two-phase mixture are given by

$$\overline{V} = 1/\rho = (X/\rho_v) + [(1 - x)/\rho_c] \ , \tag{110}$$

where units are as defined above. For multicomponent, multiphase flow,

$$\overline{V} = 1/\rho = \Sigma X_i/\rho_i \ , \tag{111}$$

where

X_i = mass fraction of component i,

ρ_i = density of component i (the same chemical species is considered a separate component for each phase in which it exists), lb/ft^3.

For solid-vapor flow, the viscosity of the mixture is assumed to be the viscosity of the vapor. For liquid-vapor flow, Hewitt (Ginoux 1978) recommends Dukler's correlation,

$$\mu_m = \left[\frac{X\mu_v}{\rho_v} + \frac{(1-x)\mu_l}{\rho_l} \right] \rho \ .$$

For multicomponent liquid-vapor flow,

$$\mu_m = \Sigma Y_i \mu_i \ , \tag{113}$$

where

$$Y_i = X_i \rho / \rho_i \ , \tag{114}$$
μ_i = viscosity of component i, lb_m/ft-hr.

In the event of three-phase, multicomponent flow, the solids are assumed to be associated with the liquid and μ_v and μ_l are defined as follows for use in Eq. 112,

$$\mu_v = (\Sigma Y_i \mu_i / \Sigma Y_i)|_{i \text{ in vapor phase}} \tag{115}$$

and

$$\mu_l = (\Sigma Y_i \mu_i / \Sigma Y_i)|_{i \text{ in liquid phase}} \ . \tag{116}$$

Thus, the viscosity of the liquid-solid mixture is taken as the viscosity of the liquid flowing alone.

The overall analysis procedure to determine the mass release rate $\dot{m}$ is as follows.

1. Assume a value of mass velocity G. (Note that if pipe diameter changes, G changes, but $\dot{m}$ remains constant.)

2. Determine the inlet pressure drop using Eq. 103 and a fluid specific volume at $P_2 = P_1 + \Delta P$.
3. Evaluate pressure drop along the piping system:
   a. Use Eq. 101 to evaluate pressure drop over the length of pipe between point features such as expansions, contractions, valves, and fittings. Use several increments of pressure, and average properties for each increment of pressure, to find increments of length summing to the total length. Note restrictions in preceding discussion and Table 9.
   b. Use Eq. 103 to evaluate pressure drop across expansions, valves, and fittings using the fluid specific volume at the upstream conditions, and across contractions using the downstream pressure.
4. Determine if assumed G is correct, or assume new G and return to Step 2:
   a. If flow is controlled by pressure, G is obtained when the total pressure drop is expended over the total pipe length, including the entrance, exit, and point features.
   b. If flow is choked, G is obtained when an infinitesimal increment of pressure drop yields a zero or negative pipe length given that the last increment of pressure brought the total length to the length of the system. This is equivalent to satisfying Eq. 102, the choke flow criterion.
5. When G is obtained, determine the mass release rate $\dot{m}$ from Eq. 100.

The procedure outlined in the preceding paragraph has, for the most part, been incorporated into the subroutine PIPSYS. The first step, assuming a mass velocity, is taken outside PIPSYS by determining the maximum value of G which would result if a breach in containment had the initial diameter of the piping system. This value is obtained using the subroutine BREACH, which will be discussed in the next section. The assumed value of G is used until a choking condition occurs (i.e., G too large) or the piping system length is exceeded (i.e., G too small), then a new value of G is chosen. When the total pressure drop is exactly expended over the entire piping system or choking occurs at the outlet of the piping system, G is determined.

Special consideration must be given when the triple point is encountered, which is often the case because liquid releases are usually considered and the triple point exceeds atmospheric pressure. If the UF_6 triple-point pressure (22.04 psia) is between the inlet and outlet pressures of the entrance of any fitting or valve or of a sudden expansion or contraction and if any liquid is present in the stream at the inlet pressure, the liquid is assumed to flash to solid and vapor within that element. If, for an estimated mass velocity, the triple point is predicted to occur within a length of pipe between point features, the change in specific volume from a liquid-vapor mixture to a solid-vapor mixture will result in a negative incremental pipe length from Eq. 101. In this case, the estimated mass velocity is considered too high and a new, lower value is chosen for evaluation. In a complex piping system, this approach may lead to an underestimation of the mass release rate because it tends to force the triple point toward the outlet end of the piping system, unless the triple point is crossed in evaluating the pressure drop across a point feature.

In addition to supplying an initial guess of G, the program calling PIPSYS must input values for the pressure, temperature, molecular weight, and phase mass fractions of UF_6 entering the release pathway; the pressure of the surroundings; and the UF_6 triple-point temperature and vapor pressure. The calling program must pass to PIPSYS the resistance coefficients and nominal diameters of fittings and valves, the resistance coefficients of sudden expansions and contractions, and the length and inside diameters of pipe segments. The PIPSYS subroutine outputs the predicted mass velocity through the piping system. A listing of PIPSYS appears in Appendix B.

3.2.2 Flow rates through a breach in containment

Flow through a breach in containment is modeled essentially as flow through a piping system except that the flow path length is assumed infinitesimal. Referring to Fig. 18, Eq. 103 can be used to evaluate G and P_i by using a specific volume corresponding to P_i, provided the flow is controlled by the pressure drop. Thus,

$$G = \{[6177.4(P_1 - P_2)]/\overline{V_i}\}^{0.5} \tag{117}$$

$$= \{[18532(P_1 - P_i)]/\overline{V_i}\}^{0.5}$$

$$= \{[9266.1(P_i - P_2)/\overline{V_i}\}^{0.5} ,$$

where the first equality is referenced to the total pressure drop and a K of 1.5, the second equality refers to the entrance pressure drop with a K of 0.5, and the third equality refers to the exit pressure drop with a K of 1.0. The equation is applicable to flashing flow because K values are based on conditions inside the pipe. Because the flow path length is assumed negligible, conditions inside the pipe based on P_i are assumed to be the same for evaluating entrance and exit pressure drops. By rearranging the various expression for G, which can be obtained from Eq. 117, an expression for the intermediate pressure P_i can be obtained,

$$P_i = (2P_1 + P_2)/3 . \tag{118}$$

ORNL–DWG 85-14589
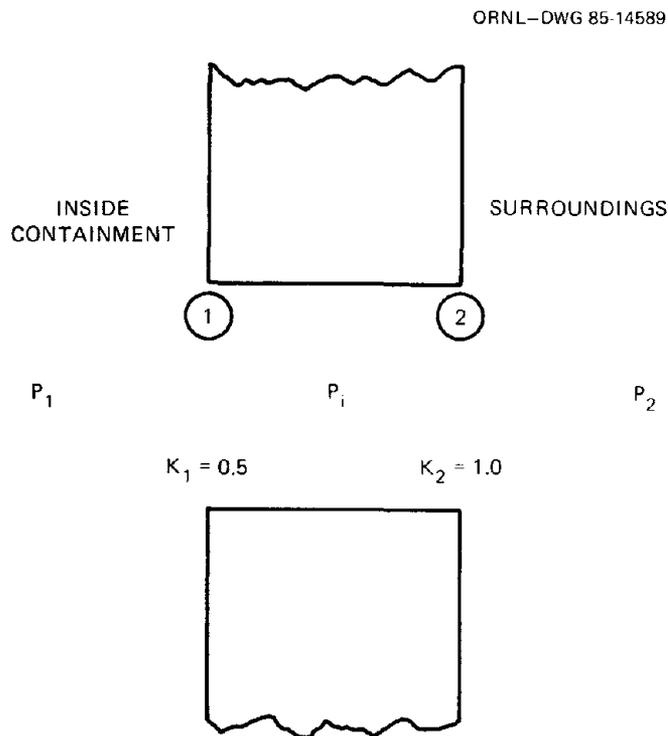
Fig. 18. Model used for evaluating flow through a breach in containment.

If the mass velocity G is limited by choke flow, two of the three equalities of Eq. 117 do not apply. Choke flow requires that G satisfy both Eq. 103, evaluated for the entrance pressure drop $(\Delta P = P_i - P_1)$, the mixture specific volume $\overline{V}_i$ at P_i, and $K = 0.5$ and Eq. 102, where ΔP and $\Delta \overline{V}$ are evaluated over a small ΔP using P_i as the upstream pressure. Thus,

$$G_{\max} = \left[\frac{18532(P_1 - P_i)}{\overline{V}_i} \right]^{0.5} = [-4633.1(\Delta P / \Delta \overline{V}_i)]^{0.5} \ . \tag{119}$$

As with Eq. 117, this equation is also applicable to flashing flow.

Because of the tremendous difference that occurs in specific volume if P_i is slightly above the triple point vs slightly below the triple point, it was decided to restrict P_i to no less than the triple point if a liquid release were being simulated. In practice, the minimum value is higher than the triple-point pressure by the differential pressure used to evaluate the choke flow condition so that both specific volumes are restricted to liquid-vapor mixtures.

The procedure for finding the mass velocity G for a release through a breach in containment is as follows. First, calculate the intermediate pressure P_i, using Eq. 118. If P_i is less than the triple-point pressure (~ 22.04 psi), set it equal to the triple-point pressure. Next, evaluate $\overline{V}_i$ and P_i, and then calculate G from Eq. 117. Using the second expression for $G_{\max}$ given by Eq. 119, evaluate $G_{\max}$ at P_i. If $G \leqslant G_{\max}$, the flow is controlled by pressure drop and G is the predicted mass velocity. If $G > G_{\max}$, the flow is choked. Using Eq. 119, select values of P_i iteratively until the same value for $G_{\max}$ is obtained from both the first and second parts of Eq. 119. The value of $G_{\max}$ thus obtained is the predicted mass velocity.

The above procedure has been implemented in the subroutine BREACH. The program calling BREACH must input values for the pressure, temperature, molecular weight, and phase mass fractions of UF_6 entering the release pathway, the pressure of the surroundings; and the UF_6 triple point temperature and vapor pressure. Also, the calling program must input an integer value indicating that constant enthalpy is assumed in the flash calculations. The BREACH subroutine outputs the calculated value of mass velocity and the corresponding pressure, temperature, and phase mass fractions of UF_6 at the intermediate or choke flow conditions. Also, the subroutine outputs an integer value indicating whether the mass velocity was controlled by pressure drop or by the choke flow criterion. Further documentation is provided in the program listing found in Appendix B.

3.3 MAIN PROGRAM FOR EVALUATING RELEASE RATES FROM A CYLINDER

A main program, CYLIND, has been developed to evaluate mass release rates from a cylinder through a breach or piping system. A simplified logic flow diagram for this main program is shown in Fig. 19. CYLIND prepares as input for the subroutines the data describing the cylinder, the release pathway, and physical conditions including the initial temperature, pressure, total mass of UF_6, and mass fractions in each phase in the cylinder, and the ambient pressure. Input requirements and format for CYLIND are listed in Table 12. CYLIND also controls the number and length of time steps and the output of results. A few simple calculations are done in the main program, including the initial mass balance (specifically the initial vapor mass fraction, see Eq. 83) and the conversion of steady state mass velocities predicted by BREACH and PIPSYS subroutines for each time step to mass flow rates in pounds of UF_6 per second. Output from CYLIND includes

ORNL- DWG 85-14587
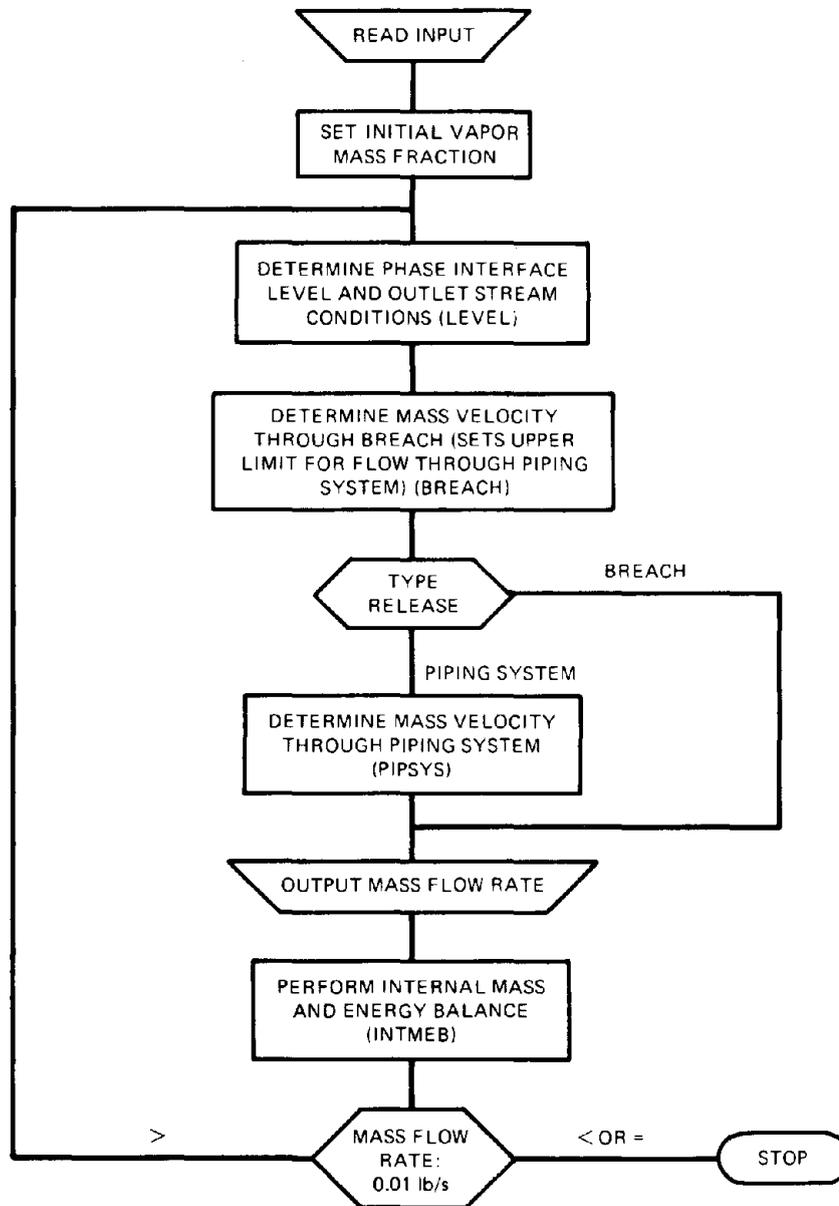
Fig. 19. Simplified logic flow diagram for CYLIND.

information on the UF_6 in containment (mass of UF_6 in each phase and temperature) and mass release rates as well as a data file suitable for input to the compartment models. Examples of CYLIND output are given in Table 24 and in Appendix C. Any computer program or subroutine incorporating the contents of CYLIND may use the four subroutines described in this chapter. A descriptive listing of the program and the required data files is included in Appendix A.

Table 12. Input required for CYLIND

/
/ CARD 1.   READ TITLE (LIMITED TO 80 CHARACTERS).

/
/ CARD 2.   READ FLASH BASIS, CYLINDER TYPE, CYLINDER ORIENTATION,
           AND NUMBER OF ELEMENTS IN RELEASE PATHWAY.

           FLASH BASIS (ISEN)

           0   ISENTROPIC
           1   ISENTHALPIC

           ISEN = 1 IS RECOMMENDED SINCE THE FLASHING PROCESS WAS
           ASSUMED TO BE ISENTHALPIC IN THE DERIVATION OF THE
           CORRELATION USED IN THE SUBROUTINE PIPSYS FOR PRESSURE
           DROP IN A PIPE.

           CYLINDER TYPE (ICYL)

           0   USER SPECIFIED
           1   TYPE 5A CYLINDER
           2   TYPE 8A CYLINDER
           3   TYPE 12B CYLINDER
           4   TYPE 30B CYLINDER (2.5 TON)
           5   TYPE 48X CYLINDER (10 TON)
           6   TYPE 48Y CYLINDER (14 TON)

           IF A NEGATIVE VALUE OF ICYL IS READ (-1, -2, -3, -4, -5,
           -6), THE USER MAY SUBSEQUENTLY SPECIFY A TOTAL MASS OF UF6
           DIFFERENT FROM THE DEFAULT VALUE (SEE CARD 4).

           CYLINDER ORIENTATION (IVERT)

           -1   CYLINDER STANDS ON END -- RELEASE FROM TOP END
           0   CYLINDER LIES ON SIDE -- RELEASE FROM END
           1   CYLINDER STANDS ON END -- RELEASE FROM BOTTOM END

           NUMBER OF ELEMENTS IN RELEASE PATHWAY (IPIG)

           IF IPIG = 2, THE RELEASE PATHWAY IS A BREACH IN THE
           CYLINDER. IF THE RELEASE PATHWAY IS A PIPING SYSTEM, IPIG
           IS GREATER THAN 2.

/
/ CARD 3.   -- USE THIS CARD ONLY IF ICYL = 0 --

           READ MASS OF UF6 IN THE CYLINDER (LB); VOLUME (FT**3),
           INTERNAL DIAMETER (IN), AND INTERNAL LENGTH (IN) OF THE
           CYLINDER; RADIUS FROM THE CYLINDER CENTERLINE TO THE VALVE
           (BREACH) (IN); AND THE VALVE (BREACH) DIAMETER (IN).

Table 12. (continued)

/
/ CARD 4.   -- USE THIS CARD ONLY IF ICYL IS NEGATIVE --

READ MASS OF UF6 IN CYLINDER (LB).

/
/ CARD 5.   READ PRESSURE (PSIA), TEMPERATURE (DEG F), LIQUID MASS
FRACTION OF THE NONVAPOR FRACTION (--), MOLECULAR WEIGHT
(LB/LB MOLE), AND THE ANGLE MEASURED FROM A VERTICAL VECTOR
PASSING THROUGH THE CENTER OF THE END AND A VECTOR FROM THE
CENTER OF THE END AND THE ENTRANCE TO THE RELEASE PATHWAY
(DEG). IF PRESSURE IS SPECIFIED AS ZERO AND/OR TEMPERATURE
IS SPECIFIED AS NONZERO, THEN THE PRESSURE WILL BE SET EQUAL
TO THE VAPOR PRESSURE. IF PRESSURE IS SPECIFIED AS NONZERO
AND TEMPERATURE IS SPECIFIED AS ZERO, THEN THE EQUILIBRIUM
TEMPERATURE CORRESPONDING TO THE SPECIFIED PRESSURE WILL BE
CALCULATED. IF THE TRIPLE POINT TEMPERATURE IS SPECIFIED
(147.306561 DEG F), THEN A NONZERO VALUE FOR THE LIQUID MASS
FRACTION OF THE NONVAPOR FRACTION CAN BE SPECIFIED;
OTHERWISE, THE VALUE READ AS INPUT WILL BE SET BY THE
PROGRAM TO THE APPROPRIATE VALUE. THE DEFAULT VALUE FOR
MOLECULAR WEIGHT IS 352.025 -- IF THIS VALUE IS ACCEPTABLE,
A ZERO MAY BEPECIFIED FOR THIS VARIABLE.

/
/ CARD 6.   -- USE THIS CARD ONLY IF IPIG = 2 --

READ AMBIENT PRESSURE (PSIA). A ZERO VALUE DEFAULTS TO
14.7 PSIA.

/
/ CARD 7.   -- USE ONLY IF IPIG IS GREATER THAN 2 --

READ AS MANY CARDS AS THE VALUE OF IPIG TO SPECIFY THE
PIPING SYSTEM. EACH CARD CONTAINS (1) A VALUE SPECIFYING
ELEMENT TYPE, (2) ELEMENT LENGTH (FT) OR RESISTANCE
COEFFICIENT (--), AND (3) DIAMETER (IN), EXCEPT FOR THE LAST
CARD. THE THIRD VALUE ON THE LAST OF THE "CARD 7" CARDS IS
THE AMBIENT PRESSURE (PSIA).

ELEMENT TYPE (PIGRAY(I,1))

    1   SPECIFIES A PIPE SEGMENT (EXCEPT FIRST "CARD 7" WHERE
         IT SPECIFIES THE ENTRANCE)
    2   SPECIFIES A PIPING SYSTEM FEATURE (SUDDEN EXPANSION,
         VALVE, BEND, ETC.) FOR WHICH A RESISTANCE COEFFICIENT
         IS SUPPLIED
    3   SPECIFIES A SUDDEN CONTRACTION FOR WHICH A RESISTANCE
         COEFFICIENT IS SUPPLIED

Table 12 (continued)

RESISTANCE COEFFICIENT (PIGRAY(I,2))

    THIS VALUE MUST BE CALCULATED BY THE USER.

DIAMETER (PIGRAY(I,3))

    (NOTE: PIGRAY(IPIG,3) IS THE EXHAUST PRESSURE, PSIA.)

    FOR A SUDDEN CONTRACTION, SPECIFY THE DOWNSTREAM DIAMETER
    FOLLOWING THE CONTRACTION. FOR A SUDDEN EXPANSION, SPECIFY
    THE UPSTREAM DIAMETER BEFORE THE EXPANSION.

/
/ CARD 8.   READ SIMULATION TIME INTERVAL (SEC) AND MAXIMUM
         SIMULATION TIME (SEC).

/
/ CARD 9.   -- THESE CARDS ARE OPTIONAL --

    ENTER DRAWING NUMBERS (LIMITED TO 20 CHARACTERS--THE LAST
    CHARACTER MUST BE A DOLLAR SIGN ($)). THESE NUMBERS ARE
    ENTERED IN A FILE FOR CYLPLT PROCESSING.

    1ST CARD 9 = PHASE MASSES AND TOTAL MASS OF UF6 INSIDE
               CYLINDER
    2ND CARD 9 = PHASE AND TOTAL MASS RELEASE RATES FROM
               CYLINDER
    3RD CARD 9 = TEMPERATURE AND PRESSURE INSIDE CYLINDER
    4TH CARD 9 = EXHAUST TEMPERATURE

3.4 CYLINDER MODEL PLOTTING PROGRAM

A program has been written to read data from the primary output file of CYLIND (e.g., see Table 24 in Chap. 5) and to plot the results. This program, CYLPLT, is written using DISSPLA version 9.0.[*] An input file listing drawing numbers is also required to execute CYLPLT; an appropriate file is produced by CYLIND. Examples of output from CYLPLT are given in Chap. 5 illustrating results of Examples 1, 2, and 3. A listing of CYLPLT is provided in Appendix A.

---

[*]Integrated Software Systems Corporation, San Diego, California, 1981.

4. COMPARTMENT MODELS

Accident scenarios involving the postulated release of UF_6 can occur both indoors and outdoors. For indoor releases, compartment models are needed that can handle the effects of chemical reactions and vapor liquid equilibrium, including changes in temperature and pressure within a compartment. The compartment models presented herein were developed on the assumption of homogeneous behavior; that is, at a given instant in time, the composition, temperature, and pressure within a compartment are the same; hence, there is no spatial variation. Because the characteristics of a particular site are unique, an extensive set of subroutines was written so that specialized transient models tailored to simulate specific building ventilation configurations could be quickly developed by writing only a main program. Two transient models and one batch model have been developed for inclusion in this report.

