Designation: F2815 – 10 (Reapproved 2014)

Standard Practice for Chemical Permeation through Protective Clothing Materials: Testing Data Analysis by Use of a Computer Program[1]

This standard is issued under the fixed designation F2815; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers the calculations of all the permeation parameters related to Test Method F739, ISO 6529, and Practice D6978 standards by use of a computer program, referred to as "Permeation Calculator" (DHHS (NIOSH) Publication No. 2007 – 143c).[2,3]

1.2 The practice is applicable to both open loop and closed loop permeation tests. The closed loop test includes continuous sampling and discrete sampling. The discrete sampling includes tests when sample volume is replaced and also when sample volume is not replaced. For an open loop permeation test, the computer program also allows permeation data files with variable sampling flow rate. Refer to Test Method F739 for more details about the different types of the permeation testing systems.

1.3 This practice is applicable to the most typical permeation behavior, that is, Type A, where the permeation rate stabilizes at a "steady-state" value. It does not apply to the other types of permeation behaviors. Refer to Test Method F739 for more details about the various permeation behaviors.

1.4 This practice is not applicable to Test Method F1383 because the permeation behavior is different under conditions of intermittent contact than under conditions of continuous contact.

1.5 This practice does not address the procedure of permeation testing. Refer to Test Method F739, ISO 6529, or Practice D6978 for the procedures in detail if needed.

2. Referenced Documents

2.1 *ASTM Standards:*[4]

D6978 Practice for Assessment of Resistance of Medical Gloves to Permeation by Chemotherapy Drugs

F739 Test Method for Permeation of Liquids and Gases through Protective Clothing Materials under Conditions of Continuous Contact

F1194 Guide for Documenting the Results of Chemical Permeation Testing of Materials Used in Protective Clothing

F1383 Test Method for Permeation of Liquids and Gases through Protective Clothing Materials under Conditions of Intermittent Contact

F1494 Terminology Relating to Protective Clothing

2.2 *ISO Standards:*[5]

ISO 6529 Protective Clothing—Protection against Chemicals—Determination of Resistance of Protective Clothing Materials to Permeation by Liquids and Gases

3. Terminology

3.1 *Definitions:*

3.1.1 *analytical technique, n*—a procedure whereby the concentration of a challenge chemical in a collection medium is quantitatively determined.

3.1.1.1 *Discussion*—The detailed steps for these procedures are often specific to individual chemical and collection medium combinations. Applicable techniques include but are not limited to flame ionization, photo ionization, electro-chemical, and ultraviolet and infrared spectrophotometry, gas and liquid chromatography, colorimetry, length-of-stain detector tubes, and radionuclide tagging/detection counting.

3.1.2 *breakthrough detection time, n*—the elapsed time measured from the start of the test to the sampling time that immediately precedes the sampling time at which the test chemical is first detected.

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[1] This practice is under the jurisdiction of ASTM Committee F23 on Personal Protective Clothing and Equipment and is the direct responsibility of Subcommittee F23.30 on Chemicals.

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[2] Gao P, Weise T, and Tomasovic B [2009] Development of a computer program for permeation testing data analysis. *Journal of Occupational & Environmental Hygiene*, 6(6): 363-373.

[3] The computer program is available at no-charge either on the National Institute for Occupational Safety and Health website at http://www.cdc.gov/niosh/npptl/PermeationCalculator/permeationcalc.html or on CD by request. Phone: 1-800-CDC-INFO (1-800-232-4636), Fax: 1-888-232-6348, or E-mail: CDCInfo@cdc.gov.

[4] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[5] Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, http://www.ansi.org.

3.1.2.1 *Discussion*—For this practice the breakthrough detection time is calculated by a computer algorithm and is dependent on the sensitivity of the analytical method.

3.1.3 *breakthrough point, n*—the point at which the breakthrough occurs during a permeation test.

3.1.3.1 *Discussion*—The computer program determines the breakthrough point based on the approach shown in 6.2.1 through 6.2.4. The breakthrough point is determined as the first data point used in the last slope's calculation as described in 6.2.3. Note that BP is not an absolute number but rather is dependent on the sensitivity of the analytical method.

3.1.4 *closed loop, adj*—refers to a testing mode in which the collection medium volume is fixed.

3.1.5 *collection medium, n*—a liquid, gas, or solid that absorbs, adsorbs, dissolves, suspends, or otherwise captures the challenge and does not affect the measured permeation.

3.1.6 *minimum breakthrough detection time, n*—the time in minutes measured from the start of the test to the sampling time at which the permeation rate reaches 0.01 µg/cm^2/min.