1. FODRFT simulates the transient behavior of a release in a building having forced-draft ventilation.
2. INDRFT simulates the transient behavior of a release in a building having induced-draft ventilation.
3. BATCH evaluates final conditions in a closed room with an option (open compartment) to base final conditions on the ambient pressure while allowing the compartment volume to be changed.

The "open compartment" option identified for BATCH allows for the simulation of a steady-state release into a constant volume air flow rate ventilation system exhausting to the outside.

A simplified logic diagram for the transient models is shown in Fig. 20. The following list provides a brief description of the purpose of each subroutine as well as the section of this report in which background material and the subroutine are discussed.

1. COMPRT performs final mass and energy balances for a compartment, including reaction and heat transfer given input and output flow rates and initial conditions (see Sect. 4.5.2).
2. DENTHL calculates total enthalpy with respect to reference conditions, given composition, temperature, and pressure (see Sect. 2.4).
3. DENUF6 calculates densities of UF_6, given temperature, pressure, and molecular weight (see Sects. 2.1.3 and 2.1.12).
4. DPFLOW calculates mass flow and enthalpy rates through a pressure-drop-controlled duct or vent given the pressure drop, a resistance term, and upstream conditions (see Sect. 4.2.2).
5. EQTUF6 calculates the temperature that would yield a given pressure as the vapor pressure of UF_6 (see Sects. 2.1.1 and 2.1.12).
6. FLASH calculates the resulting final solid-liquid-vapor split of UF_6, given the initial composition, temperature, and pressure and the final pressure (see Sect. 2.1.11).
7. HCOEFF calculates a heat transfer coefficient required to maintain steady-state conditions, given steady-state compartment and inlet stream data (see Sect. 4.5.1).
8. HFPOLY calculates effective molecular weight and monomer, trimer, and hexamer weight fractions, given the temperature and partial pressure of HF (see Sects. 2.2.1 and 2.2.7).
9. HHFH2O calculates liquid and vapor enthalpies of HF-H_2O mixtures, given temperature and composition (see Sects. 2.2.4, 2.2.5, and 2.2.7).
10. HUF6 calculates UF_6 enthalpies, given temperature, pressure, and molecular weight (see Sects. 2.1.7 and 2.1.12).

59

ORNL–DWG 85-14586

```
                    ┌─────────┐
                    │  START  │
                    └─────────┘
                         │
              ┌────────────────────────┐
              │  INITIALIZE ARRAYS     │
              │      SETRAY            │
              └────────────────────────┘
                         │
              ╱──────────────────────╲
              ╲    READ INPUT DATA    ╱
               ──────────────────────
                         │
         ┌───────────────────────────────┐
         │  EXPAND STEADY-STATE DATA      │
         │  READ IN TO PROVIDE INITIAL    │
         │  CONDITIONS FOR TRANSIENT      │
         │      RELEASE ANALYSIS          │
         │           HUMID                │
         │           ROOM                 │
         │           SSBLOW               │
         │           RESIST               │
         │           DENTHL               │
         │           HCOEFF               │
         │           STERM*               │
         └───────────────────────────────┘
                         │
                  ┌─────────────┐
                  │  TIME = 0   │
                  └─────────────┘
                         │
         ┌─────────────────────────────┐
         │  ESTABLISH FLOW RATES        │
         │         STERM*               │
         │         TRBLOW               │
         │         DPFLOW               │
         │         REMOVE               │
         └─────────────────────────────┘
                         │
         ┌─────────────────────────────┐
         │  SET SOURCE TERM TO ZERO     │
         │  IF RELEASE TIME EXCEEDED    │
         └─────────────────────────────┘
                         │
         ┌─────────────────────────────┐
         │  OUTPUT COMPARTMENT MODEL    │
         │  MASS, TEMPERATURE, AND      │
         │      PRESSURE DATA           │
         └─────────────────────────────┘
                         │
         ┌─────────────────────────────┐
         │  TIME = TIME + DELT          │
         └─────────────────────────────┘
                         │
              ╱──────────────────╲   YES   ┌────────┐
              ╲   TIME > MAXTIM   ╱────────│  STOP  │
               ──────────────────          └────────┘
                         │ NO
         ┌─────────────────────────────┐
         │  PERFORM COMPARTMENT MASS    │
         │  AND ENERGY BALANCES         │
         │        COMPRT                │
         └─────────────────────────────┘
```

*STERM IS CALLED BEFORE TRANSIENT ANALYSIS BEGINS UNLESS CODING
FOR A QUASI-TRANSIENT SOURCE TERM IS REQUIRED.

Fig. 20. Simplified logic diagram for transient compartment models.

11. HUMID calculates the molar ratio of water vapor to moist air, given the ambient temperature, pressure, and relative humidity (see Sect. 4.5.1).

12. MIXFLW combines up to four streams including reaction effects and exhausts at a given pressure, given initial stream data (see Sect. 4.2.3).

13. PHASE performs a vapor-liquid equilibrium mass balance for an HF-H$_2$O system, given total masses of HF and H$_2$O, volume, and temperature (see Sects. 2.2.6 and 2.2.7).

14. PHFH2O calculates partial and total vapor pressures for the HF-H$_2$O system, given liquid-phase composition and temperature (see Sect. 2.2.2, 2.2.3, and 2.2.7).

15. REMOVE evaluates removal rate of condensate from a compartment, given the composition in the compartment and the floor area of the compartment (see Sect. 4.4).

16. RESIST calculates a resistance term for pressure-drop-controlled vents, given either a resistance coefficient and flow area or steady-state mass flow rate, density, and pressure differential (see Sect. 4.2.1).

17. ROOM calculates the initial mass of air and water vapor in a compartment, given the ambient-water-vapor-to-moist-air ratio and the temperature, pressure, and volume of the compartment (see Sect. 4.5.1).

18. SETRAY initializes arrays (see Sect. 4.1.1).

19. SSBLOW calculates initial flow rates of air and water vapor through a constant volume blower, given the ambient-water-vapor-to-moist-air ratio, the upstream temperature and pressure, and the blower volumetric flow rate (see Sect. 4.2.1).

20. STERM sets up source term data for the transient compartment models, given input data read by main program (see Sect. 4.3).

21. SUF6 calculates entropies of UF$_6$ given temperature, pressure, and molecular weight (see Sects. 2.1.8 and 2.1.12).

22. TRBLOW calculates mass flow and enthalpy rates through a constant volume blower, given upstream compartment conditions and blower volumetric flow rate (see Sect. 4.2.2).

23. VPRUF6 evaluates UF$_6$ vapor pressure for a given temperature (see Sects. 2.1.1 and 2.1.12).

24. ZUF6 calculates UF$_6$ vapor compressibility, given temperature and pressure (see Sects. 2.1.2 and 2.1.12).

In addition to these subroutines, subroutines CPUF6, THCUF6, and VISUF6—which calculate UF$_6$ heat capacities, thermal conductivities, and viscosities, respectively—are available but not used in the current compartment models (see Sects. 2.1.6, 2.1.5, and 2.1.4, respectively, as well as Sect. 2.1.12). VISUF6 is used in the flow rate models discussed in Chap. 3.

A general discussion of the structure of the main programs is given in Sect. 4.1; however, the specific programs (FODRFT, INDRFT, and BATCH) are not discussed until Sect. 4.6. COMPLT, a program to plot output from FODRFT and INDRFT, is presented in Sect. 4.7. Listings of these main programs are provided in Appendix A. A discussion of physical and thermodynamic properties required for the compartment models has been provided earlier in Chap. 2. Ventilation system subroutines are discussed in Sect. 4.2, including a stream mixing model. A source term model which develops input values for a finite duration release is described in Sect. 4.3. Section 4.4 discusses condensate deposition. Subroutines for performing compartment mass and energy balances are presented in Sect. 4.5. Listings of all subroutines are included in Appendix B.

4.1 MAIN PROGRAM STRUCTURE

The general structure of a main program to perform transient compartment analyses is described in this section. This description includes certain elements of coding required in any transient program. Many elements would need to be added to develop a suitable main program for a particular application. Examples of such additional elements of coding, as well as how these elements fit together with those presented in this section, are best seen by comparing the subsequent discussion in this section to the program listings of FODRFT and INDRFT included in Appendix A. A generalized logic diagram for the aforementioned main programs is given in Fig. 21. The overall structure of a main program is

1. initialize arrays and read input data (Sects. 4.1.1 and 4.1.2),
2. develop initial steady state conditions existing prior to the release that are derived from input data (Sect. 4.1.3), and
3. perform the transient analysis and output results (Sect. 4.1.4).

Special features of the programs developed for inclusion in this report are discussed in Sect. 4.6.

4.1.1 Initial Statements

All subroutines discussed in this report are written in double precision FORTRAN. The following coding is required in all main programs.

```
      IMPLICIT REAL*8 (A-H,J-Z)
C
      LOGICAL CHECK
C
      DIMENSION FLAREA(30), ACFM(30), RATE(9)
C
      COMMON /LBMASS/ MASS(30,9), RH
      COMMON /COMPTP/ TC(30), PC(30), TSURF(30)
      COMMON /MOLWT/ WMOL(9)
      COMMON /VOLUME/ VOL(30), KRCOEF(30), DPAREA(30), DEPVEL
      COMMON /ENTHAL/ H(30), QRATE(30), QCOOL(30), HTCOEF(30),
     *      HTAREA(30)
      COMMON /ISTRMS/ IIN(30,4), IOUT(30,4)
      COMMON /CONTRL/ AMINLN, TIME, DELT, MAXTIM, IFLAG, TRELS
      COMMON /POLYMR/ C1, C3, C6, WMBHF
      COMMON /MISCEL/ ITYPE, SOURCE, ISEN
      COMMON /RVFLOW/ TSTART(30), TSTOP(30)
C
      EQUIVALENCE (VOL(1),ACFM(1),FLAREA(1))
C
      CALL SETRAY(INODES, INOUT)
```

Definitions and units for the variables shown in the preceding coding, as well as for other variables appearing in this chapter, are given in Table 13. Note the call to SETRAY, which initializes many of the variables to appropriate values including the array of molecular weights. As currently imple-

ORNL—DWG 85-14588

START

INITIALIZE ARRAYS
SETRAY

READ INPUT DATA

CALCULATE WATER VAPOR
TO MOIST AIR RATIO
HUMID

CALCULATE INITIAL MASS OF
AIR AND WATER VAPOR AND
INITIAL TOTAL ENTHALPY
IN EACH COMPARTMENT
ROOM

CALCULATE STEADY-STATE
MASS AND ENERGY FLOW
RATES THROUGH BLOWERS
SSBLOW

PERFORM STEADY-STATE MASS
BALANCE TO DETERMINE INITIAL
MASS FLOW RATES THROUGH
PRESSURE-DROP-CONTROLLED VENTS

EVALUATE RESISTANCE TERMS FOR
PRESSURE-DROP-CONTROLLED VENTS
RESIST

EVALUATE ENTHALPY RATES FOR
PRESSURE-DROP-CONTROLLED VENTS
DENTHL

EVALUATE "HEAT TRANSFER
COEFFICIENT" FOR EACH
COMPARTMENT
HCOEFF

QUASI-TRANSIENT
SOURCE TERM? ———NO——— EVALUATE SOURCE TERM
STERM

YES

A

Fig. 21. Logic diagram for transient compartment models. (Sheet 1 of 2).

*WHEN ICOUNT EQUALS IFLAG, COMPARTMENT AND STREAM OUTPUT
IS PRINTED. IFLAG IS THE PRINT INTERVAL DIVIDED BY THE
SIMULATION INTERVAL.

Fig. 21. Logic diagram for transient compartment models. (Sheet 2 of 2).

Table 13. Variables required in a main program

Variable	Dimension	Definition and Units
ACFM	(30)	VOLUMETRIC FLOW RATE, FT**3/MIN
AMINLN		NATURAL LOG OF MINIMUM NUMBER ACCEPTED BY THE COMPUTER
C1		WEIGHT FRACTION OF HF MONOMER TO TOTAL HF VAPOR
C3		WEIGHT FRACTION OF HF TRIMER TO TOTAL HF VAPOR
C6		WEIGHT FRACTION OF HF HEXAMER TO TOTAL HF VAPOR
DELT		TIME INTERVAL USED FOR TRANSIENT SIMULATION, SEC
DEPVEL		DEPOSITION VELOCITY, FT/SEC
DPAREA	(30)	DEPOSITION AREA, FT**2
FLAREA	(30)	FLOW AREA FOR PRESSURE-DROP-CONTROLLED NODE, FT**2
H	(30)	NODE ENTHALPY, BTU, OR ENTHALPY RATE, BTU/(DELT)
HTAREA	(30)	HEAT TRANSFER AREA, FT**2
HTCOEF	(30)	HEAT TRANSFER COEFFICIENT, BTU/SEC-FT**2-DEG F
ICOUNT		COUNTER TO CONTROL PRINTING OF OUTPUT
IFLAG		FLAG TO CONTROL PRINTING OF OUTPUT
IIN	(30,4)	INLET STREAM NODE NUMBER
INODES		MAXIMUM NUMBER OF NODES ALLOWED BY CODING OF SUBROUTINES
INOUT		MAXIMUM NUMBER OF INLET STREAMS AND OUTLET STREAMS
IOUT	(30,4)	OUTLET STREAM NODE NUMBER
ISEN		VARIABLE TO SPECIFY ISENTROPIC OR ISENTHALPIC RELEASE, SEE CARD 5
KRCOEF	(30)	RESISTANCE COEFFICIENT, --, OR RESISTANCE TERM, RESISTANCE TERM, PSI-SEC**2/LB-FT**3

Table 13 (continued)

Variable	Dimension	Definition and Units
MASS	(30,9)	NODE MASS, LB, OR MASS FLOW RATE, LB/(DELT)
MAXTIM		MAXIMUM SIMULATION TIME, SEC
PC	(30)	NODE PRESSURE, PSIA
QCOOL	(30)	COOLING RATE, BTU/HR (INPUT) OR BTU/SEC (INTERNAL)
QRATE	(30)	HEAT TRANSFER RATE, BTU/SEC OR BTU/(DELT)
RATE	(9)	COMPONENT MASS RELEASE RATE, LB/SEC
RATIO		RATIO OF MOLES OF WATER VAPOR TO TOTAL MOLES OF MOIST AIR
RH		RELATIVE HUMIDITY, % (AS INPUT) OR FRACTION (INTERNAL)
SOLIDS		MASS FLOW RATE OF UF6 SOLIDS ONTO THE FLOOR, LB/(DELT)
SOURCE		TOTAL MASS OF RELEASE, LB
TC	(30)	NODE TEMPERATURE, DEG F
TIME		CUMULATIVE SIMULATION TIME, SEC
TRELS		TOTAL RELEASE TIME, SEC
TSTART	(30)	START OF REVERSE FLOW IN NODE
TSTOP	(30)	END OF REVERSE FLOW IN NODE
TSURF	(30)	NODE HEAT TRANSFER SURFACE TEMPERATURE, DEG F
VOL	(30)	NODE VOLUME, FT**3
WMBHF		MOLECULAR WEIGHT OF HF MONOMER, LB/LB MOLE
WMOL	(9)	COMPONENT MOLECULAR WEIGHTS, LB/LB MOLE

mented, a system of up to 28 nodes plus an ambient node and a null node* (30 total) can be accommodated. Nine "components" have been defined which are listed in Table 14. Up to four input streams can be accommodated by a compartment or mix node, and a compartment node can have four output streams. All values in the input and output arrays, IIN and IOUT, are initialized to 30 (the array element number corresponding to the null node) by SETRAY and are then modified by statements of the following form,

```
      IIN(I,J)  = N
C
      IOUT(I,J) = N
```

where

$$IIN(I,J) = \text{the J-th inlet stream to node I,}$$
$$IOUT(I,J) = \text{the J-th outlet stream from node I,}$$
$$N = \text{the node number corresponding to the J-th inlet/outlet stream for node I.}$$

The subroutine SETRAY is listed in Appendix B.

4.1.2 Input Data Requirements

The type of input data required for a compartment model and the units used in main programs written to date are shown in Table 15. In a few cases, units used internally have been different from those of the input. Coding used to obtain the proper units, which must follow the READ statement supplying the data, are discussed in the next several paragraphs.

The ambient relative humidity is entered as a percentage value, whereas a fractional value is used within the code. A conditional statement has been included that allows any percentage relative humidity greater than 1 or any fractional relative humidity less than or equal to 1 to be entered. That statement is as follows:

```
      IF (RH.GT.1.D0) RH = RH/1.D2
```

The input value for the cooling rate is Btu/hr; however, because the time unit used internally is the second, the cooling rate must be converted to Btu/sec. The following statement has been used:

```
      QCOOL(IROOM) = QCOOL(IROOM)/3.6D3
```

Note that a heating rate can be entered as a negative cooling rate. Variables such as IROOM, which describe certain nodes, are given in Table 16.

---

*Use of a "null node" permitted generalization of coding such that the number of inlet or outlet nodes to a given node would not need to be specified.

**Table 14. Components incorporated into
the transient models**

Number	Species	Phase	Molecular weight	Foot-note
1	Air	Vapor	28.966	
2	H_2O	Liquid	18.016	
3	H_2O	Vapor	18.016	
4	HF	Liquid	20.008	
5	HF	Vapor		*a*
6	UF_6	Solid	352.025	*b*
7	UF_6	Liquid	352.025	*b*
8	UF_6	Vapor	352.025	*b*
9	UO_2F_2	Solid	308.025	*b*

*a*The effective molecular weight of HF vapor varies with temperature and the partial pressure of HF.

*b*Default values for UF_6 and UO_2F_2 molecular weights are shown.

The default molecular weight for UF_6 may need to be changed, particularly for high enrichments of [235]U. If the molecular weight for UF_6 is changed, then that of UO_2F_2 must also be changed. Appropriate coding for modifying the molecular weights previously set by the call to SETRAY is the following:

```
      IF (MW.LT.100.D0) GO TO 10
C
      WMOL(9) = WMOL(9) - WMOL(6) + MW
      WMOL(6) = MW
      WMOL(7) = MW
      WMOL(8) = MW
C
   10 CONTINUE
```

The print interval for output data should be input as an integer multiple of the interval input for simulating the transient. Internally, ICOUNT is used as an index that permits output to be printed when ICOUNT equals IFLAG (see subsequent listing under Sect. 4.1.4). To avoid potential rounding errors resulting in a print interval other than that desired, the following statement is used to calculate IFLAG:

```
      IFLAG = IDINT(PRINT/DELT+0.01D0)
```

Table 15. Input conditions required
for a compartment model

Ambient conditions
    Temperature, °F
    Pressure, psia
    Relative humidity, %

Compartment conditions
    Temperature, °F
    Pressure, psia
    Volume, ft^3
    Floor area, ft^2
    Heat transfer area, ft^2
    Surface Temperature, °F
    Cooling rate, Btu/hr

Stream conditions
    Flow area, ft^2
    Resistance coefficient
      or
    Volume flow rate, acfm

Source-term conditions
    Type of source
        4   Liquid HF
        5   Vapor HF
        7   Liquid UF_6 (vapor source term)
      −7   Liquid UF_6 (vapor/solid source term)
        8   Vapor UF_6
    Temperature, °F
    Pressure, psia
    Mass, lb
    Release duration, sec
    Basis for flash
        0   Isentropic
        1   Isenthalpic
    Molecular weight (for UF_6), lb/lb-mole

Time variables
    Time step for simulation, sec
    Maximum time for simulation, sec
    Print interval, sec

4.1.3 Steady-State Conditions

Before the transient analysis of a postulated release can begin, it is necessary that all initial conditions existing prior to the release be established. The next section of coding must establish these conditions. The mole ratio of water vapor to moist air, which is assumed to exist both outside and inside the compartment, is established by a call to HUMID. An "ambient volume" is defined*

---

*The ambient volume specified is arbitrary; it need not be 1 billion (ft^3) as subsequently shown.

**Table 16. Definitions of variables representing
node numbers to be specified in subroutine cells**

Variable	Definition
IROOM	Compartment node number
IAMB	Ambient node number
IBLOW	Blower node number
IVENT	Vent or duct node number
ISOURC	Source node number
IINLET	Array element corresponding to a specific inlet stream
IDEP	Deposition node number
ISTRM	Stream node number
IFLOOR	Floor node number

and component masses and a total enthalpy for that volume are evaluated by a call to ROOM for subsequent use when material is drawn into the compartment from the environment. The following statements establish ambient conditions:

```
      CALL HUMID(IAMB, RH, RATIO)
C
      VOL(IAMB) = 1.D9
C
      CALL ROOM(IAMB, RATIO)
```

Next, calls to ROOM and SSBLOW are made to establish initial conditions in compartments and constant volume blowers, respectively. ROOM determines the masses of air and water vapor as well as the total enthalpy of the compartment atmosphere. SSBLOW establishes mass and enthalpy flow rates based on the temperature and pressure of the upstream node as well as on the water-vapor-to-moist-air ratio and the time increment to be used in the subsequent transient analysis. These calls take the following form:

```
      CALL ROOM(IROOM, RATIO)
C
      CALL SSBLOW(IBLOW, RATIO)
```

When mass flow rates are known for constant-volume blowers that feed or draw air from the compartment, a mass balance must be incorporated into the coding to determine mass flow rates through those openings through which flow occurs by pressure differential. The mass flow rates established by SSBLOW are based on the simulation interval, DELT (i.e., flow rates are in lb/ses only if DELT = 1.); likewise, the mass flow rates obtained from user-supplied coding must be based on DELT. Once these flow rates are established, the subroutine RESIST is used to calculate

a resistance term for determining mass flow rates occurring during the transient analysis. A call to DENTHL must be made to determine the enthalpy flow rate for the steady-state pressure-drop-controlled flow. Representative statements for calls to these subroutines follow.

```
      CALL RESIST(IVENT)
C
      CALL DENTHL(TC(IVENT), PC(IVENT), IVENT, H(IVENT))
```

As a transient simulation continues after a release is stopped, it is expected that the conditions in the compartment will return to their initial steady-state values. When temperatures of the compartment and ambient surroundings are different, a heat transfer model may be required. A call to HCOEFF can be made to determine a heat transfer coefficient. The subroutine call takes the following form:

```
      CALL HCOEFF(IROOM)
```

In many simple models, a constant source term is used. If this is the case, source term characteristics may be established before the transient analysis begins. Coding for more complex sources is discussed in Sect. 4.3. The subroutine call to establish source term characteristics is the following:

```
      CALL STERM(ISOURC, IROOM, SOLIDS)
```

4.1.4 Transient Analysis

The transient analysis is performed by (1) determining the flow rates into and out of a compartment at the beginning of a time interval, (2) adding and removing material and energy based on these flow rates over the time interval, (3) reacting components to the extent possible within the compartment after material has been added and removed, (4) determining heat transfer based on the temperature of the compartment and heat transfer surface at the beginning of the time step, and (5) determining the final-phase equilibrium, temperature, and pressure in the compartment at the end of the time step. Several subroutines are used for the first item, whereas the subroutine COMPRT performs the last four functions.

Coding for the transient analysis section of the main program begins with the following statements:

```
      TIME = 0.D0
C
      ICOUNT = IFLAG
C
  100 CONTINUE
C
      IF (TIME.GE.TRELS) IIN(IROOM,IINLET) = INODES
```

By setting ICOUNT equal to IFLAG, the initial steady-state conditions will be printed. The 100 CONTINUE statement is the point to which the program returns to begin the next time step. If the cumulative time exceeds the source release time, the value of IIN corresponding to the source term inlet node into the compartment node is set equal to INODES so that the source term subsequently corresponds to the null node.

Next, a series of subroutine calls is made to determine transient flow rates. The subroutines TRBLOW and DPFLOW evaluate flows through a constant volume blower and a pressure-drop-controlled pathway, respectively. Deposition rates of condensed phases are calculated by REMOVE. The following statements show the form of these subroutine calls:

```
      CALL TRBLOW(IBLOW)
C
      CALL DPFLOW(IVENT)
C
      CALL REMOVE(IROOM,IDEP)
```

Once flow rates have been determined at the beginning of a time interval, which time corresponds to the end of the previous interval, data corresponding to that time can be output. It should be noted that flow rate data must be converted to a per-second basis before being output because those data are internally treated on a per-"time interval" basis.* Coding for that purpose, as well as for determining whether or not to output data for that time, is shown in the following sequence of statements:

---

*The "time interval" is DELT.

```
        IF (ICOUNT.LT.IFLAG) GO TO 190
C
        WRITE ( . . .                *** output compartment data ***
               .
               .
               .

        DO 170 I170=1,9
C
            RATE(I170) = MASS(I180,I170)/DELT
C
   170 CONTINUE
C
        HRATE = H(I180)/DELT
C
        WRITE ( . . .                *** output data for node ISTRM ***
               .
               .
               .

        ICOUNT = 0
C
   190 CONTINUE
C
        TIME = TIME + DELT
C
        IF (TIME.GT.MAXTIM) STOP
C
        ICOUNT = ICOUNT + 1
```

After conditions for desired streams and compartments have been output for a given time, the program stops execution if the maximum time for the simulation has been reached, as indicted in the preceding coding. Otherwise, compartment conditions at the end of the time interval should be evaluated, and condensed materials being deposited on the floor should be accumulated. Note that compartment models developed to date simply accumulate condensed materials on the floor and that they are removed from any further material or energy-balance considerations. The following sequence of statements concludes all required coding for a main program for a compartment model using the methods described herein:

```
      CALL COMPRT(IROOM, INOUT, INODES)
C
      DO 200 I200=1,9
C
         MASS(IFLOOR,I200) = MASS(IFLOOR,I200) + MASS(IDEP,I200)
C
  200 CONTINUE
C
      IF (ITYPE.EQ.7 .AND. TIME.LE.TRELS) MASS(IFLOOR,6) =
     *    MASS(IFLOOR,6) + SOLIDS
C
      GO TO 100
C
      END
```

4.1.5 Other Considerations

The four preceding sections have outlined the structure of a main program for a transient compartment model. Multicompartment models can also be assembled following the preceding outline. The transient models discussed in Sect. 4.6 include additional coding to provide specialized output. Following sections in this chapter will discuss the various aspects of the compartment models in greater detail.

4.2 VENTILATION SYSTEM

The ventilation system is modeled in a simplistic manner. Four subroutines, which are discussed in Sects. 4.2.1 and 4.2.2, have been written to evaluate steady-state and transient conditions. A mixing subroutine was also written to combine flows from several sources; it is discussed in Sect. 4.2.3. Listings of all subroutines discussed in this section are included in Appendix B.

4.2.1 Steady-State Analysis

The subroutine SSBLOW is used to establish the initial component mass flow rates and the enthalpy rate for moist air flowing through a constant-volume blower. The total moles of moist air passing through the blower over the time interval used for subsequent transient analysis are evaluated using the ideal gas law and the temperature and pressure of the inlet node. Thus,

$$\Delta n_T = (P_i \dot{V}_b \Delta T)/(R T_{R,i} 60) \ , \tag{120}$$

where

Δn_T = total moles passing through blower in time interval Δt,

P_i = inlet pressure, psia,

$\dot{V}_b$ = volumetric flow rate of blower, acfm,

Δt = time interval for transient simulation, sec,

R = ideal gas constant, psia-ft^3/lb mole-°R

= 10.73,

$T_{R,i}$ = inlet temperature, °R.

The ratio of moles of water vapor to moles of moist air calculated by HUMID (see Sect. 4.5.1) is then used to determine the mass flow rate of water vapor and dry air. The mass of water vapor passing through the blower is given by

$$\Delta m_{H_2O} = \Delta n_T r M W_{H_2O} \ , \tag{121}$$

where

Δm = mass passing through the blower in time interval Δt, lb,
r = ratio of moles of water vapor to moles of moist air,
MW = molecular weight,
H_2O = subscript referring to water.

Similarly, the mass of dry air passing through the blower is given by,

$$\Delta M_{air} = \Delta n_T (1 - r) M W_{air} \ , \tag{122}$$

where

air = subscript referring to air.

The enthalpy rate is calculated by a call to DENTHL (see Sect. 2.4).

A general expression for pressure drop obtained from Eq. 103 is,

$$\Delta P = -K(\dot{m}^2/9266.1 \, \rho A^2) \ , \tag{123}$$

where

ΔP = pressure drop, psi,
K = resistance coefficient,
$\dot{m}$ = mass flow rate, lb/sec
    = $\Delta m/\Delta t$,
ρ = density, lb/ft^3,
A = flow area, ft^2.

A resistance term that remains constant throughout the analysis can be defined by

$$\phi = K/(9266.1 \, A^2) \ , \tag{124}$$

where

ϕ = resistance term, psi-sec^2/lb-ft^3.

This term is directly evaluated by the subroutine RESIST if a positive resistance coefficient and flow area are specified as input. Otherwise, ϕ is evaluated using the mass flow rate, inlet density, and pressure difference without specific knowledge of the flow area or resistance coefficient by,

$$\phi = -\Delta P \rho / \dot{m}^2 \ . \tag{125}$$

4.2.2 Transient Analysis

The mass flow and enthalpy rates of streams are assumed to be proportional to the total mass and enthalpy of the node (compartment) feeding the stream. The transient subroutines TRBLOW and DPFLOW calculate volume and mass ratios, respectively, to obtain stream flow rates based on the simulation time interval. In the case of TRBLOW, the volume ratio is given by

$$f_v = (\dot{V}_b \Delta t / 60) / V_i \ , \tag{126}$$

where

f_v = volume ratio,

V_i = volume of inlet node (e.g., compartment volume), ft^3.

The mass of each component in the compartment node, as well as the total enthalpy of that node, is multiplied by this volume fraction to obtain the stream rates for the blower node. Thus,

$$\Delta m_{j,b} = f_v m_{j,k} \tag{127}$$

and

$$\Delta H_b = f_v H_i \ , \tag{128}$$

where

j = subscript referring to a particular component,

b,i = subscripts referring to blower (or later, vent) and inlet nodes, respectively,

ΔH = enthalpy of mass passing through the blower in the time interval Δt, Btu/lb,

H = enthalpy, Btu/lb.

The temperature and pressure of the blower node are taken to be same as the compartment node from which it draws.

The overall approach for determining stream rates resulting from pressure-drop-controlled flow is similar. In this case, Eq. 125 is rearranged, and the mass flow rate term is split into a mass term and time term to yield

$$\Delta m = \Delta t \sqrt{|\Delta P| \rho / \phi} \ , \tag{129}$$

where

Δm = total mass flowing through a pressure drop controlled flow node over the time interval Δt, lb,

ΔP = pressure difference, psi,

ρ = density, lb/ft^3,

ϕ = resistance term calculated by RESIST, psi-sec^2/lb-ft^3,

Δt = time interval used for transient simulation, sec.

The mass ratio, which is applied in DPFLOW in an analogous fashion to the volume fraction in TRBLOW, is then obtained from

$$f_m = \Delta m / m_{T_i} \ ,$$

(130)

where

f_m = mass ratio,

m_{T_i} = total mass in the inlet node.

Thus, Eqs. 127 and 128 apply if f_v is replaced by f_m. Note that, if the normal direction of flow is reversed by either an increase in the normal downstream pressure or by a decrease in the upstream pressure, then the mass fraction, f_m is made negative and is applied to the normal outlet node. This change of sign and use of the outlet node as the effective inlet makes an inlet stream act as an outlet stream and vice versa. The temperature and pressure of the stream node are those of the effective inlet node.

4.2.3 Stream Mixing

Stream mixing is handled in several ways in the compartment models. When several streams combine and the combined stream enters another compartment, it is reasonable to skip the mixing step by making each individual stream an inlet stream to the downstream compartment. If the combined streams exhaust to the atmosphere, however, the streams need to be mixed such that reactions are allowed to occur and phase equilibrium is established at atmospheric pressure. Such a well-mixed stream can then become a source term for atmospheric dispersion modeling.

The subroutine MIXFLW is used to combine up to four streams and exhaust them at the pressure of the node to which the combined streams exhaust. All streams should originate from blowers because no criteria have been established or implemented in this modeling effort to address flow splitting or the occurrence of backflow in a multipath, induced-draft system (except for a single stream as described in Sect. 4.2.2). The total enthalpy and individual component masses found in the mixed stream before reactions are considered* are calculated by using the following summations:

$$H_m = \sum H_i$$

(131)

---

*Reaction effects are evaluated by COMPRT.

and

$$m_{j,m} = \sum m_{j,i} \quad , \tag{132}$$

where

  m,i = subscripts referring to the mixed stream and inlet streams, respectively.

Phase composition is determined by iterating on volume while calling the subroutine COMPRT (see Sect. 4.5.2) which calculates temperature, pressure, and phase composition in a volume, given the total enthalpy and component masses. Volume is varied until the predicted pressure corresponds to the known outlet pressure.

4.3 SOURCE-TERM SUBROUTINE

A simplified source-term subroutine is currently used in the compartment models. Because the coding being developed for the compartment models was required to handle HF, in addition to UF_6, the source-term subroutine, STERM, was written to supply either UF_6 or HF data. For UF_6, three types of source terms can be specified, two for liquid UF_6 and one for vapor. If liquid is released from containment, it is allowed to flash—either isentropically or isenthalpically—to the pressure of the compartment in which the release occurs; however, use of an isenthalpic flash is recommended because such a flash is consistent with the release rate models described in Chap. 3. The difference in the two liquid source terms is that, in one case, the solids formed are assumed to immediately fall to the floor, while in the other case the solid particles are assumed to be dispersed in the compartment atmosphere. Thus, in the latter case, the solids are subsequently considered in the mass and energy balances of the compartment, whereas in the former case they are treated as inert solids which accumulate on the floor. If UF_6 vapor is released from containment, it is allowed to expand with a resulting increase in temperature. The subroutine FLASH (see Sect. 2.1.11) is called from STERM to perform the flashing and expansion calculations.

While information on the results of flashing or expansion are of interest, such information is not necessarily a requirement when such processes are assumed to occur isenthalpically within a compartment. Under this assumption, all the energy released with the source material, whether liquid or vapor, becomes a part of the total energy within the compartment. Such an assumption is applied to HF releases. The subroutine STERM determines the release rate and the enthalpy rate of the material being released, based on the initial temperature and pressure and whether the HF is specified to be liquid or vapor.

The release rate determined by STERM may be represented by

$$\Delta m = (M/T)\Delta t \quad , \tag{133}$$

where

  Δm = mass of material released per time increment Δt, lb,
  M = total mass of source, lb,
  T = release duration, sec,
  Δt = time increment used for transient simulation, sec.

In the case of a UF_6 liquid release, Δm is subdivided into a solid term and a vapor term. For HF as well as UF_6 vapor releases, the specified phase of the source is the phase assigned to the Δm term. The subroutine DENTHL (see Sect. 2.4) is used to calculate the enthalpy rate for the source term, given the value of Δm assigned to the appropriate component of the mass vector as well as the appropriate temperature and pressure. For UF_6 releases, the appropriate temperature and pressure are those obtained after flashing or expansion, whereas the temperature and pressure supplied as input to STERM are used for HF releases. A listing of STERM appears in Appendix B.

The preceding discussion has described the evaluation of a single set of source-term characteristics. Although a source-term subroutine interfacing the release rate models discussed in Chap. 3 with the compartment models described in this chapter has not been developed, two quasi-transient source-term methods have been incorporated into the main programs FODRFT and INDRFT. Incorporation of these methods allows the user (1) to input several sets of constant conditions via the primary input file so that a transient release can be approximated or (2) to read a secondary source-term file (see Tables 18 and 19 in Sect. 4.6 for a description of this secondary file). The required coding is outlined in Table 17. Note that the source term is reevaluated periodically within the transient section of the main program rather than prior to the transient analysis. The source-term vector is replaced by the null vector at the end of the release.

4.4 CONDENSATE DEPOSITION SUBROUTINE

A very simple condensate deposition model has been used in the subroutine REMOVE, which is listed in Appendix B. The model assumes a constant deposition velocity for all condensed phases of 1 cm/sec, which is specified in SETRAY as 0.033 (ft/sec). All condensed material within a slab having a volume specified by the product of the deposition area, the deposition velocity, and the time interval used for the transient simulation is assumed to be removed over the time interval. Thus, the amount deposited is given by

$$\Delta m_{j,d} = [(A_f v_d \Delta t)/V_c]m_{j,c} \quad , \tag{134}$$

where

$\quad m_{j,d}$ = mass of component j deposited over the time interval Δt,
$\quad A_f$ = deposition (floor) area, ft^2,
$\quad v_d$ = deposition velocity, ft/sec,
$\quad \Delta t$ = time interval for transient simulation, sec,
$\quad V_c$ = compartment volume, ft^3,
$\quad m_{j,c}$ = mass of component j present in compartment, lb.

Equation 134 applies only to condensed components. It is important to remember that the compartment volume from which the condensed material is deposited is assumed to be well mixed, so the amount of material removed by deposition in each time interval is (in general) continually varying.

4.5 COMPARTMENT MASS AND ENERGY BALANCE SUBROUTINES

Conditions within a compartment at any specific time are assumed to be homogeneous. In other words, the temperature, pressure, component concentrations, and phase splits are uniform

Table 17. Additional coding for quasi-transient source term

```
                    *** Initial Statements ***


        DIMENSION MSOURC(5), TSOURC(5), TEMP(5), PRES(5)


                    *** Read Statements ***


        READ (40,*) ITYPE, IRELST, ISEN, MW
C
        IF (MW.LT.100.D0) GO TO 10
C
        WMOL(9) = WMOL(9) - WMOL(6) + MW
        WMOL(6) = MW
        WMOL(7) = MW
        WMOL(8) = MW
C
     10 CONTINUE
C
        MWURAN = WMOL(6) - 113.99D0
C
        IF (ITYPE.EQ.22) GO TO 30
C
        READ (40,*) (TSOURC(I), MSOURC(I), TEMP(I), PRES(I), I=1,IRELST)
C
        TRELS = 0.D0
C
        MRELS = 0.D0
C
        DO 20 I20=1,IRELST
C
            TRELS = TRELS + TSOURC(I20)
C
            MRELS = MRELS + MSOURC(I20)
C
            IF (ITYPE.EQ.5) CALL PHFH2O(TEMP(I20), 1.D0, 0.D0, PTEST,
     *          0.D0, 0.D0)
            IF (ITYPE.EQ.8) CALL VPRUF6(TEMP(I20), PTEST)
C
            IF (PRES(I20).GT.PTEST .OR. PRES(I20).LE.0.D0)
     *          PRES(I20) = PTEST
C
     20 CONTINUE
C
     30 CONTINUE



                    *** Transient Analysis ***


        IRELS = 1
C
        TRELS = 0.D0
C
        IF (ITYPE.EQ.22) READ (22,*) DELTAT
C
    100 CONTINUE
C
        IF (TIME.LT.TRELS) GO TO 140
C
        IF (ITYPE.NE.22) GO TO 120
C
```

Table 17 (continued)

```
      READ (22,*,END=140) TRELS, (RATE(I),I=1,9),TC(IIN(1,2)),
     *     PC(IIN(1,2))
C
      DO 110 I110=1,9
C
         MASS(IIN(1,2),I110) = RATE(I110)*DELT
C
  110 CONTINUE
C
      TRELS = TRELS + DELTAT
C
      GO TO 140
C
  120 CONTINUE
C
      IF (IRELS.GT.IRELST) GO TO 140
C
      TRELS = TSOURC(IRELS)
C
      SOURCE = MSOURC(IRELS)
C
      TC(3) = TEMP(IRELS)
C
      PC(3) = PRES(IRELS)
C
      CALL STERM(3, 1, SOLIDS)
C
      TRELS = 0.D0
C
      DO 130 I130=1,IRELS
C
         TRELS = TRELS + TSOURC(I130)
C
  130 CONTINUE
C
      IRELS = IRELS + 1
C
  140 CONTINUE
C
      IF (TIME.GE.TRELS) IIN(1,2) = INODES
```

throughout the compartment volume at any specific time. Within the overall compartment model structure, compartment conditions are determined for two circumstances. First, normal steady-state initial conditions must be established; second, conditions must be evaluated at the end of each time interval of the transient simulation. Sect. 4.5.1 discusses the steady-state mass and energy balance; Sect. 4.5.2 discusses evaluation of transient conditions.

4.5.1 Initial Conditions

Initial conditions within a compartment are determined on the basis of ambient temperature, pressure, and relative humidity; compartment temperature, pressure, and volume; and the assumption that the ideal gas law applies. First, the ratio of moles of water vapor to moles of moist air is calculated using ambient conditions and the following equation:

$$r = [RH(P_{H_2O}°)]/P \quad , \tag{135}$$

where

r = molar ratio of water vapor to moist air,

RH = fractional relative humidity,

$P_{H_2O}^{\circ}$ = vapor pressure of water, psia,

P = total pressure, psia.

The subroutine HUMID calculates r using the subroutine PHFH2O (see Sects. 2.2.3 and 2.2.7) to evaluate $P_{H_2O}^{\circ}$. Note that it is assumed that all compartments and streams, as well as the ambient surroundings, have the same composition prior to a release.

Once the molar ratio is determined, the mass quantities of air and water for each node can be determined. The procedure for evaluating these quantities for ventilation system nodes has been outlined in Sect. 4.2.1. For a compartment, the total moles of vapor contained in the compartment at a given temperature and pressure are calculated assuming the ideal gas law,

$$n_T = PV/RT_R \ , \tag{136}$$

where

n_T = total number of moles in a compartment,

P = compartment pressure, psia,

V = compartment volume, ft^3,

R = ideal gas constant, psia-ft^3/lb-moles-$^{\circ}$R

= 10.73,

T_R = compartment temperature,$^{\circ}$R.

The water-vapor-to-moist-air-molar ratio is then applied along with the molecular weights of water and air to obtain the component masses of air and water vapor in the compartment node using the following relationships,

$$m_{H_2O} = n_T r M W_{H_2O} \tag{137}$$

and

$$m_{air} = n_T(1 - r)MW_{air} \ , \tag{138}$$

where

m = mass, lb,

MW = molecular weight,

H_2O, air = superscripts referring to water and air, respectively.

A call to DENTHL (see Sect.2.4) is made to evaluate the total enthalpy of the compartment node. These calculations for a compartment are programmed into the subroutine ROOM.

To close the energy balance for the compartment, heat transfer from process equipment or other heat sources within a compartment must be considered; otherwise, in the subsequent transient simulation, the temperature will eventually approach ambient temperature rather than the initial room temperature. The subroutine HCOEFF has been written to evaluate a heat transfer coefficient, based on normal steady-state conditions, which is used in the transient simulation. The coding has been written to handle up to four inlet streams. The heat added to a compartment by heat transfer is found from

$$Q = [H_c(\dot{m}_i/m_c) - \dot{H}_i + Q_{cool}\Delta t]/\Delta t \quad , \tag{139}$$

where

Q = heat transferred from process equipment, Btu/sec,
H_c = total enthalpy of compartment atmosphere, Btu,
$\dot{m}_i$ = total inlet mass flow rate of all inlet stream, lb/Δt,
m_c = total mass of compartment atmosphere, lb,
$\dot{H}_i$ = total inlet enthalpy rate of all inlet streams, Btu/Δt,
Q_{cool} = cooling rate, Btu/sec,
Δt = time interval for transient simulation, sec.

Note that inlet mass flow and enthalpy rates are based on the time interval used for the transient simulation and that a negative cooling rate is a heating rate. The heat transfer coefficient is then determined from

$$h = Q/[A(T_s - T_c)] \quad , \tag{140}$$

where

h = heat transfer coefficient, Btu/sec-ft^2-°F,
A = heat transfer surface area, ft^2,
T_s = heat transfer surface temperature, °F,
T_c = temperature of compartment atmosphere, °F.

Of the variables h, A, and T_s, T_s is probably most important. The product of h and A is assumed to remain constant throughout the analysis.

Listings of HUMID, ROOM, and HCOEFF appear in Appendix B.

4.5.2 Transient Behavior

The procedure for analyzing transient behavior is divided between the main program and the subroutine COMPRT. The approach is to determine various mass flow and enthalpy rates based on conditions at the beginning of the time step, then to accumulate mass and energy terms for the compartment and react components to the extent possible, and finally to determine temperature, pressure, and phase compositions at the end of the time step. Mass flow and enthalpy rates, except for heat transfer rates, are evaluated in subroutines called from the main program. The other calculations are carried out in COMPRT.

COMPRT can be divided into two sections. In the first, mass and energy terms are accumulated and components are reacted to determine the final overall composition and total enthalpy. In the latter section, the final temperature, pressure, and phase composition are determined iteratively using assumed temperatures as the basis for iteration and total enthalpy as the basis for closure. Accumulating mass and energy terms is done by adding inlet stream terms and subtracting outlet stream terms from the comparable compartment node terms. Thus, for each component (and prior to considering the effect of chemical reactions),

$$m_j\big|_f = m_j\big|_i + \sum_{in=1}^{4} \Delta m_j\big|_{in} - \sum_{out=1}^{4} \Delta m_j\big|_{out} \ , \tag{141}$$

where

m = mass of a component in a compartment, lb,

Δm = mass passing through a node over the transient simulation time interval Δt, lb,

f, i = subscripts referring to final and initial conditions, respectively,

in, out = summation indices for inlet and outlet streams, respectively.

Up to four inlet and four outlet streams can be assigned for each compartment. If reverse flow occurs in a pressure drop controlled node, the subroutine DPFLOW (see Sect. 4.2.2) assigns negative mass flow and energy rates so that when COMPRT accumulates terms the proper results are obtained.

The only reaction currently considered in COMPRT is the reaction of UF_6 and H_2O. It is assumed to go to completion, being limited only by the exhaustion of one of the reactants, according to the following equation:

$$UF_6(v) + 2\,H_2O(v) \rightarrow UO_2F_2(s) + 4\,HF(v) \ . \tag{142}$$

The heat released by this reaction is 25,199 Btu/lb-mole of H_2O reacted based on a reference temperature of 77°F (see Sect. 2.1.10). If H_2O is the limiting reactant,

$$m_{UF_6}\big|_f = m_{UF_6}\big|_i - m_{H_2O}\big|_i MW_{UF_6}/(2\,MW_{H_2O}) \ , \tag{143}$$

$$m_{UO_2F_2}\big|_f = m_{UO_2F_2}\big|_i + m_{H_2O}\big|_i MW_{UO_2F_2}/(2\,MW_{H_2O} \ , \tag{144}$$

$$m_{HF}\big|_f = m_{HF}\big|_i + 2\,m_{H_2O}\big|_i MW_{HF\,monomer}/MW_{H_2O} \ , \tag{145}$$

$$m_{H_2O}\big|_f = 0 \ , \tag{146}$$

$$\Delta H_{rxn} = 25199\,m_{H_2O}\big|_i/MW_{H_2O} \ , \tag{147}$$

where

ΔH_{rxn} = heat released by the reaction of UF$_6$ with H$_2$O, Btu.