3.1.7 *minimum detectable mass permeated, n*—the smallest mass of test chemical that is detectable with the complete permeation test system.

3.1.7.1 *Discussion*—This value is not necessarily the sensitivity of the analytical instrument.

3.1.8 *minimum detectable permeation rate, n*—the lowest rate of permeation that is measurable with the complete permeation test system.

3.1.8.1 *Discussion*—This value is not necessarily the sensitivity of the analytical instrument.

3.1.9 *normalized breakthrough detection time, n*—in an open-loop test, it is the elapsed time at which the permeation rate reaches 1.0 µg/ cm^2/min. In a closed-loop test, it is the time at which the mass of chemical permeation reaches 2.5 µg/cm^2.

3.1.10 *open loop, adj*—refers to a testing mode in which fresh collection medium flows continuously through the collection chamber of the test cell.

3.1.11 *penetration, n*—for chemical protective clothing, the movement of substances through voids in a chemical protective clothing material or item on a non-molecular level.

3.1.11.1 *Discussion*—Voids include gaps, pores, holes and imperfections in closures, seams, interfaces and protective clothing materials. Penetration does not require a change of state; solid chemicals move through voids in the materials as solids, liquids as liquids, and gases as gases. Penetration is a distinctly different mechanism from permeation.

3.1.12 *permeation, n*—for chemical protective clothing, the movement of chemicals as molecules through protective clothing materials by the processes of (*1*) absorption of the chemical into the contact surface of the material, (*2*) diffusion of the absorbed molecules throughout the material, and (*3*) desorption of the chemical from the opposite surface of the material.

3.1.12.1 *Discussion*—Permeation is a distinctly different mechanism from penetration.

3.1.13 *protective clothing, n*—an item of clothing that is specifically designed and constructed for the intended purpose of isolating all or part of the body from a potential hazard; or isolating the external environment from contamination by the wearer of the clothing.

3.1.14 *standardized breakthrough time, n*—the first time at which the permeation rate reaches 0.1 µg/cm^2/min.

3.1.15 *steady-state permeation rate, n*—a constant rate of permeation that occurs after breakthrough when all forces affecting permeation have reached equilibrium.

3.1.16 *test chemical, n*—solid, liquid, gas or mixture thereof, used to evaluate the performance of a protective clothing material.

4. Summary of Practice

4.1 The computer program used in this practice calculates all the permeation parameters listed in Test Method F739, ISO 6529, and Practice D6978, including standardized breakthrough time, normalized breakthrough detection time, breakthrough detection time, minimum breakthrough detection time (if applicable), steady-state permeation rate, cumulative permeation at a given elapsed time, elapsed time at a given cumulative permeation, average permeation rate, and maximum permeation rate if it is an open loop permeation test.

4.2 The operation of the computer program involves the following steps:

4.2.1 *Data Input to the Computer Program*—Input a permeation testing data file that contains data points in time versus concentration. The data must be in a spreadsheet software file with a minimum of seven data points before the breakthrough point and the total number of data points can not exceed 5000. The number of significant figures used for the input data will affect the number of significant figures reported for the permeation parameters, so appropriate significant figures should be used. Refer to Appendix X1 for details in data file requirements.

4.2.2 *Analysis*—After importing the data file and entering required information, the program determines the permeation parameters based on a series of strategies and approaches.

4.2.3 *Output*—Upon completion, the program displays all the permeation parameters together with relevant information and the permeation curve in a spreadsheet software or a text file-formatted report.

5. Significance and Use

5.1 Data analysis for chemical protective clothing permeation testing involves a number of equations and experimental factors. Possible calculation errors are critical issues when determining permeation parameters. Because the calculations of some of the permeation parameters are mathematically complex, this computer program will be useful.

5.2 This practice is to help researchers and industrial hygienists avoid labor intensive hand calculations of the permeation parameters. From a standardization point of view, this practice prevents variability or inconsistency caused by different experimenters thus ensuring identical permeation parameters or results will be obtained from a given permeation test data file.

5.3 Protective clothing manufacturers worldwide will benefit since they must inform customers about the permeation parameters of their products in a consistent manner. The practice will also help diagnostic laboratories and research centers involved in the chemical protective clothing testing.