If UF$_6$ is the limiting reactant,

$$m_{\mathrm{H_2O}}\big|_f = m_{\mathrm{H_2O}}\big|_i - 2\, m_{\mathrm{UF_6}}\big|_i MW_{\mathrm{H_2O}}/MW_{\mathrm{UF_6}} \ , \tag{148}$$

$$m_{\mathrm{UO_2F_2}}\big|_f = m_{\mathrm{UO_2F_2}}\big|_i + m_{\mathrm{UF_6}}\big|_i MW_{\mathrm{UO_2F_2}}/MW_{\mathrm{UF_6}} \ , \tag{149}$$

$$m_{\mathrm{HF}}\big|_f = m_{\mathrm{HF}}\big|_i + 4\, m_{\mathrm{UF_6}}\big|_i MW_{\mathrm{HF\,monomer}}/MW_{\mathrm{UF_6}} \ , \tag{150}$$

$$m_{\mathrm{UF_6}}\big|_f = 0 \ , \tag{151}$$

$$\Delta H_{rxn} = 50398\, m_{\mathrm{UF_6}}\big|_f / MW_{\mathrm{UF_6}} \ . \tag{152}$$

In Eqs. 143 through 152, initial masses correspond to the final masses obtained from Eq. 141. Note that, although the compartment model in general treats each phase of a chemical component as an individual component, all phase components of a chemical component are combined prior to evaluating the effects of chemical reactions. Subsequently, the amount of a chemical component in each phase is reallocated in the process of determining the final temperature and pressure.

The amount of heat transferred from process equipment is given by

$$Q_{\Delta t} = hA(T_s - T_c)\Delta t \ , \tag{153}$$

where $Q_{\Delta t}$ is the amount of heat transferred over the time interval used for the transient simulation. The units of $Q_{\Delta t}$ are Btu/(Δt), which is consistent with other enthalpy rate terms calculated internally by the various compartment model subroutines.

Once the heat of reaction and heat transferred from process equipment have been determined, the total enthalpy with respect to the reference conditions is given by,

$$H\big|_f = H\big|_i + \sum_{in=1}^{4} H_{in} - \sum_{out=1}^{4} H_{out} + \Delta H_{rxn} + Q_{\Delta t} - Q_{cool}\Delta t \ , \tag{154}$$

where

H_{in}, H_{out} = enthalpy rates of inlet and outlet streams Btu/Δt,
Q_{cool} = cooling rate, Btu/sec,
Δt = time interval for transient simulation, sec.

Note that ΔH and $Q_{\Delta t}$ in effect have the units of Btu because Δt has already been accounted for in calculating these values.

The iterative procedure to determine the temperature, pressure, and phase composition at the end of the time step begins by assuming a final temperature. For condensible components, their respective vapor pressures are calculated, at the assumed final temperature and the amount of each component in the compartment is compared with the maximum amount of that component allowed in the compartment on the basis of the assumed temperature and calculated vapor pressure and the assumption the ideal gas law applies. If the amount of the component exceeds the maximum, the excess is placed in the condensed phase. For UF_6, the calculation is performed in COMPRT except for the calculation of vapor pressure, which is done by a call to VPRUF6. For the HF-H$_2$O subsystem, these calculations are performed in PHASE which is described in Sects. 2.2.6 and 2.2.7. The number of moles in the vapor phase is determined and a total pressure is obtained using the ideal gas law and the assumed temperature. Given the phase composition and pressure at the assumed temperature, a total enthalpy is calculated. If the total enthalpy calculated for the assumed temperature exceeds the total enthalpy calculated by Eq. 154, a lower "assumed" temperature is selected, or vice versa, and the process is repeated until the two values of enthalpy agree. When the enthalpies agree, then the conditions determined for the last assumed temperature are known to be the conditions for the end of the time step.

Listings of COMPRT and PHASE are given in Appendix B.

4.6 COMPARTMENT MODEL MAIN PROGRAMS

The main programs described in this section represent specialized models developed to simulate ventilation patterns likely to be encountered in buildings where UF_6 is handled. The structure of these programs follows the general outline presented in Sect. 4.1. Listings of all main programs described in this section are provided in Appendix A.

4.6.1 Forced-Draft Compartment

The transient forced-draft compartment model, FODRFT, is based on the schematic shown in Fig. 22. Input data requirements and format for executing the program are listed in Table 18. The

ORNL—DWG 85-14582
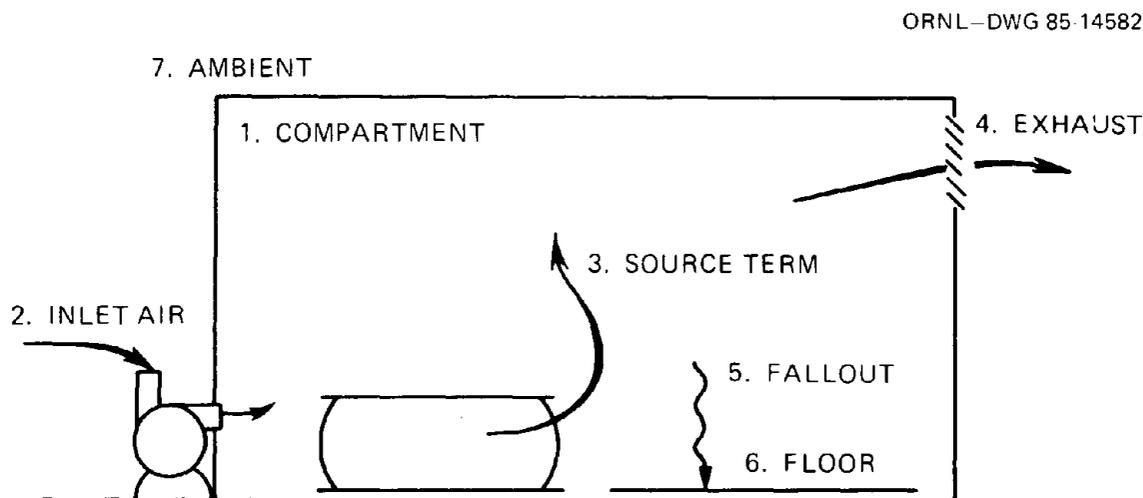
Fig. 22. Schematic for the transient forced-draft compartment model FODRFT.

Table 18. Input data requirements and format for FODRFT

ALL INPUT DATA EXCEPT THAT ON CARDS 1 AND 9 ARE READ IN FREE FORMAT. ON CARDS 1 AND 9, COUNT CHARACTERS STARTING IN COLUMN 1.

/
/ CARD 1.   READ TITLE (MAXIMUM OF 80 CHARACTERS).

/
/ CARD 2.   READ AMBIENT TEMPERATURE (F), PRESSURE (PSIA), AND RELATIVE HUMIDITY (%).

/
/ CARD 3.   READ COMPARTMENT TEMPERATURE (F), PRESSURE (PSIA), VOLUME (FT**3), AND FLOOR (DEPOSITION) AREA (FT**2).

/
/ CARD 4.   READ INLET AIR BLOWER FLOW RATE (ACFM).

/
/ CARD 5.   READ HEAT TRANSFER SURFACE AREA IN COMPARTMENT (FT**2), HEAT TRANSFER SURFACE TEMPERATURE (F), AND COOLING RATE (BTU/HR). A NEGATIVE COOLING RATE IMPLIES A HEATING RATE. WHILE THE VALUE OF THE SURFACE AREA IS NOT PARTICULARLY IMPORTANT BECAUSE THE PRODUCT OF THE SURFACE AREA AND THE HEAT TRANSFER COEFFICIENT TO BE CALCULATED WILL BE CONSTANT, A SURFACE TEMPERATURE GREATER THAN THE COMPARTMENT TEMPERATURE MUST BE SPECIFIED.

/
/ CARD 6.   READ SOURCE TYPE, NUMBER OF RELEASES, BASIS FOR FLASH, AND MOLECULAR WEIGHT. SOURCE TYPE IS GIVEN BY THE FOLLOWING:

4	LIQUID HF
5	VAPOR HF
7	LIQUID UF6 (VAPOR SOURCE TERM GENERATED)
-7	LIQUID UF6 (VAPOR/SOLID SOURCE TERM GENERATED)
8	VAPOR UF6
22	INPUT PROVIDED IN FOR22.DAT

IF SOURCE TYPE 22 IS SPECIFIED, SET NUMBER OF RELEASES TO ZERO. NO MORE THAN FIVE RELEASES MAY BE SPECIFIED, WHICH ARE TO RUN CONSECUTIVELY. THE BASIS FOR THE FLASH IS GIVEN BY THE FOLLOWING:

0	ISENTROPIC
1	ISENTHALPIC

THE DEFAULT MOLECULAR WEIGHT FOR UF6 IS 352.025; ENTER A VALUE LESS THAN 100 IF THAT VALUE IS ACCEPTABLE.

Table 18 (continued)

/
/ CARD 7.   -- DO NOT USE "CARD 7" CARDS IF ITYPE = 22. --

            READ FOR EACH INCREMENTAL RELEASE THE DURATION (SEC), MASS
            (LB), TEMPERATURE (DEG F), AND PRESSURE (PSIA). SPECIFY AS
            MANY SETS OF DATA AS THE NUMBER OF RELEASES (IRELST). IF
            THE PRESSURE GIVEN IS LESS THAN OR EQUAL TO ZERO OR GREATER
            THAN THE VAPOR PRESSURE, THE PRESSURE IS SET EQUAL TO THE
            VAPOR PRESSURE FOR THAT INCREMENT.

/
/ CARD 8.   READ TIME INTERVAL FOR CALCULATIONS (SEC), DURATION OF
            SIMULATION (SEC), AND PRINT INTERVAL (SEC).

/
/ CARD 9.   -- THESE CARDS ARE OPTIONAL. --

            READ DRAWING NUMBERS FOR PLOTS (LIMITED TO 20 CHARACTERS--
            THE LAST CHARACTER MUST BE A DOLLAR SIGN ($)).

            1ST CARD 9 = CUMULATIVE URANIUM RELEASED
            2ND CARD 9 = CUMULATIVE HF RELEASED
            3RD CARD 9 = URANIUM CONCENTRATION IN COMPARTMENT
            4TH CARD 9 = HF CONCENTRATION IN COMPARTMENT
            5TH CARD 9 = TEMPERATURE IN COMPARTMENT
            6TH CARD 9 = PRESSURE IN COMPARTMENT

THE OPTIONAL SOURCE TERM INPUT IS READ FROM A DIFFERENT FILE THAN THE
PRECEEDING INPUT.

/
/ OPTIONAL SOURCE TERM INPUT: CARD 1.   ENTER TIME INTERVAL FOR SOURCE
            TERM INPUT (SEC).

/
/ OPTIONAL SOURCE TERM INPUT: CARD 2.   ENTER INITIAL TIME FOR RELEASE
            INTERVAL (SEC); MASS FLOW RATE (LB/SEC) FOR EACH OF THE NINE
            COMPONENTS IN THE FOLLOWING ORDER: AIR, H2O(L), H2O(V),
            HF(L), HF(V), UF6(S), UF6(L), UF6(V), UO2F2; SOURCE TERM
            TEMPERATURE FOR INTERVAL (DEG F); AND SOURCE TERM PRESSURE
            FOR THE INTERVAL (PSIA).

general outline of the main program given in Sect.4.1 has been followed, except that the quasi-transient source-term coding outlined in Sect. 4.3 and Table 17 has been used. The general outline has been supplemented to include WRITE statements that provide title blocks for each output file. These WRITE statements are included just before the transient analysis section of the code. Coding to provide summary data on the cumulative amount of uranium and HF released, as well as the densities of uranium and HF in the compartment, has also been added. Similar data are also written to a special file for plotting using COMPLT (see Sect. 4.7). Examples of FODRFT input and output are provided in Sect. 5.2 and Appendixes C.4 and C.5.

4.6.2 Induced Draft Compartment

The transient induced-draft compartment model, INDRFT, is based on the schematic shown in Fig. 23. Input data required for executing the program are listed in Table 19. The quasi-transient source-term coding outlined in Sect. 4.3 has been incorporated into the general main program outline of Sect. 4.1, as has special coding to read from a source-term input file. Also, the general outline has been supplemented to add title blocks, additional summary data, and a plot data file in a manner similar to those described for FODRFT.

Besides the rather straightforward modifications to the general outline, the modeling of an induced-draft system presented several problems. Initially, coding was added to allow the calculation of the internal compartment pressure (based on mass flow rate, specified inlet area, and resistance coefficients) or the internal pressure could be specified. Allowing INDRFT to calculate the internal pressure, though, generally leads to such a small pressure difference between the compartment and the surroundings under steady-state conditions that subsequent transient analysis is usually unstable. Specifying a pressure about 0.05 to 0.1 psi lower than ambient pressure avoids long-term instability (note that the resistance term for Node 2 would be based on Eq. 152), whereas little difference is found in results obtained over such a range of initial internal pressures. Short-term

ORNL—DWG 85-14580
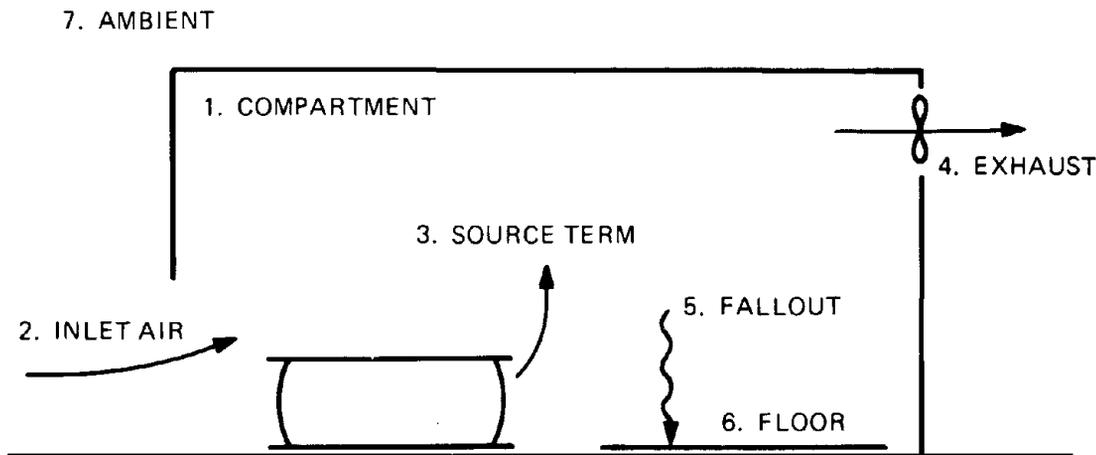
Fig. 23. Schematic for the transient induced-draft compartment model INDRFT.

Table 19. Input data requirements and format for INDRFT

ALL INPUT DATA EXCEPT THAT ON CARDS 1 AND 9 IS READ IN FREE FORMAT. ON CARDS 1 AND 9, COUNT CHARACTERS STARTING IN COLUMN 1.

/
/ CARD 1.   READ TITLE (MAXIMUM OF 80 CHARACTERS).

/
/ CARD 2.   READ AMBIENT TEMPERATURE (F), PRESSURE (PSIA), AND RELATIVE HUMIDITY (%).

/
/ CARD 3.   READ COMPARTMENT TEMPERATURE (F), PRESSURE (PSIA), VOLUME (FT**3), AND FLOOR (DEPOSITION) AREA (FT**2). IF THE COMPARTMENT PRESSURE IS NOT KNOWN AND IS TO BE CALCULATED, SPECIFY A PRESSURE GREATER THAN OR EQUAL TO THE AMBIENT PRESSURE OR LESS THAN OR EQUAL TO ZERO.

/
/ CARD 4.   READ EXHAUST FLOW RATE (ACFM), INLET FLOW AREA (FT**2), AND INLET RESISTANCE COEFFICIENT (--). IF THE PROGRAM IS TO CALCULATE THE RESISTANCE COEFFICIENT, A COMPARTMENT PRESSURE GREATER THAN OR EQUAL TO THE AMBIENT PRESSURE OR LESS THAN OR EQUAL TO ZERO MUST HAVE BEEN ENTERED, AND AN INLET AREA AND RESISTANCE COEFFICIENT MUST BE GIVEN. A RESISTANCE COEFFICIENT COEFFICIENT OF 1.5 REPRESENTS A SUDDEN CONTRACTION FOLLOWED BY A SUDDEN EXPANSION.

/
/ CARD 5.   READ HEAT TRANSFER SURFACE AREA IN COMPARTMENT (FT**2), HEAT TRANSFER SURFACE TEMPERATURE (F), AND COOLING RATE (BTU/HR). A NEGATIVE COOLING RATE IMPLIES A HEATING RATE. WHILE THE VALUE OF THE SURFACE AREA IS NOT PARTICULARLY IMPORTANT BECAUSE THE PRODUCT OF THE SURFACE AREA AND THE HEAT TRANSFER COEFFICIENT TO BE CALCULATED WILL BE CONSTANT, A SURFACE TEMPERATURE GREATER THAN THE COMPARTMENT TEMPERATURE MUST BE SPECIFIED.

/
/ CARD 6.   READ SOURCE TYPE, NUMBER OF RELEASES, BASIS FOR FLASH, AND MOLECULAR WEIGHT. SOURCE TYPE IS GIVEN BY THE FOLLOWING:

            4   LIQUID HF
            5   VAPOR HF
            7   LIQUID UF6 (VAPOR SOURCE TERM GENERATED)
           -7   LIQUID UF6 (VAPOR/SOLID SOURCE TERM GENERATED)
            8   VAPOR UF6
           22   INPUT PROVIDED IN FOR22.DAT

Table 19 (continued)

IF SOURCE TYPE IS SET EQUAL TO 22, SET NUMBER OF RELEASES TO ZERO. NO MORE THAN FIVE RELEASES MAY BE SPECIFIED, WHICH ARE TO RUN CONSECUTIVELY. THE BASIS FOR THE FLASH IS GIVEN BY THE FOLLOWING:

    0   ISENTROPIC
    1   ISENTHALPIC

THE DEFAULT MOLECULAR WEIGHT FOR UF6 IS 352.025; ENTER A VALUE LESS THAN 100 IF THAT VALUE IS ACCEPTABLE.

/
/ CARD 7.   -- DO NOT USE "CARD 7" CARDS IF ITYPE = 22. --

READ FOR EACH INCREMENTAL RELEASE THE DURATION (SEC), MASS (LB), TEMPERATURE (DEG F), AND PRESSURE (PSIA). SPECIFY AS MANY SETS OF DATA AS THE NUMBER OF RELEASES (IRELST). IF THE PRESSURE GIVEN IS LESS THAN OR EQUAL TO ZERO OR GREATER THAN THE VAPOR PRESSURE, THE PRESSURE IS SET EQUAL TO THE VAPOR PRESSURE FOR THAT INCREMENT.

/
/ CARD 8.   READ TIME INTERVAL FOR CALCULATIONS (SEC), DURATION OF SIMULATION (SEC), AND PRINT INTERVAL (SEC).

/
/ CARD 9.   -- THESE CARDS ARE OPTIONAL. --

READ DRAWING NUMBERS FOR PLOTS (LIMITED TO 20 CHARACTERS-- THE LAST CHARACTER MUST BE A DOLLAR SIGN ($)).

    1ST CARD 9 = CUMULATIVE URANIUM RELEASED
    2ND CARD 9 = CUMULATIVE HF RELEASED
    3RD CARD 9 = URANIUM CONCENTRATION IN COMPARTMENT
    4TH CARD 9 = HF CONCENTRATION IN COMPARTMENT
    5TH CARD 9 = TEMPERATURE IN COMPARTMENT
    6TH CARD 9 = PRESSURE IN COMPARTMENT

THE OPTIONAL SOURCE TERM INPUT IS READ FROM A DIFFERENT FILE THAN THE PRECEEDING INPUT.

/
/ OPTIONAL SOURCE TERM INPUT: CARD 1. ENTER TIME INTERVAL FOR SOURCE TERM INPUT (SEC).

/
/ OPTIONAL SOURCE TERM INPUT: CARD 2. ENTER INITIAL TIME FOR RELEASE INTERVAL (SEC); MASS FLOW RATE (LB/SEC) FOR EACH OF THE NINE COMPONENTS IN THE FOLLOWING ORDER: AIR, H2O(L), H2O(V), HF(L), HF(V), UF6(S), UF6(L), UF6(V), UO2F2; SOURCE TERM TEMPERATURE FOR INTERVAL (DEG F); AND SOURCE TERM PRESSURE FOR THE INTERVAL (PSIA).

transient instabilities resulting from reverse flow (occurring when internal pressure exceeds external pressure) were overcome by limiting the amount of material exhausted over a time step to that quantity that would reduce the compartment pressure to the ambient pressure, given the conditions existing in the compartment at the beginning of the time step. Coding for these special conditions appears between the statements CALL DPFLOW(2) and 160 CONTINUE (see listing in Appendix A.2). The bases for this latter section of coding are the following volumetric relationships

$$V_{max} = P_i V_i / P_{amb} \tag{155}$$

$$\Delta V_{max} = V_{max} - \dot{V}_b \Delta t / 60 - V_i \ , \tag{156}$$

where

V_{max} = volume of compartment contents if expanded to ambient pressure, ft^3,

P_i = compartment pressure, psia,

V_i = compartment volume, ft^3,

P_{amb} = ambient pressure, psia,

ΔV_{max} = maximum volume of compartment contents that can be exhausted via reverse flow through the inlet over the transient simulation time interval Δt, ft^3,

$\dot{V}_b$ = blower volumetric flow rate, acfm,

Δt = time interval for transient simulation, sec.

If the product of the fraction defined by the ratio of ΔV_{max} to V_{max} and the mass of material in the compartment is less than the mass of material that would be exhausted based on the results of the call to DPFLOW, then the mass of each component exhausted by reverse flow through the inlet is limited to the product of the fraction $\Delta V_{max}/V_{max}$ and the component mass in the compartment. The enthalpy rate is also limited, if the mass exhausted is limited, to the product of the fraction $\Delta V_{max}/V_{max}$ and the enthalpy of the compartment.

Examples of INDRFT input and output are provided in Sect. 5.2 and Appendix C.4.

4.6.3 Closed Compartment/Ventilation System

The BATCH program can be used to simulate releases into a closed room or steady-state releases into a ventilation system. When UF_6 or HF is released into a closed compartment, the final pressure may increase above the ambient pressure. For steady-state releases the batch model assumes that the source term represents a constant release rate and that the specified "compartment" volume is a constant volume flow rate. The two streams are mixed and exhausted at the ambient pressure using the MIXFLW subroutine (see Sect. 4.2.3). Input conditions required for BATCH are listed in Table 20. This particular program is interactive in contrast to the main programs previously discussed which require input files. Examples of BATCH input and output are provided in Sect. 5.3.

Table 20. Input data required for batch

Title

Ambient data
  Temperature, °F
  Pressure, psia
  Relative humidity, %

Compartment data
  Temperature, °F
  Pressure, psia
  Volume, ft^3
  Open or closed

Source term data
  Type
  Temperature, °F
  Pressure, psia
  Molecular weight, lb/lb-mole (for UF$_6$)
  Mass, lb

4.7 COMPARTMENT MODEL PLOTTING PROGRAM

COMPLT, a program for plotting results from FODRFT and INDRFT, has been written using DISSPLA version 9.0. Results plotted as a function of time include (1) cumulative uranium released from the compartment, (2) cumulative HF released from the compartment, including that subsequently formed from UF$_6$ released from the compartment, (3) the concentration of uranium in the compartment, (4) the concentration of HF in the compartment, (5) the temperature inside the compartment, and (6) the pressure inside the compartment. The only input required for COMPLT is that provided as output from FODRFT and INDRFT. Note that data output from the compartment models for use by COMPLT is generally written to the output file more frequently than the print interval supplied as input to compartment models because of the rapid transients occuring during the release.

5. EXAMPLE PROBLEMS

Several example problems are included in this chapter to illustrate the use and application of the various main programs (CYLIND, FODRFT, INDRFT, and BATCH) described in preceding chapters. Section 5.1 describes the simulation of releases from cylinders through breaches (including sheared valves) and piping systems. The simulation of releases inside buildings is described in Sect. 5.2. Simulation of a release into a ventilation system is described in Sect. 5.3. Example results are illustrated with CYLPLT and COMPLT generated plots.

5.1 RELEASE FROM A CYLINDER

Releases from cylinders can occur through two pathways: (1) a breach in containment (including a sheared valve) and (2) a ruptured piping system. Section 5.1.1 illustrates the use of CYLIND to simulate (1) a release through a sheared valve and (2) a release through an irregular breach. The latter example is used as input for the compartment model examples of Sect. 5.2. Section 5.1.2 illustrates the use of CYLIND to simulate a rupture in a piping system.

5.1.1 Release Through a Breach in Containment

This section illustrates two types of releases that may be simulated as a breach in containment. Such releases could occur when a hot cylinder is being transported from the cylinder fill area to a cool-down storage area. The first example represents a release through a sheared valve. This example may be simulated immediately from information supplied in the example statement. The second example is based on an historical accident insofar as the breach geometry is concerned and illustrates several approximations and assumptions made in applying CYLIND to simulate the release.

Example 1

Problem statement. The valve of a 48X cylinder containing the maximum allowable mass of UF_6 is struck in such a manner that it is sheared off leaving a hole in the end of the containment. The cylinder is lying on its side and the initial UF_6 temperature is 200°F. Simulate the release using a 60-sec simulation interval and a maximum release time of 2 hr. Compare results for the breach location being in the 6, 9, and 12 o'clock positions (see Fig. 24). Also, compare the release from the 6 o'clock position to a release from a cylinder in the 6 o'clock position containing UF_6 at 250°F.

CYLIND input. Input to CYLIND for the four cases outlined in this example are given in Table 21. The first line of input (the title) corresponds to Card 1 input of Table 12 (see Chap. 3). The second line corresponds to Card 2 input of Table 12. The value for ISEN was specified as 1 (i.e., isenthalpic release) because this is consistent with the derivation of the method used for evaluating flow through a piping system. This example specifies a 48X cylinder filled with the maximum allowable mass of UF_6 as well as a sheared valve; default values for cylinder characteristics are invoked by specifying ICYL equal to 5. The cylinder is lying on its side (IVERT = 0) and IPIG is specified as 2 to identify that the release occurs through a breach. Because ICYL is greater than 0, Card 3 and Card 4 (see Table 12) are not used. The third line corresponds to Card 5 of Table 12. Because the subroutine INTMEB assumes saturated conditions inside the cylinder, either the initial pressure or the initial temperature may be specified (if both

95

ORNL—DWG 85-14585
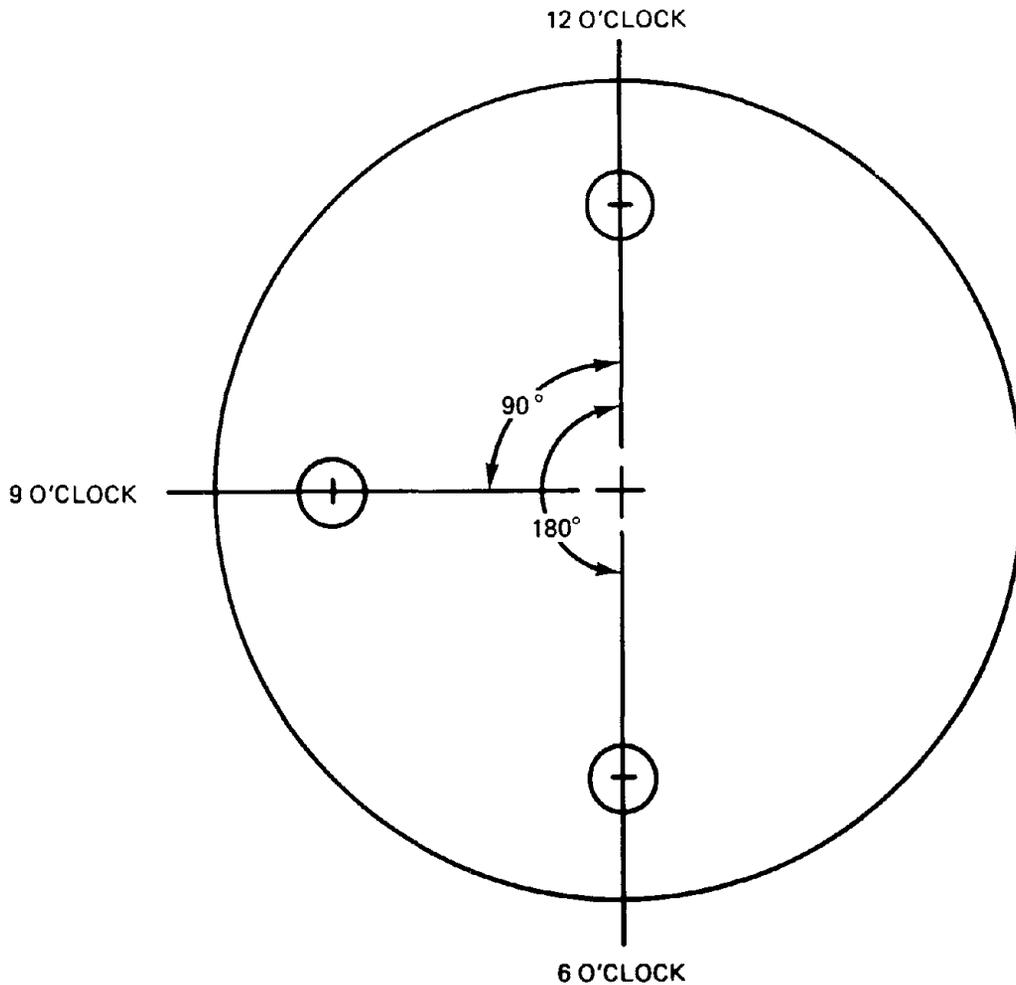
Fig. 24. End view of a cylinder illustrating 6, 9, and 12 o'clock valve positions and measurement of the angle α.

are specified, pressure is ignored). Because the initial temperature is given in this example, 0 is entered for pressure and 200 (Cases 1 through 3) or 250 (case 4) is entered for temperature. The next value, that of liquid mass fraction is important only if initial conditions correspond to the triple point; it has been set equal to 1 because the initial temperature exceeds the triple-point temperature (and since a value must be entered). The zero value corresponding to molecular weight invokes a default value of 352.025. The last value on the third line specifies the breach position relative to the cylinder center line (see Fig. 24). The 6 o'clock position corresponds to 180° (note cases 1 and 4 in Table 21). The zero in the fourth line corresponding to Card 6 of Table 12 defaults to an ambient pressure of 14.7 psia. Card 7 is not used because ICYL = 2. The fifth line, corresponding to Card 8, specifies that the time interval for simulation is 60 sec and that the simulation is limited to 7200 sec. The sixth through ninth lines, corresponding to Card 9, for Cases 2 and 3 provide drawing numbers for plots subsequently used to illustrate results.

Table 21. CYLIND input files for simulating the four cases of Example 1

```
L  C                              COLUMN
I  A
N  R        1         2         3         4         5         6
E  D  1234567890123456789012345678901234567890123456789012345678901234567

      INPUT FOR CASE 1

1  1  EX. 1, CASE 1. 10-TON CYL, SHEARED VALVE AT 6 O'CLOCK, UF6 AT 200 F
2  2  1,5,0,2
3  5  0,200,1,0,180
4  6  0
5  8  60,7200

      INPUT FOR CASE 2

1  1  EX. 1, CASE 2. 10-TON CYL, SHEARED VALVE AT 9 O'CLOCK, UF6 AT 200 F
2  2  1,5,0,2
3  5  0,200,1,0,90
4  6  0
5  8  60,7200
6  9  ORNL-DWG-85c-15268$
7  9  ORNL-DWG-85c-15269$
8  9  ORNL-DWG-85c-15270$
9  9  ORNL-DWG-85c-15271$

      INPUT FOR CASE 3

1  1  EX. 1, CASE 3. 10-TON CYL, SHEARED VALVE AT 12 O'CLOCK, UF6 AT 200 F
2  2  1,5,0,2
3  5  0,200,1,0,0
4  6  0
5  8  60,7200
6  9  ORNL-DWG-85c-15272$
7  9  ORNL-DWG-85c-15273$
8  9  ORNL-DWG-85c-15274$
9  9  ORNL-DWG-85c-15275$

      INPUT FOR CASE 4

1  1  EX. 1, CASE 4. 10-TON CYL, SHEARED VALVE AT 6 O'CLOCK, UF6 AT 250 F
2  2  1,5,0,2
3  5  0,250,1,0,180
4  6  0
5  8  60,7200
```

Results. The results of the four cases outlined in this example are summarized in Table 22. Complete output for the four cases of this example are included in Appendix C.1. The results of Case 2 are also plotted in Figs. 25 through 28, which are similar (at least in general profile) to Cases 1 and 4 also. Figure 25 shows the total mass and phases of UF_6 present inside the cylinder. Figure 26 shows the mass release rate of UF_6 in which the phase composition corresponds to the ambient pressure. The temperature and corresponding vapor pressure of UF_6 inside the cylinder are shown in Fig. 27, and the exhaust temperature is shown in Fig. 28. The rapid change in mass release rate at about 1500 sec (see Fig. 26) corresponds to the passage of the vapor-condensate interface across the breach. As the interface drops below the breach, the temperature of UF_6 inside the cylinder falls rapidly as UF_6 vapor escapes through the breach (see Fig. 27) until the triple point is reached. Solids then begin to form in the condensate (see Fig. 25). When no liquid remains, the release is considered ended. The temperature spike seen in Fig. 28 corresponds to the passage of the phase interface across the breach and subsequent rapid cooling of UF_6 inside the cylinder. A solid-vapor mixture is being formed prior to the temperature spike; whereas vapor only is released subsequent to the spike. Results of Case 3, which begins with a vapor release since the phase interface is initially below the breach, are shown in Figs. 29 through 32.

Example 2

Problem statement. Simulate the release of UF_6 from a 48Y cylinder containing 25,900 lb of UF_6 at 190°F when it is dropped onto an object resulting in an 8-in. breach next to a stiffening ring as is illustrated by Fig. 33. While one side of the breach retains the approximate contour of the cylinder cross section, the other side is dented in to approximately mirror the original contour. Compare results using simulation time intervals of 10, 20, and 60 sec.

Preliminary calculations. Because the described breach is neither circular nor in the end of the cylinder, an "equivalent" breach in the end of the cylinder must be developed. The area of the breach can be approximated as follows because of the described nature of the dent. First, calculate the angle θ (see Fig. 33) subtended by the arc of the breach,

$$\theta = (360a/2\pi R) = [360°(8\,\text{in.})]/[2\pi(24\,\text{in.})] = 19.10°. \tag{157}$$

The area of the cylinder cross section enclosed by the angle θ is given by

$$A_1 = (\theta\pi R^2)/(360) = (19.10°/360°)[\pi(24\,\text{in.})^2] = 96.01\,\text{in.}^2. \tag{158}$$

The "height" of a triangle formed by joining the ends of the breach and the center of the cylinder cross section is given by

$$h = R\cos(\theta/2) = 24\cos(19.10/2) = 23.67\,\text{in.}, \tag{159}$$

and the base is given by

$$b = 2R\sin(\theta/2) = 2[24\sin(19.10/1)] = 7.96\,\text{in.} \tag{160}$$

Table 22. Summary of results for Example 1—release
UF$_6$ Through the Sheared Valve of a 48X cylinder
initially containing 21,030 lb of UF$_6$

Case	1	2	3	4
Valve position, o'clock	6	9	12	6
Initial temperature, °F	200	200	200	250
Initial release rate, lb/sec	6.33	6.33	2.57[a]	10.71

Conditions as phase interface approaches top of breach

Time, sec	2940	1380		1740
UF$_6$ remaining, lb	2807	12368		2963
Temperature, °F	194.8	198.5		241.4
Release rate, lb/sec	5.88	6.14		9.60

Conditions as phase interface drops below bottom of breach

Time, sec	3060	1560		1860
UF$_6$ remaining, lb	2105	11402		1840
Temperature, °F	194.1	196.9		238.8
Release rate, lb/sec	2.37	2.46		4.20

Conditions as temperature reaches triple point (147.3°F)

Time, sec	3360	2820	2340	2160
UF$_6$ remaining, lb	1636	9404	17247	1103
Release rate, lb/sec	0.896	0.896	0.896	0.896

Conditions at end of simulation[b]

Time, sec	~3960	~6840	7200	~2580
UF$_6$ remaining, lb	~1045	~5747	12891	~726
Temperature, °F	<147.3	<147.3	147.3	<147.3
Release rate, lb/sec	0	0	0.896	0

[a]The initial release phase for Case 3 is vapor since the breach is above the phase interface.

[b]The simulation was terminated when the temperature of UF$_6$ inside the cylinder dropped below the triple point or when the specified duration for the simulation (i.e., 7200 sec) was reached.
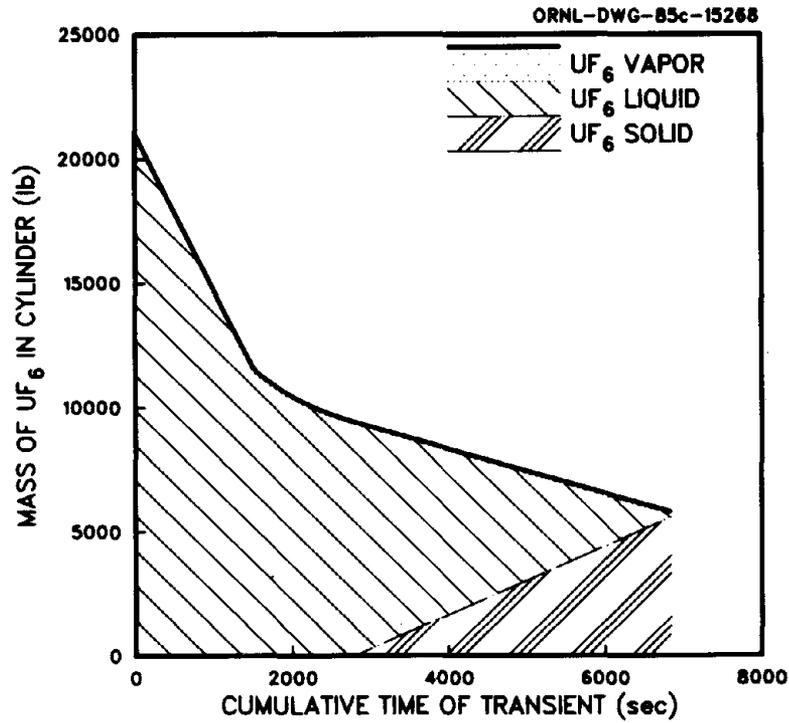
Fig. 25. UF$_6$ inventory in a 48X (10-ton) cylinder following the shearing of a valve in the 9 o'clock position (Example 1, Case 2).
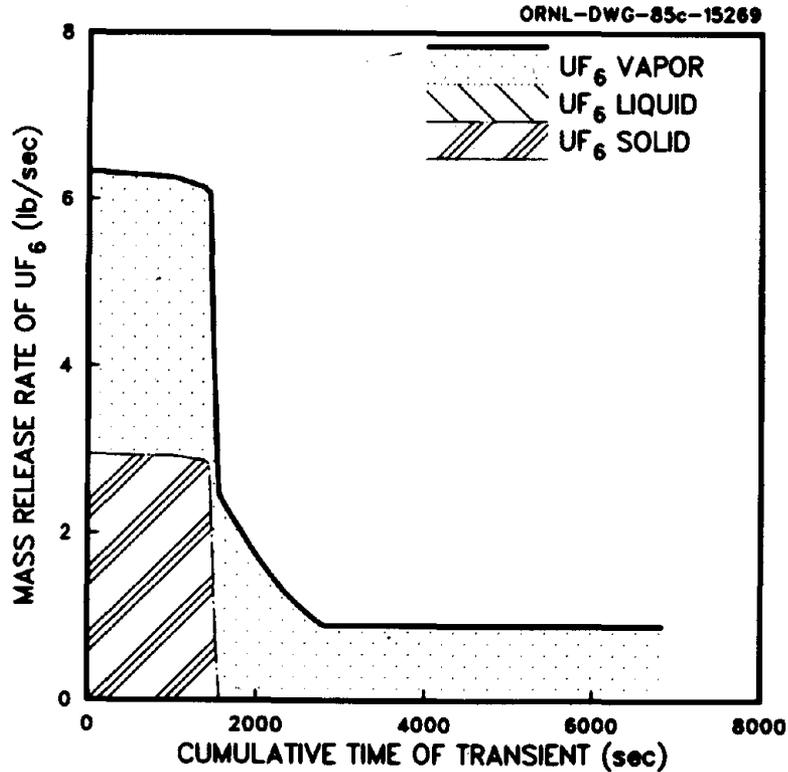
Fig. 26. Mass Release Rates of UF$_6$ from a 48X (10-ton) cylinder following the shearing of a valve in the 9 o'clock position (Example 1, Case 2).

ORNL-DWG-85c-15270
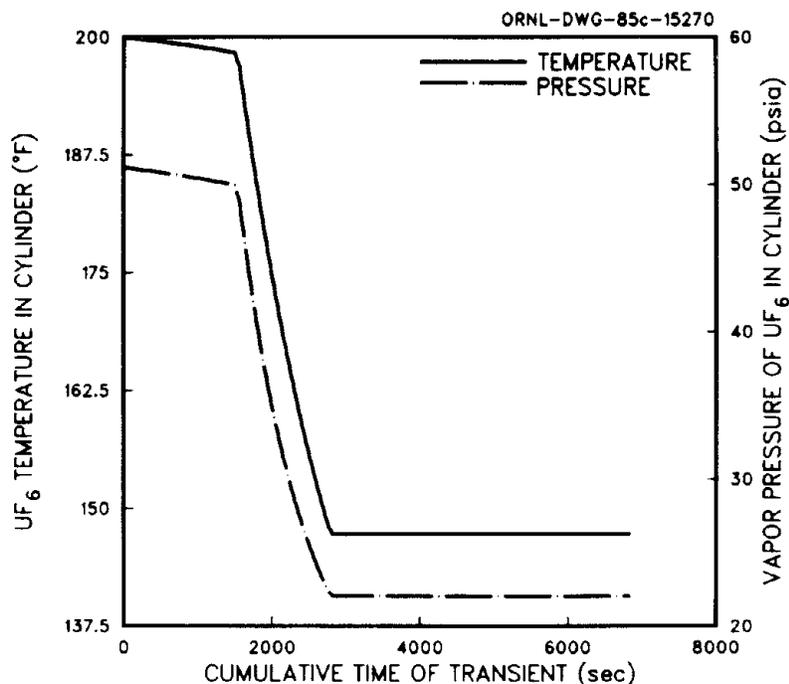
Fig. 27. Temperature and Pressure Inside a 48X (10-ton) cylinder following the Shearing of a valve in the 9 o'clock position (Example 1, Case 2).

ORNL-DWG-85c-15271
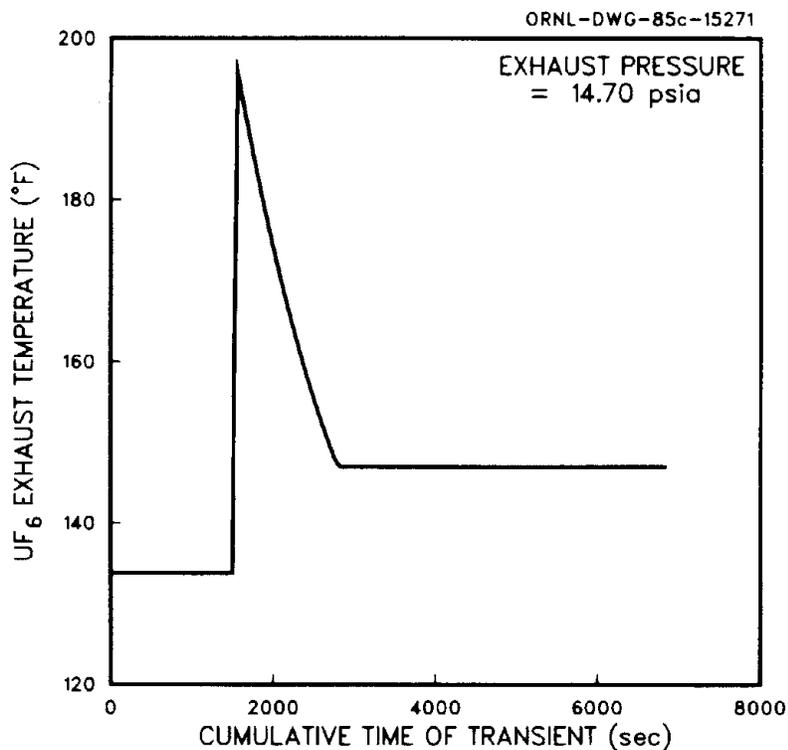
Fig. 28. Exhaust temperature of UF_6 exiting the sheared valve of a 48X (10-ton) cylinder (Example 1, Case 2). The valve is in the 9 o'clock position. A vapor-solid mixture is being released prior to the temperature spike; thereafter, a vapor release occurs.
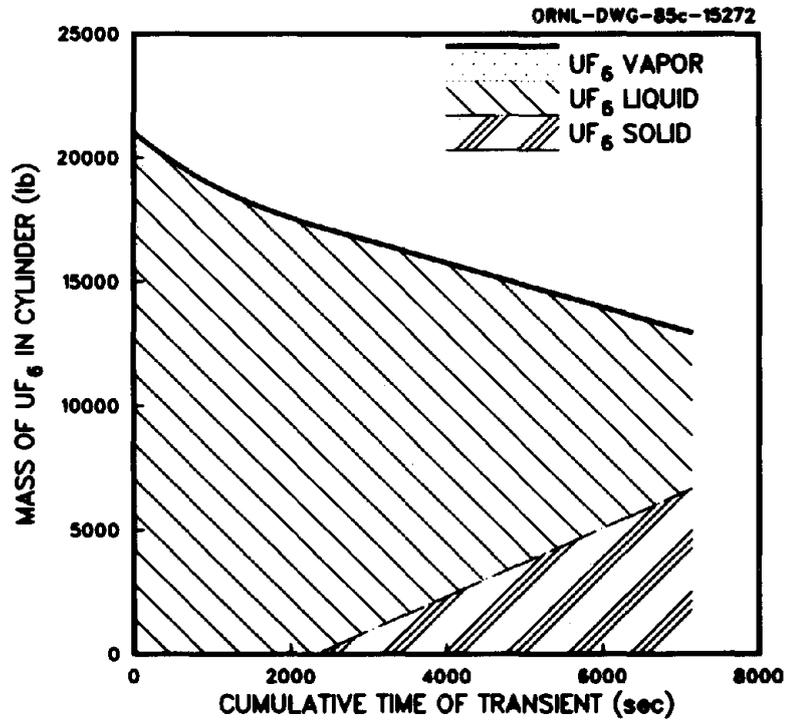
Fig. 29. Inventory of UF$_6$ in a 48X (10-ton) cylinder following the shearing of a valve in the 12 o'clock position (Example 1, Case 3).
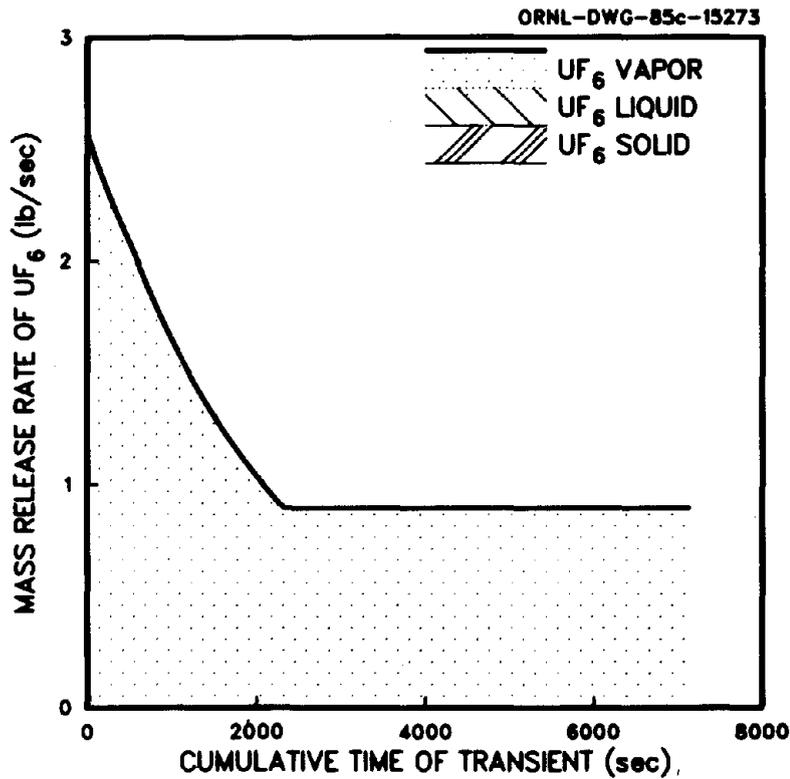
Fig. 30. Mass release rate of UF$_6$ from a 48X (10-ton) cylinder following the shearing of a valve in the 12 o'clock position (Example 1, Case 3). Only vapor is released. Conditions inside the cylinder are at the triple point when the mass release rate becomes constant.

ORNL-DWG-85c-15274
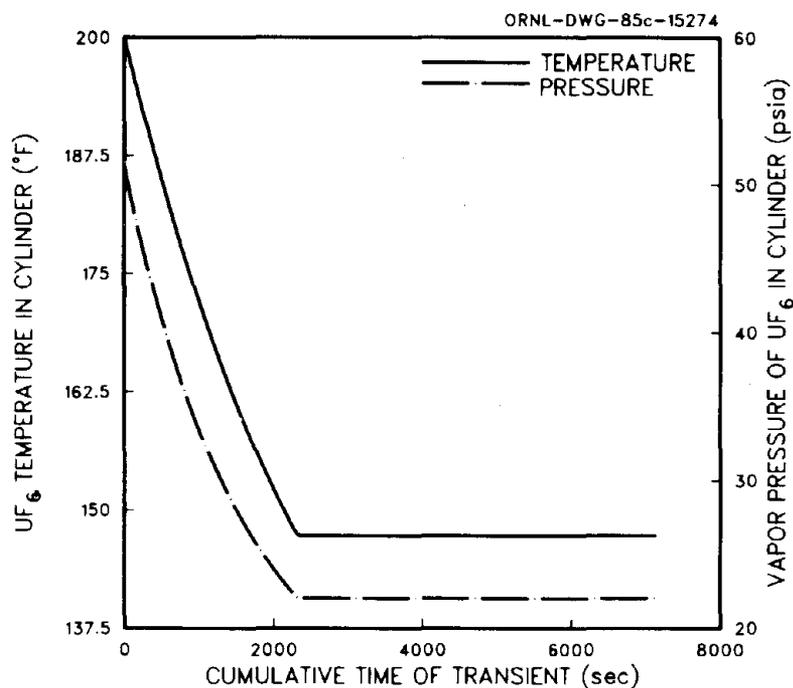
Fig. 31. Temperature and pressure inside a 48X (10-ton) cylinder following the shearing of a valve in the 12 o'clock position (Example 1, Case 3).

ORNL-DWG-85c-15275
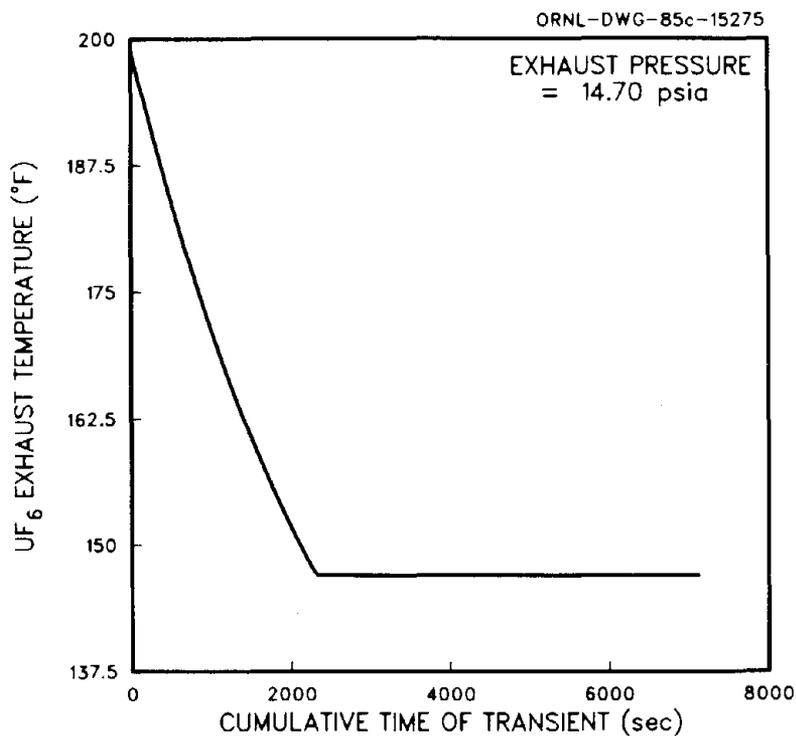
Fig. 32. Exhaust temperature of a UF_6 vapor exiting the sheared valve of a 48X (10-ton) cylinder (Example 1, Case 3). The valve is in the 12 o'clock position.

ORNL–DWG 85-14584

BREACH LOCATION

R = 24 in.

θ

h

a = 8 in.

b

BASIS FOR CALCULATING
BREACH AREA

r

d

"EQUIVALENT" BREACH IN
END OF CYLINDER
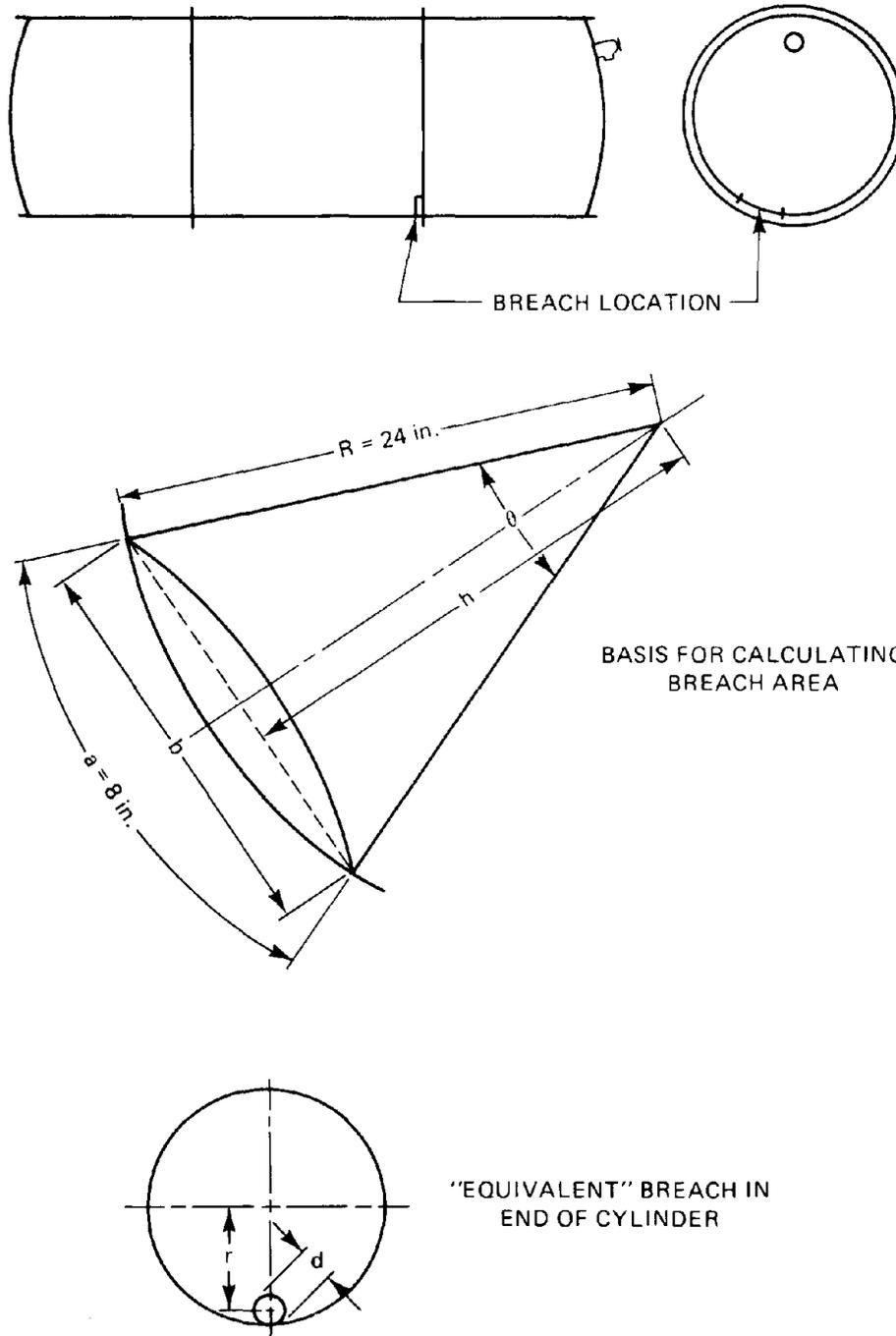
Fig. 33. Diagrams of breach location and basis for simulation for Example 2.

The area of this triangle is

$$A_2 = hb/2 = [23.67(7.96)]/2 = 94.21 \text{ in.}^2. \tag{161}$$

Because the dented side of the breach approximately mirrors the original location, the area of the breach is about twice the difference of A_1 and A_2,

$$A = 2(A_1 - A_2) = 2(96.01 - 94.21) = 3.60 \text{ in.}^2, \tag{162}$$

and the "equivalent" breach diameter is

$$d = 2\sqrt{A/\pi} = 2.14 \text{ in.} \tag{163}$$

Because the breach is basically facing downward, the radius from the center line of the cylinder to the center line of the hole is taken to be the cylinder radius minus the radius of the hole,

$$r = R - (d/2) = 22.93 \text{ in.}, \tag{164}$$

and the breach is assumed to be in the 6 o'clock position ($\alpha = 180°$).

CYLIND input. Input for simulating this example using the CYLIND program are shown in Table 23. The three cases are identical except for the simulation time interval and specified drawing numbers. The first line is the title corresponding to Card 1 of Table 12. The second line, corresponding to Card 2, specifies that the flash basis is isenthalpic (1), cylinder geometry and mass characteristics will be supplied by the user (0), the cylinder is lying on its side (0), and that the release pathway is a breach (2). Because the cylinder type was specified as 0, Card 3 is used to specify mass and cylinder geometry. Several values needed in the third line can be obtained from Table 8. The mass is obtained from the problem statement (25900); the cylinder internal volume, internal diameter, and internal length for a 48Y cylinder are obtained from Table 8 (142.7, 48, 136.27); the radius from the cylinder center line to the breach and the breach diameter are obtained from the preliminary calculations of the preceding paragraph (22.9, 2.14). Card 4 input is not used. The fourth line of input, corresponding to Card 5, shows a zero pressure since the initial pressure will be calculated from the initial temperature (190), the liquid mass fraction (1), acceptance of the default molecular weight of 352.025 (0), and the breach position (180). Line 5 gives the ambient pressure (see Card 6) and line 6 specifies the simulation interval (10, 20, or 60 for Case 1, 2, or 3, respectively) and maximum duration (3600) (see Card 8). Card 7 type input is not required. Lines 7 and 8 (see Card 9) for Case 2 specify drawing numbers for plots subsequently used to illustrate results.

Results. The output from CYLIND for Example 2, Case 2 is given in Table 24. Results for Cases 1 and 3 are given in Appendix C.2. In all three cases, the last line of output is one simulation time interval short of 780 sec. At some point between the final printout and 780 sec, the temperature of UF_6 remaining in the cylinder fell below the triple point terminating the simulation. Comparison of output for the various release times shows that increasing the simulation time

Table 23. CYLIND input files for simulating the three cases of Example 2

```
L   C                              COLUMN
I   A
N   R        1         2         3         4         5         6         7
E   D   12345678901234567890123456789012345678901234567890123456789012345678901234

        INPUT FOR CASE 1

1   1   EX. 2, CASE 1. RELEASE FROM 8" BREACH IN SIDE OF 14-T CYL (AS HOLE IN END)
2   2   1,0,0,2
3   3   25900,142.7,48.,136.27,22.9,2.14
4   5   0,190,1,0,180
5   6   14.7
6   8   10,3600

        INPUT FOR CASE 2

1   1   EX. 2, CASE 2. RELEASE FROM 8" BREACH IN SIDE OF 14-T CYL (AS HOLE IN END)
2   2   1,0,0,2
3   3   25900,142.7,48.,136.27,22.9,2.14
4   5   0,190,1,0,180
5   6   14.7
6   8   20,3600
7   9   ORNL-DWG-85c-15276$
8   9   ORNL-DWG-85c-15277$

        INPUT FOR CASE 3

1   1   EX. 2, CASE 3. RELEASE FROM 8" BREACH IN SIDE OF 14-T CYL (AS HOLE IN END)
2   2   1,0,0,2
3   3   25900,142.7,48.,136.27,22.9,2.14
4   5   0,190,1,0,180
5   6   14.7
6   8   60,3600
```

interval effectively increases the release rate; for example, at 720 sec the amounts of UF_6 remaining in the cylinder for Cases 1, 2, and 3 are 2180, 2176, and 2157 lb, respectively. Figures 34 and 35 show the inventory of UF_6 remaining in the cylinder and the mass release rate of UF_6, respectively, for Case 2. Results of this example are used as input for Examples 4 and 5.

5.1.2 Release Through a Ruptured Piping System

This section illustrates the use of CYLIND to simulate the release of UF_6 from containment through a ruptured piping system. Such releases could be postulated for several areas within UF_6 production facilities as well as in the UF_6 feed area of a fuel fabrication facility. The example problem is based on the cylinder fill area of a production facility.

Example 3

Problem statement. A type 48Y cylinder is being filled from a cold trap. Near the end of the fill cycle, the pigtail connecting the fixed piping to the cylinder is ruptured. The amount of UF_6 remaining in the cold trap is negligible. The cylinder, which contains 26,000 lb of UF_6 at 200°F, is

Table 24. Output from CYLIND for Example 2, Case 2

| | ****** CONDITION OF UF6 IN CONTAINMENT ****** | | | | | | PATHWAY | | | ****** CONDITION OF UF6 EXHAUSTED ****** | | | | | |
| | ******** MASS (LB) ******** | | | ****** | | | | INLET | FLOW | **** RELEASE RATE (LB/SEC) **** | | | | | |
TIME (SEC)	SOLID	LIQUID	VAPOR	TOTAL	TEMP (DEG F)	PRES (PSIA)	RELEASE PHASE	PRES (PSIA)	RATE BASIS	SOLID	LIQUID	VAPOR	TOTAL	TEMP (DEG F)	PRES (PSIA)
0.	0.0	25850.6	49.4	25900.0	190.000	44.136	LIQUID	48.687	CHOKE	16.396	0.000	17.275	33.671	14.700	133.780
20.	0.0	25170.8	55.8	25226.6	189.934	44.092	LIQUID	48.521	CHOKE	16.388	0.000	17.256	33.645	14.700	133.780
40.	0.0	24491.5	62.2	24553.7	189.866	44.047	LIQUID	48.357	CHOKE	16.380	0.000	17.237	33.617	14.700	133.780
60.	0.0	23812.8	68.6	23881.3	189.797	44.002	LIQUID	48.194	CHOKE	16.372	0.000	17.218	33.589	14.700	133.780
80.	0.0	23134.6	74.9	23209.5	189.726	43.955	LIQUID	48.033	CHOKE	16.363	0.000	17.198	33.561	14.700	133.780
100.	0.0	22457.0	81.3	22538.3	189.653	43.906	LIQUID	47.873	CHOKE	16.354	0.000	17.177	33.531	14.700	133.780
120.	0.0	21780.1	87.6	21867.7	189.578	43.857	LIQUID	47.714	CHOKE	16.345	0.000	17.156	33.501	14.700	133.780
140.	0.0	21103.7	93.9	21197.7	189.500	43.806	LIQUID	47.554	CHOKE	16.335	0.000	17.135	33.470	14.700	133.780
160.	0.0	20428.1	100.2	20528.3	189.421	43.753	LIQUID	47.395	CHOKE	16.326	0.000	17.112	33.438	14.700	133.780
180.	0.0	19753.0	106.5	19859.5	189.339	43.700	LIQUID	47.235	CHOKE	16.316	0.000	17.090	33.405	14.700	133.780
200.	0.0	19078.7	112.7	19191.4	189.254	43.644	LIQUID	47.074	CHOKE	16.305	0.000	17.066	33.371	14.700	133.780
220.	0.0	18405.0	118.9	18524.0	189.167	43.587	LIQUID	46.913	CHOKE	16.295	0.000	17.042	33.336	14.700	133.780
240.	0.0	17732.1	125.1	17857.3	189.077	43.528	LIQUID	46.750	CHOKE	16.283	0.000	17.017	33.300	14.700	133.780
260.	0.0	17060.0	131.3	17191.3	188.984	43.467	LIQUID	46.586	CHOKE	16.272	0.000	16.991	33.263	14.700	133.780
280.	0.0	16388.6	137.4	16526.0	188.888	43.403	LIQUID	46.420	CHOKE	16.260	0.000	16.964	33.224	14.700	133.780
300.	0.0	15718.0	143.5	15861.5	188.787	43.338	LIQUID	46.252	CHOKE	16.248	0.000	16.936	33.184	14.700	133.780
320.	0.0	15048.3	149.6	15197.9	188.683	43.270	LIQUID	46.081	CHOKE	16.235	0.000	16.907	33.142	14.700	133.780
340.	0.0	14379.4	155.6	14535.0	188.575	43.199	LIQUID	45.908	CHOKE	16.222	0.000	16.877	33.099	14.700	133.780
360.	0.0	13711.4	161.6	13873.0	188.463	43.126	LIQUID	45.733	CHOKE	16.208	0.000	16.846	33.054	14.700	133.780
380.	0.0	13044.4	167.6	13211.9	188.345	43.049	LIQUID	45.553	CHOKE	16.193	0.000	16.813	33.007	14.700	133.780
400.	0.0	12378.3	173.5	12551.8	188.222	42.969	LIQUID	45.371	CHOKE	16.178	0.000	16.779	32.958	14.700	133.780
420.	0.0	11713.3	179.4	11892.7	188.093	42.886	LIQUID	45.184	CHOKE	16.162	0.000	16.744	32.906	14.700	133.780
440.	0.0	11049.3	185.2	11234.5	187.957	42.798	LIQUID	44.992	CHOKE	16.146	0.000	16.707	32.852	14.700	133.780
460.	0.0	10386.5	191.0	10577.5	187.814	42.705	LIQUID	44.795	CHOKE	16.128	0.000	16.667	32.795	14.700	133.780
480.	0.0	9724.8	196.7	9921.6	187.663	42.608	LIQUID	44.592	CHOKE	16.109	0.000	16.626	32.735	14.700	133.780
500.	0.0	9064.5	202.4	9266.9	187.503	42.505	LIQUID	44.383	CHOKE	16.090	0.000	16.582	32.672	14.700	133.780
520.	0.0	8405.4	208.0	8613.4	187.333	42.395	LIQUID	44.165	CHOKE	16.069	0.000	16.535	32.604	14.700	133.780
540.	0.0	7747.8	213.5	7961.3	187.151	42.278	LIQUID	43.939	CHOKE	16.046	0.000	16.486	32.532	14.700	133.780
560.	0.0	7091.7	219.0	7310.7	186.955	42.153	LIQUID	43.703	CHOKE	16.022	0.000	16.433	32.454	14.700	133.780
580.	0.0	6437.3	224.4	6661.6	186.743	42.017	LIQUID	43.455	CHOKE	15.996	0.000	16.375	32.371	14.700	133.780
600.	0.0	5784.6	229.6	6014.2	186.513	41.871	LIQUID	43.193	CHOKE	15.967	0.000	16.313	32.280	14.700	133.780
620.	0.0	5133.9	234.7	5368.6	186.261	41.710	LIQUID	42.915	CHOKE	15.936	0.000	16.245	32.181	14.700	133.780
640.	0.0	4485.3	239.7	4725.0	185.981	41.533	LIQUID	42.616	CHOKE	15.901	0.000	16.169	32.071	14.700	133.780
660.	0.0	3839.0	244.6	4083.6	185.668	41.335	LIQUID	42.293	CHOKE	15.863	0.000	16.085	31.948	14.700	133.780
680.	0.0	3195.5	249.2	3444.6	185.311	41.110	LIQUID	41.937	CHOKE	15.818	0.000	15.990	31.808	14.700	133.780
700.	0.0	2555.0	253.5	2808.5	184.896	40.850	LIQUID	41.539	CHOKE	15.767	0.000	15.880	31.646	14.700	133.780
720.	0.0	1918.1	257.5	2175.5	184.400	40.542	LIQUID	41.083	CHOKE	15.705	0.000	15.749	31.454	14.700	133.780
740.	0.0	1285.5	260.9	1546.5	183.784	40.160	LIQUID	40.539	CHOKE	15.624	0.000	15.583	31.207	14.700	133.780
760.	0.0	658.7	263.6	922.3	182.967	39.659	LIQUID	39.849	CHOKE	15.408	0.000	15.257	30.665	14.700	133.780

108
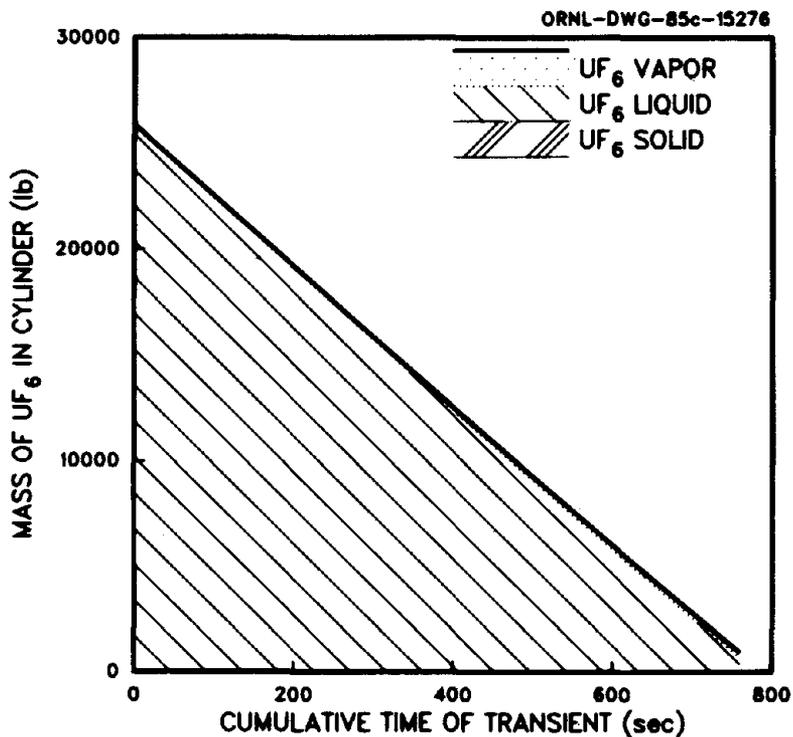
Fig. 34. UF$_6$ inventory in a 48Y (14-ton) cylinder following formation of a large breach (Example 2, Case 2).
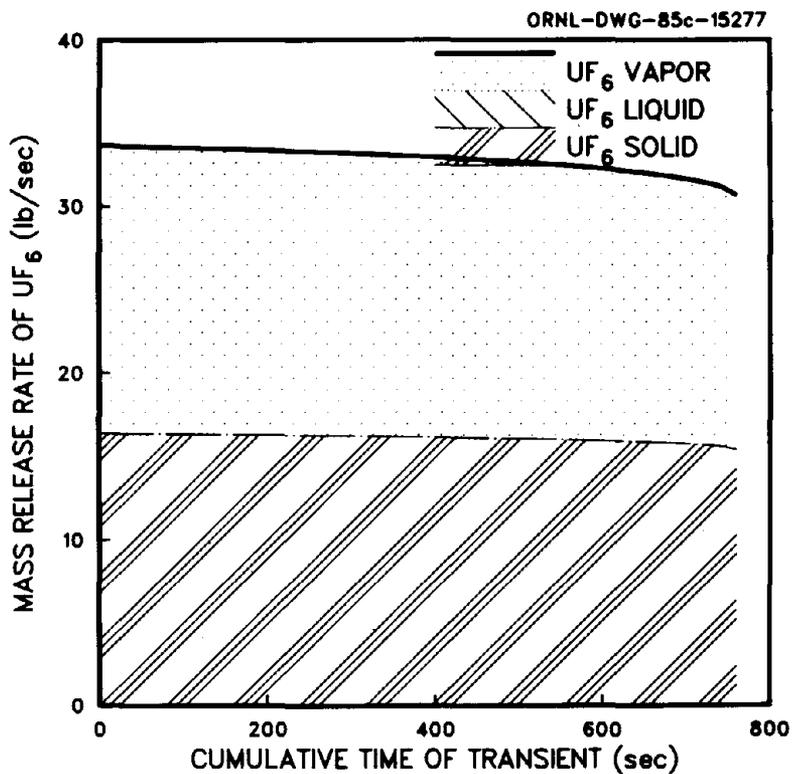
Fig. 35. Mass release rates of UF$_6$ from a 48Y (14-ton) cylinder following formation of a large breach (Example 2, Case 2).

lying on its side with the valve in the 11 o'clock position. Determine the total amount of UF$_6$ released assuming the release is stopped within 15 min for pigtail lengths of 6 in. 2 ft, and 4 ft.

CYLIND input. Input data sets for the use of CYLIND are given in Table 25. The only difference in the three data sets is the pigtail length, which appears in the title line and the second to last line of the data. The title is the first line of input, corresponding to Card 1 of Table 12. In

Table 25. CYLIND input files for simulating the three cases of Example 3

```
L  C                          COLUMN
I  A
N  R           1        2        3        4        5
E  D    123456789012345678901234567890123456789012345678901234567890 12

        INPUT FOR CASE 1

1  1    EX. 3, CASE 1. 14-TON CYL W/ RUPTURED PIGTAIL (6 IN)
2  2    1,-6,0,4
3  4    26000
4  5    0,200,1,0,30
5  7    1,0.5,0.875
6  7    2,0.316,0.875
7  7    1,0.5,0.875
8  7    2,1.0,14.7
9  8    30,900

        INPUT FOR CASE 2

1  1    EX. 3, CASE 2. 14-TON CYL W/ RUPTURED PIGTAIL (2 FT)
2  2    1,-6,0,4
3  4    26000
4  5    0,200,1,0,30
5  7    1,0.5,0.875
6  7    2,0.316,0.875
7  7    1,2.0,0.875
8  7    2,1.0,14.7
9  8    30,900

        INPUT FOR CASE 3

1   1   EX. 3, CASE 3. 14-TON CYL W/ RUPTURED PIGTAIL (4 FT)
2   2   1,-6,0,4
3   4   26000
4   5   0,200,1,0,30
5   7   1,0.5,0.875
6   7   2,0.316,0.875
7   7   1,4.0,0.875
8   7   2,1.0,14.7
9   8   30,900
10  9   ORNL-DWG-85c-15278$
11  9   ORNL-DWG-85c-15279$
```

line 2 (Card 2), 1 sets the flash basis to isenthalpic , -6 calls for default values for a 48Y cylinder (except for the initial mass of UF_6), 0 specifies the cylinder is on its side, and 4 specifies the number of elements in the release pathway (entrance, valve, pipe segment, and exit). Card 3 is not included since a nonzero cylinder type was specified. In line 3 (Card 4), 26,000 specifies the mass of UF_6 initially in the cylinder. In the fourth line (Card 5), 0 specifies the initial pressure will be evaluated from the temperature, 200 is the initial temperature, 1 is the liquid mass fraction of the nonvapor fraction, 0 specifies use of the default molecular weight, and 30 specifies the valve position. Card 6 is not used because the release pathway contains more than two elements. The next four lines, one for each element of the release pathway, correspond to Card 7. Line 5 represents the entrance: 1 is used in the first "Card 7" line to specify the entrance, 0.5 is the resistance coefficient for the entrance, and 0.875 is the entrance diameter. The first of the Card 7 lines always represents an entrance effect; otherwise, a 1 in the first position represents a pipe segment. Line 6 represents the cylinder valve: 2 specifies a fitting, 0.316 specifies the resistance coefficient (see Table 10), and the third entry is the nominal diameter of the fitting. Line 7 is the pigtail element: the first and third entries on the line have been previously identified as specifying a pipe segment and the pipe diameter. The second entry specifies the pipe segment length. The eighth and last Card 7 line is the exit effect: 2 specifies that the second entry on the line is a resistance coefficient (1.0 for a sudden expansion). The third entry on line 8 (and always for the last Card 7 line) is the ambient pressure. A normal atmospheric pressure of 14.7 psia has been assumed. The last line (Card 8) specifies the simulation interval (60) and the simulation duration (900).

Results. Output for the three cases of this example are summarized in Table 26. Complete output is given in Appendix C.3. Because of the initial valve position, only UF_6 vapor is released. The total amount of UF_6 released is estimated to be 1695, 1542, and 1424 lb for Cases 1, 2, and 3 respectively. The inventory of UF_6 remaining in the cylinder and the mass release rate from the cylinder for Case 3 are given in Fig. 36 and 37, respectively.

Table 26. Summary of output from CYLIND for Example 3

Case	1	2	3
Pigtail length, ft	0.5	2	4
Initial release rate, lb/sec	2.13	1.91	1.75
Conditions at 870 sec			
UF_6 remaining, lb	24354	24504	24619
Temperature, °F	183.0	184.6	185.8
Release rate, lb/sec	1.66	1.53	1.42
Estimated conditions at 900 sec			
UF_6 remaining, lb	24305	24458	24576
Estimated total UF_6 released, lb	1695	1542	1424

ORNL-DWG-85c-15278
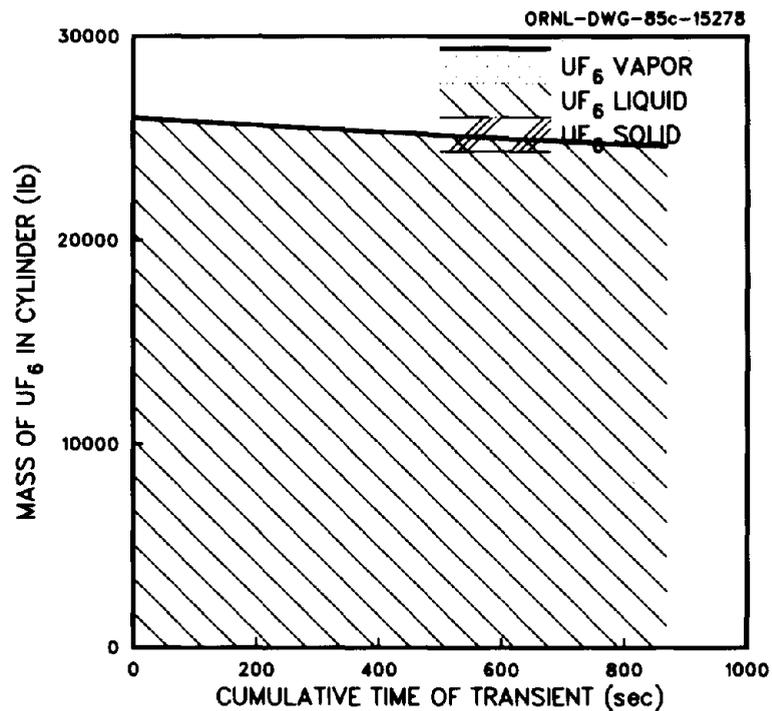
Fig. 36. UF$_6$ inventory in a 48Y (14-ton) cylinder following the rupture of a pigtail (Example 3, Case 3). The pigtail length is 4 ft and the valve is in the 11 o'clock position.

ORNL-DWG-85c-15279
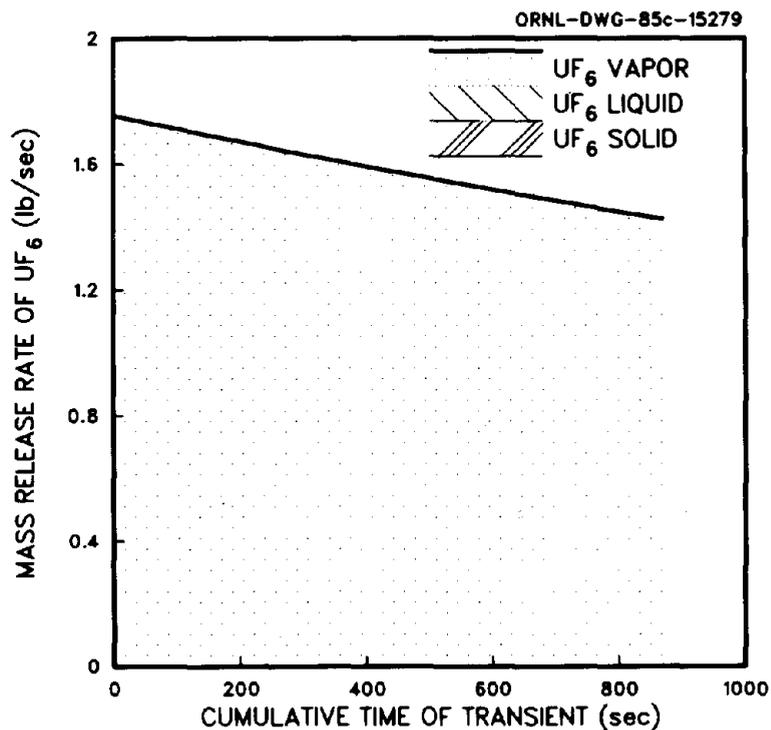
Fig. 37. Mass release rate of UF$_6$ from a 48Y (14-ton) cylinder following the rupture of a pigtail (Example 3, Case 3). The pigtail length is 4 ft and the valve is in the 11 o'clock position.

5.2 RELEASE INSIDE A COMPARTMENT

This section illustrates the use of the transient compartment models FODRFT and INDRFT. Input for these two models is almost identical, as will be illustrated in Example 4 which uses input obtained directly from the CYLIND simulation of Example 2. An alternative input data set for the same problem as Example 4 is illustrated by Example 5.

Example 4

Problem statement. Assume the release described in Example 2 occurs in a large room having a volume of 500,000 ft^3 and a floor area of 12,500 ft^2. The room air temperature is initially 90°F. Hot equipment in the room has a surface area of 2000 ft^2 and an average surface temperature of 120°F. The ambient conditions are 80°F, 14.7 psia, and 60% relative humidity. Compare the amount of uranium released if the room is ventilated in a forced-draft mode (initial pressure = 14.75 psia) vs an induced-draft mode (initial pressure = 14.65 psia). Also contrast results obtained by assuming UF$_6$ solids remain airborne and vaporize after flashing vs falling out immediately to the floor of the room. The blower flow rate for all cases is 80,000 acfm.

Compartment model input. The following four cases are outlined in the problem statement.

Case	Ventilation mode	Initial Pressure (psia)	UF$_6$ solids	Model
1	Force	14.75	Airborne	FODRFT
2	Induced	14.65	Airborne	INDRFT
3	Forced	14.75	Floor	FODRFT
4	Induced	14.65	Floor	INDRFT

Building schematics showing the initial conditions cited in the problem statement for forced- and induced-draft ventilation modes are shown in Figs. 38 and 39, respectively. For Cases 1 and 2, the source-term input file generated by CYLIND for Example 2, Case 2 was used directly. For Cases 3 and 4, the source-term file was modified by replacing the solid release rates generated by CYLIND with zeros. With the exception of the title and drawing numbers, Cases 1 and 3 use the same FODRFT input file, whereas Cases 2 and 4 use the same INDRFT input file. These input files are shown in Table 27.

Input file requirements for FODRFT and INDRFT are listed in Tables 18 and 19, respectively (see Sect. 4.6). These files follow the same structure except for Card 4 and some provisions noted in Card 3 of the INDRFT input file. The first line (Card 1) in each input file is the title. The second line (Card 2) lists the ambient temperature (80), pressure (14.7), and relative humidity (60). The third line (Card 3) lists the compartment temperature (90), pressure [14.75 for FODRFT (Cases 1 and 3) and 14.65 for INDRFT (Cases 2 and 4)], volume (5.D5), and floor area (12500). The fourth line of input for Cases 1 and 3 (Card 4 of FODRFT input) gives the inlet blower flow rate (8.D4); the trailing zeros are ignored (they were copied over from the INDRFT input). The fourth line of input for Cases 2 and 4 (Card 4 of INDRFT input) gives the exhaust blower rate (8.D4), whereas the trailing zeros along with a specified internal pressure of 14.65 psia indicate that a resistance term is calculated from pressure and flow conditions rather than from the inlet area and

ORNL—DWG 85-14583
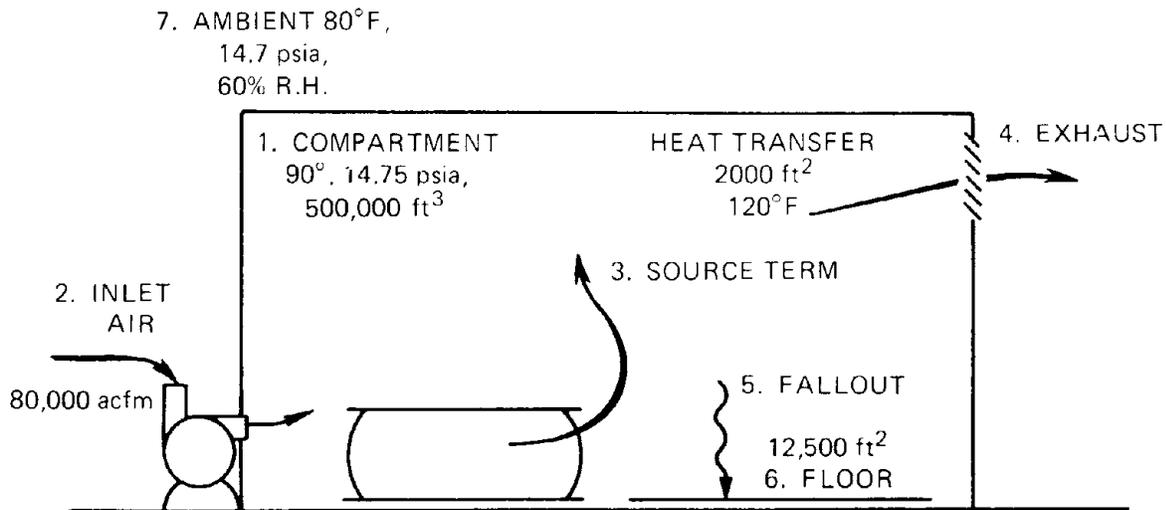
Fig. 38. Building schematic and initial conditions from Example 4 for
simulation of a release in a forced-draft ventilated room.

ORNL—DWG 85-14581
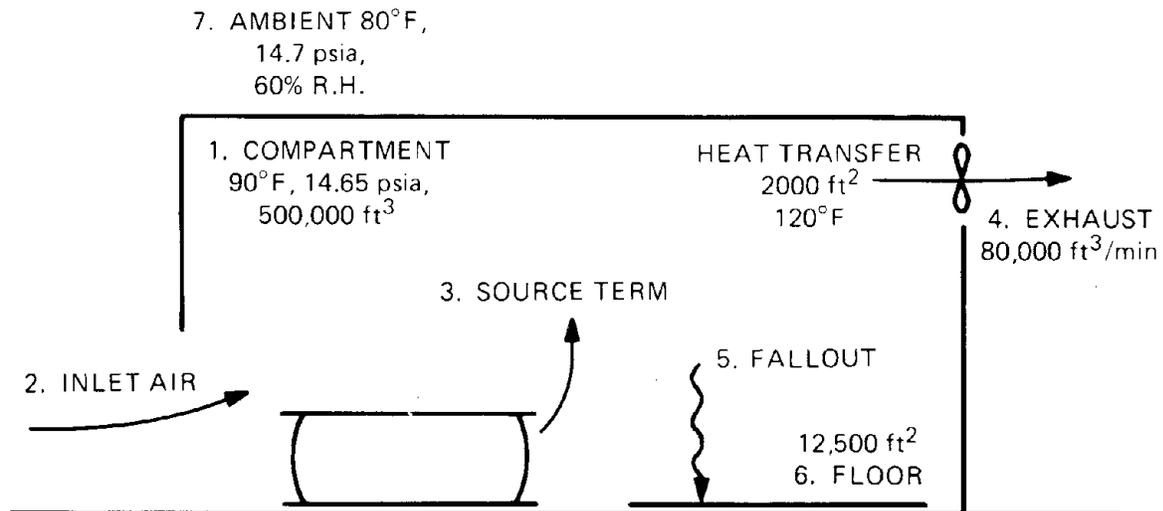
Fig. 39. Building schematic and initial conditions from Example 4 for
simulation of a release in an induced-draft ventilated room.

resistance coefficient (see Sect. 4.2.1). Note that trailing zeros in excess of the input required (e. g.,
in Cases 1 and 3) are not detrimental to program execution; however, exclusion of trailing zeros
(e.g., in Cases 2 and 4) when an input value is required will cause execution errors because input is
read in free format. (INDRFT would take the values 2000 and 120 from the next line if the zeros
were missing.) The next three lines of input are identical for all cases. The fifth line (Card 5)
specifies the heat transfer surface area (2000) and temperature (120) as well as the cooling rate

Table 27. Input files for simulating the release described in Example 4

```
L  C                            COLUMN
I  A
N  R        1         2         3         4         5         6
E  D  123456789012345678901234567890123456789012345678901234567890123456789012

      INPUT FOR CASE 1

 1  1  EX. 4, CASE 1. RELEASE (EX. 2.2), FORCED VENT, AIRBORNE SOLIDS
 2  2  80,14.7,60
 3  3  90,14.75,5.D5,12500
 4  4  8.D4,0,0
 5  5  2000,120,0
 6  6  22,0,0,0
 7  8  1,3600,120
 8  9  ORNL-DWG-85c-15280$
 9  9  ORNL-DWG-85c-15281$
10  9  ORNL-DWG-85c-15282$
11  9  ORNL-DWG-85c-15283$
12  9  ORNL-DWG-85c-15284$
13  9  ORNL-DWG-85c-15285$

      INPUT FOR CASE 2

 1  1  EX. 4, CASE 2. RELEASE (EX. 2.2), INDUCED VENT, AIRBORNE SOLIDS
 2  2  80,14.7,60
 3  3  90,14.65,5.D5,12500
 4  4  8.D4,0,0
 5  5  2000,120,0
 6  6  22,0,0,0
 7  8  1,3600,120

      INPUT FOR CASE 3

 1  1  EX. 4, CASE 3. RELEASE (EX. 2.2), FORCED VENT, SOLIDS TO FLOOR
 2  2  80,14.7,60
 3  3  90,14.75,5.D5,12500
 4  4  8.D4,0,0
 5  5  2000,120,0
 6  6  22,0,0,0
 7  8  1,3600,120

      INPUT FOR CASE 4

 1  1  EX. 4, CASE 4. RELEASE (EX. 2.2), INDUCED VENT, SOLIDS TO FLOOR
 2  2  80,14.7,60
 3  3  90,14.65,5.D5,12500
 4  4  8.D4,0,0
 5  5  2000,120,0
 6  6  22,0,0,0
 7  8  1,3600,120
```

(0). Because the source term is an input file generated by CYLIND, the sixth line (Card 6) specifies a release type of 22, the number of releases and the flash basis both as zero (the value entered is ignored, but a value must be entered), and use of the default molecular weight (0). Card 7 is not included because a source-term data file is used. The seventh line (Card 8) specifies the simulation interval to be used internally by FODRDT and INDRFT (1), the duration of the simulation (3600) and the print interval (120). The last six lines (Card 9) of Case 1 input provide drawing numbers for plots illustrating simulation results.

Results. Results of the four cases outlined in this example are given in Table 28. Ventilation mode makes little difference in the total amount of uranium released; however, the assumptions concerning the initial disposition of UF_6 solids result in significant differences. These latter assumptions bound expected release behavior. Complete results from all four cases are included in Appendix C.4. Figures 40 through 45 are results from Case 1 and were plotted using COMPLT (see Sect. 4.7).

Example 5

Problem statement. Repeat Example 4, Case 1 without using the input file produced by CYLIND.

Table 28. Results of Example 4. Uranium may be
in the form either UF_6 or UO_2F_2

Time (Sec)	UF_6 solids airborne (lb)		UF_6 solids to floor (lb)	
	Case 1 FODRFT	Case 2 INDRFT	Case 3 FODRFT	Case 4 INDRFT
Uranium released to atmosphere				
360	2,970	2,720	1,570	1,370
720	8,720	8,310	4,350	4,030
1,080	13,260	12,840	6,250	6,070
1,440	14,410	14,270	6,780	6,670
1,800	14,740	14,680	6,930	6,840
2,160	14,830	14,790	6,970	6,890
2,520	14,860	14,830	6,980	6,900
3,600	14,870	14,840	6,980	6,900
Uranium deposited on floor				
3,600	2,440	2,470	10,320[a]	10,400[a]

[a]A total of 17,300 lb of uranium was released from the cylinder in Example 2, Case 2. These values are obtained by difference because the solids could not be included in the input data file.
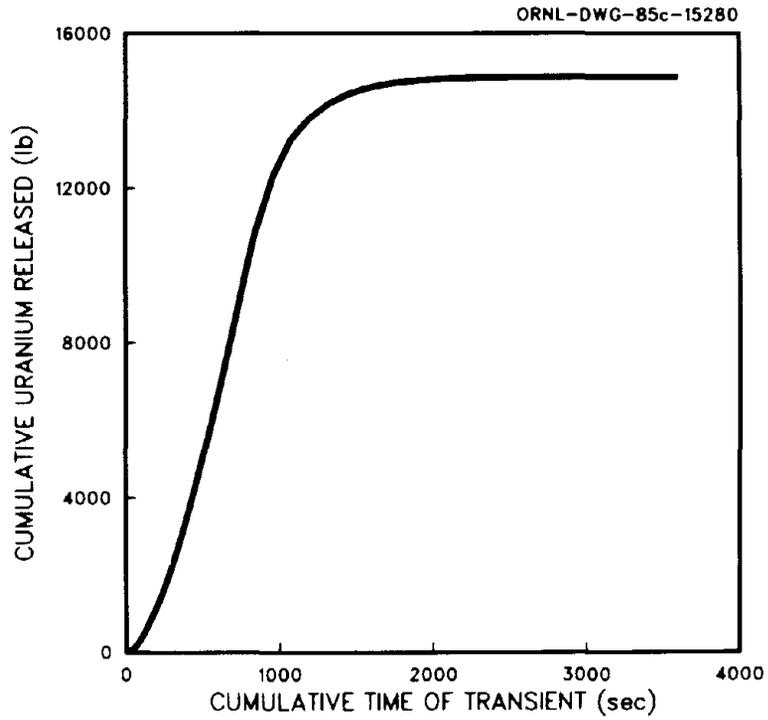
Fig. 40. Cumulative uranium released from a compartment (Example 4, Case 1).
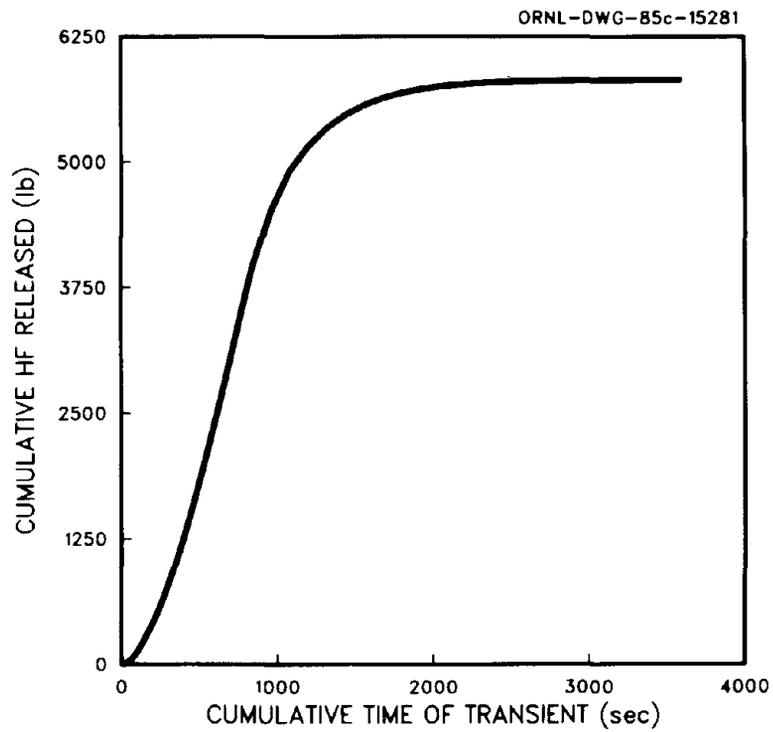
Fig. 41. Cumulative HF released from a compartment (Example 4, Case 1).
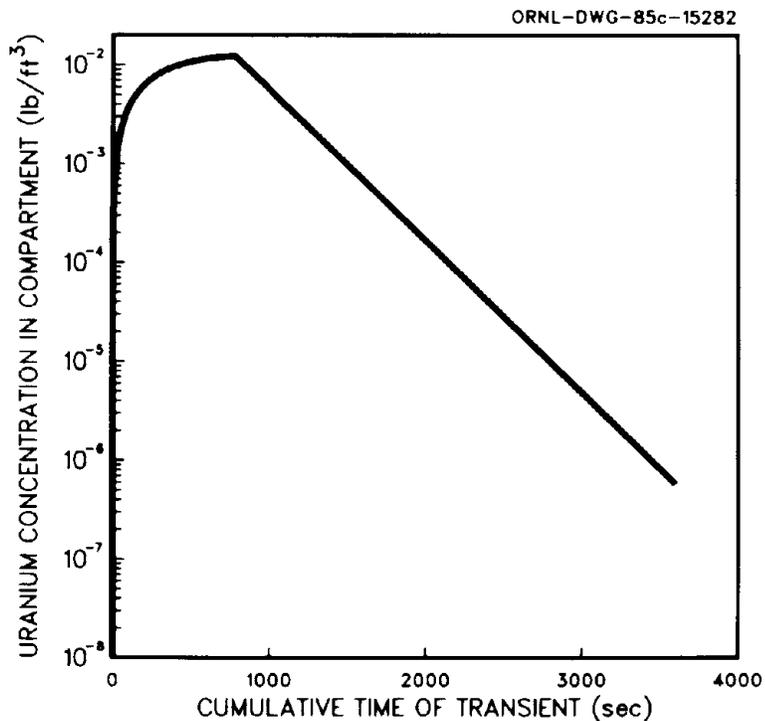
Fig. 42. Uranium concentration inside a compartment (Example 4, Case 1).
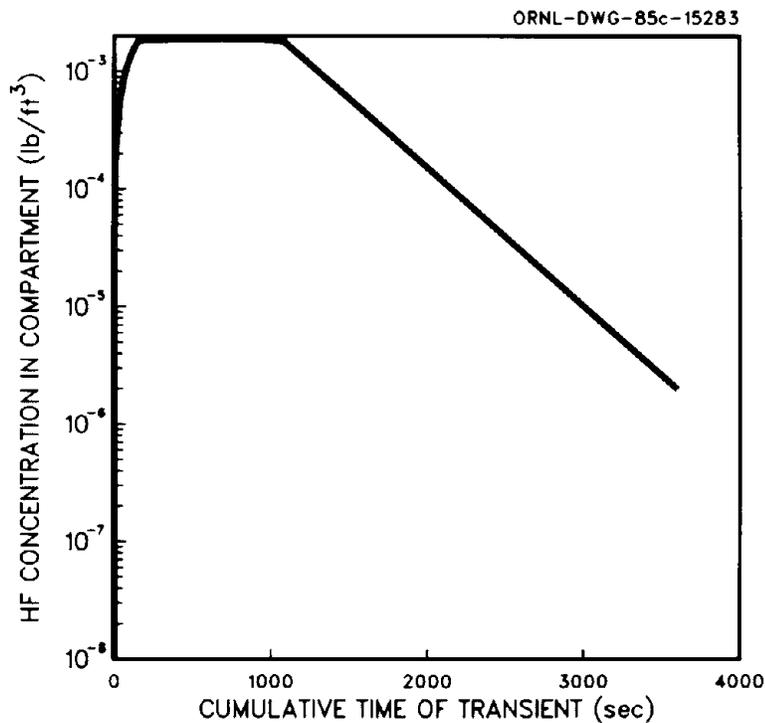
Fig. 43. HF concentration inside a compartment (Example 4, Case 1).

ORNL-DWG-85c-15284
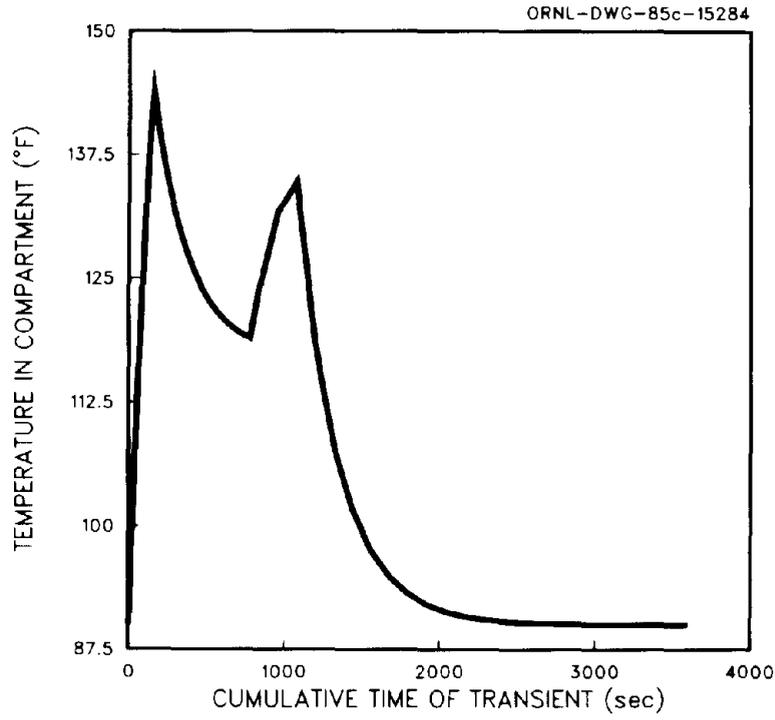
Fig. 44. Compartment temperature (Example 4, Case 1).

ORNL-DWG-85c-15285
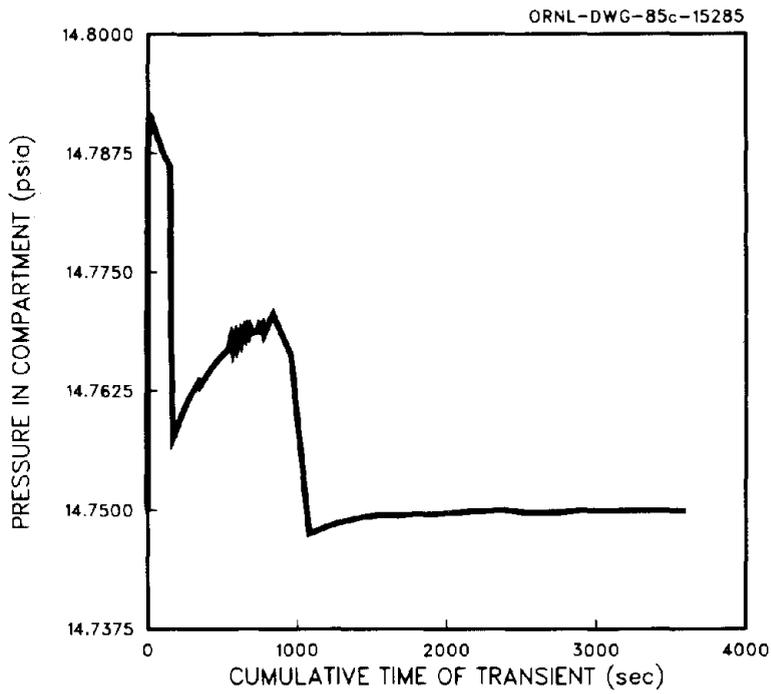
Fig. 45. Compartment pressure (Example 4, Case 1).

Preliminary calculations. Another option available in the compartment models is to specify the quantity of UF_6 released and the duration of the release in increments. Such an input format may be more appropriate for scoping studies. In this problem, information on the release of UF_6 through a large breach in a 48Y cylinder is available in Table 24 and Figs. 34 and 35. The mass release rate of UF_6 decreases slowly with no significant change until the end of the release (see Fig. 35). This obvious change at 740 sec (see Table 24) is used as one break point in developing the incremental release data. Other break points are arbitrarily selected. The following data on the mass and temperature of UF_6 in the cylinder is taken from Table 24, then the duration and mass released for each increment are obtained by difference and the temperature by averaging. Note that the final mass at 780 sec is obtained by subtracting the product of the mass rate and the simulation time interval (20 sec) from the last total mass printed at 760 sec.

Time (sec)	Mass of UF_6 in cylinder (lb)	Temperature (°F)	Increment	Time interval (sec)	Mass released (lb)	Temperature (°F)
0	25,900	190.0				
			1	200	6,709	189.6
200	19,191	189.3				
			2	200	6,639	188.7
400	12,552	188.2				
			3	200	6,538	187.3
600	6,014	186.5				
			4	100	4,728	185.1
740	1,286	183.8				
			5	40	977	183.0
780	309	<183				

FODRFT input. The input data file format is given in Table 17. The input file for this example is shown in Table 29. The first line (Card 1) contains the title. The second through fifth lines, as well as the last line (Cards 2 through 5 and Card 8), are identical to input for case 1 of Example 4. The sixth line (Card 6) specifies that a liquid release of UF_6 with a vapor/solid source term (i.e., solids remain airborne) is to be simulated (-7); the number of release increments (5); the basis for flashing the UF_6 (1), which is isenthalpic; and use of the default molecular weight for UF_6 (0). The next five lines correspond to Card 7. Each line gives the incremental duration, mass released, and temperature as shown in the preceding spot table as well as a zero, which will default to the vapor pressure.

Results. For practical purposes, the results of this example are almost identical to the results of Example 4, Case 1. Complete output from FODRFT is given in Appendix C.5.

5.3 RELEASE INTO A VENTILATION SYSTEM

This section illustrates the use of BATCH to simulate the release of UF_6 into a ventilation system.

Table 29. Input data to FODRFT for Example 5

```
L  C                        COLUMN
I  A
N  R        1         2         3         4         5
E  D    12345678901234567890123456789012345678901234567890123

1  1    EX. 5. REPEAT OF EX. 4.1 W/ RELEASE (EX. 2) SEGMENTED
2  2    80,14.7,60
3  3    90,14.75,5.D5,12500
4  4    8.D4,0,0
5  5    2000,120,0
6  6    -7,5,1,0
7  7    200,6709,189.6,0
8  7    200,6639,188.7,0                        -
9  7    200,6538,187.3,0
10 7    140,4728,185.1,0
11 7    40,977,183.,0
12 8    1,3600,120
```

Example 6

Problem statement. Assume UF_6 vapor initially at 300'F and 50 psia is released at a rate of 50 lb/min into a ventilation system duct. The inlet blower rate to the duct is 1000 acfm and the inlet air conditions in the duct immediately downstream of the blower are 90°F and 14.8 psia. Ambient conditions are 80°F, 14.7 psia, and 60% relative humidity. Assuming isenthalpic conditions along the duct, what are the temperature, volume flow rate, and composition of the mixed stream exhausted from the duct.

BATCH input. The batch program is run interactively. Input for this example is shown in Table 30. Underlined text is supplied by the user. Note that for this example, when the volume of the compartment is requested, the value input corresponds to the volume flow rate (acfm), and, when the mass of the source term is requested, the release rate (lb/min) is entered. Also note that the default molecular weight for UF_6 is used and that the output basis is specified as an "open" compartment.

Results. Complete output for this example is shown in Table 31. The final temperature is 192.3°F, and the exhaust flow rate is 1274 ft^3/min. The final composition is the following.

Component	Flow Rate (lb/min)	Weight fraction
Air	71.2	0.583
HF (v)	2.1	0.017
UF_6 (v)	40.9	0.335
UO_2F_2 (s)	7.9	0.065
	122.1	1.000

Table 30. Printout of interactive execution of BATCH on the ORNL PDP-10 for Example 6 (Underlines have been added to highlight user input)

```
.RU BATCH



     WARNING: OUTPUT APPEARS IN FOR06.DAT


     ENTER TITLE (MAXIMUM OF 48 CHARACTERS).
EXAMPLE 6. UF6 VAPOR RELEASE TO VENTILATION DUCT
     ENTER COMPARTMENT TEMPERATURE (F), PRESSURE (PSIA), AND
     VOLUME (FT**3).
90,14.8,1000
     ENTER AMBIENT TEMPERATURE (F), PRESSURE (PSIA), AND RELATIVE
     HUMIDITY (%)
80,14.7,60
     ENTER SOURCE TYPE (4=HF LIQUID, 5=HF VAPOR, 7=UF6 LIQUID WITH VAPOR
     SOURCE TERM AND SOLIDS IGNORED IN HEAT BALANCE, -7=UF6 LIQUID WITH
     VAPOR PLUS SOLID SOURCE TERM, 8=UF6 VAPOR), TEMPERATURE (F), AND
     PRESSURE (PSIA--A NEGATIVE PRESSURE OR A LIQUID RELEASE DEFAULTS
     TO THE VAPOR PRESSURE CORRESPONDING TO THE SOURCE TEMPERATURE).
8,300,50
     ENTER UF6 MOLECULAR WEIGHT (A VALUE LESS THAN 100 DEFAULTS TO
     352.025) AND BASIS FOR FLASH (0=ISENTROPIC, 1=ISENTHALPIC).
0,1
     ENTER MASS OF SOURCE TERM (LB).
50
     ENTER OUTPUT BASIS (1=CLOSED COMPARTMENT, 4=OPEN COMPARTMENT WITH
     FINAL PRESSURE EQUAL TO AMBIENT PRESSURE).
4
STOP

END OF EXECUTION
CPU TIME: 0.36   ELAPSED TIME: 1:14.83
EXIT
```

Table 31. Results of Example 6

CASE: EXAMPLE 6. UF6 VAPOR RELEASE TO VENTILATION DUCT

AMBIENT CONDITIONS

TEMPERATURE	80.000	DEG F
PRESSURE	14.700	PSIA
RELATIVE HUMIDITY	60.0	%
WATER VAPOR : MOIST AIR	0.02055	MOLE/MOLE

INITIAL COMPARTMENT CONDITIONS

TEMPERATURE	90.000	DEG F
PRESSURE	14.800	PSIA
VOLUME	1000.0	FT**3
MASS OF AIR V	71.2	LB
MASS OF H2O V	0.9	LB

SOURCE TERM: UF6 VAPOR

TEMPERATURE	300.000	DEG F
PRESSURE	50.000	PSIA
TOTAL MASS OF SOURCE	50.0	LB
MOLECULAR WEIGHT	352.025	LB/LB MOLE
BASIS FOR EXPANSION OF VAPOR	ISENTHALPIC	
TEMPERATURE AFTER EXPANSION	300.000	DEG F
MASS OF UF6 V	50.0	LB

FINAL CONDITIONS (OPEN COMPARTMENT)

TEMPERATURE	192.306	DEG F
PRESSURE	14.700	PSIA
VOLUME	1274.1	FT**3
MASS OF AIR V	71.2	LB
MASS OF HF V	2.1	LB
MASS OF UF6 V	40.9	LB
MASS OF UO2F2 S	7.9	LB
DENSITY OF FINAL MIXTURE	0.09585	LB/FT**3

REFERENCES

Barber, E. J. 1979. K/ET-194, Supplement 3, Fig. 3, Oak Ridge Gaseous Diffusion Plant, Oak Ridge, Tenn.

Barber, E. J. 1983. Oak Ridge Gaseous Diffusion Plant, Oak Ridge, Tenn., personal communication to W. R. Williams, Oak Ridge Natl. Lab., Oak Ridge, Tenn., July 13. Barber referred to K/ET-698 and K/ET-273.

Beckerdrite, J. M., Powell, D. R., and Adams, E. T. 1983. "Self-Association of Gases. 2. The Association of Hydrogen Fluoride," *J. Chem Eng. Data* **28**, 287–293.

Brosheer, J. C., Lenfesty, F. A. and Elmore, K. L. 1947. "Vapor Pressre of Hydrofluoric Acid Solutions," *Ind. Eng. Chem* **39**, 423–27.

Churchill, S. W. 1977. "Friction-Factor Equation Spans All Fluid-Flow Regimes." *Chem. Eng.* **84**(24), 91–92

Crane Company 1980. *Flow of Fluids*, Technical Papaer 410M.

Dewitt, R. 1960. *Uranium Hexafluoride: A Survey of the Physico-Chemical Properties*, GAT-280, Goodyear Atomic Corporation, Portsmouth, Ohio.

Ginoux, J. J., ed. 1978. *Two-Phase Flows and Heat Transfer*, Hemisphere Publishing Corporation, Washington, D.C., pp. 20–22.

Perry, R. H. et al. 1973. *Chemical Engineer's Handbook*, 5th Ed., McGraw-Hill Book Company, New York, pp. 5–43 through 5–44.

Popov, M. M., Kostylev, F. A., and Karpova, T. F. 1957. "The Heat of Formation of Uranyl Fluoride and the Heats of Reactions of Hexa- and Tetra-Fluorides of Uranium with Water," *J. Inorg. Chem. (USSR)* **II**(1), 9–12. (Printed in translation by the Israel Program for Scientific Translations, AEC-tr-4434, p. 9–15).

Reid, R. C., Prausnitz, J. M., and Sherwood, T. K. 1977. *The Properties of Gases and Liquids*, 3d Ed., McGraw-Hill Book Company, New York.

Siman-Tov, M. et al. 1984. *Scenarios and Analytical Methods for UF6 Releases at NRC-Licensed Fuel Cycle Facilities*, NUREG/CR-3139 (ORNL/ENG/TM-25), Oak Ridge Natl. Lab., Oak Ridge, Tenn.