6. Calculation

6.1 *Symbols*—The following symbols are used in the calculations, where:

a	=	a coefficient for a polynomial equation, Eq 1-3 and Eq 15; an arbitrary data point before data point b, Eq 6-10,
A	=	area of the material specimen contacted, cm^2, Eq 4, Eq 5, Eq 11, Eq 13, and Eq 14,
b	=	a constant for a polynomial equation, Eq 1-3 and Eq 15; an arbitrary data point after data point a, Eq 10,
c	=	a constant for a polynomial equation, Eq 1,
C	=	concentration of test chemical in collection medium, µg/L, Eq 11, Eq 13, and Eq 14,
$\bar{C}$	=	average concentration of test chemical in collection medium, µg/L, Eq 5,
CP	=	cumulative permeation beginning with initial chemical contact, $µg/cm^2$, Eq 6-11, Eq 13, and Eq 14,
F	=	flow rate of collection medium through the permeation cell, L/min, Eq 5,
i	=	data point, Eq 11-14; data point immediately before data point a or b, Eq 6-9,
m	=	a collection or a series of data points i, Eq 7 and Eq 9,
n	=	total number of data points i, Eq 11, Eq 13, and Eq 14,
P	=	permeation rate, $µg/cm^2/min$,
$\bar{P}$	=	average permeation rate for the time interval T_a to T_b, $µg/cm^2/min$, Eq 10,
R	=	correlation coefficient of a regression analysis,
$SSPR$	=	steady-state permeation rate, $µg/cm^2/min$, Eq 4 and Eq 5,
T	=	elapsed time, min, Eq 6-10,
V_i	=	remaining medium volume at t_i, Eq 12,
V_s	=	volume of discrete sample removed from the collection medium, L, Eq 11-Eq 14,
V_t	=	total volume of the collection medium, L, Eq 4, Eq 12-Eq 14,
x	=	value of x axis in a permeation curve, min, and
y	=	value of y axis in a permeation curve, µg/L, $µg/cm^2$, or $µg/cm^2/min$.

6.2 *Breakthrough detection time for open-loop permeation test and closed-loop permeation test with continuous sampling:*

6.2.1 Calculate the slope and regression correlation coefficient centered on each data point n starting at n = 8, by performing a linear regression for points n-7 to n+7.

6.2.2 Calculate the slope between the data point closest to 50 % and the data point closest to 90 % of the maximum concentration, that is, $(y_{90}-y_{50})/(x_{90}-x_{50})$. This is referred to as the largest slope.

6.2.3 Stop when all of the following conditions are met: (*1*) the slopes calculated in 6.2.1 increase consecutively for seven times, (*2*) each of these seven slopes is greater than 2 % of the largest slope calculated in 6.2.2, and (*3*) the square of the correlation coefficient (R^2) for the last slope is greater than 0.9.

NOTE 1—Conditions (*1*) and (*3*) in 6.2.3 are to filter out the background noise and Condition (*2*) is to avoid determining the breakthrough detection time in a flat region before the real breakthrough. The values specified for these three conditions were optimized using hundreds of permeation data files. Refer to Section 9 on the precision and bias. In addition, adequately predicting the real tendency of the data for determining the breakthrough detection time could not be ensured when using fewer data points for the linear regression analysis.

6.2.4 When the last slope is determined in 6.2.3, select the first data point used in that slope's calculation as the breakthrough point (BP).

6.2.5 Using the data points from BP to the point closest to 15 % of the maximum concentration, perform a regression analysis to obtain a polynomial equation ($y_{BP} = ax^2+bx+c$) as illustrated in Fig. 1(a).

NOTE 2—Calculating breakthrough detection time by taking the regression analysis and then solving the polynomial equation is to avoid reporting the standardized breakthrough time only at the times (T_i) that are shown in the data file but not really at a time within a data collection time interval (same purpose for the calculations of standardized breakthrough time and normalized breakthrough detection time as to be described below).

6.2.6 Calculate the breakthrough detection time by solving the polynomial equation for x. Take the root x1 or x2, whichever is closest to x_{BP}.

6.3 *Standardized breakthrough time:*

6.3.1 *Closed-loop permeation test with continuous sampling:*

6.3.1.1 As shown in Fig. 1(b), for a permeation curve of y ($µg/cm^2$) against x (min), the program performs a regression analysis using a range of data points to obtain a polynomial equation, that is, Eq 1. The first data point is the one with an elapsed time closest to 75 % of the time value for the BP, as determined previously for calculation of the breakthrough detection time, and the last data point is the one with a CP closest to 15 % of the maximum CP.

$$y = ax^2 + bx + c \tag{1}$$

6.3.1.2 Take the derivative to obtain the permeation rate in $µg/cm^2/min$:

$$\frac{dy}{dx} = 2ax + b \tag{2}$$

6.3.1.3 Based on the ASTM definition stated above, let

$$2ax + b = 0.1 \tag{3}$$

6.3.1.4 Solve Eq 3 for the standardized breakthrough time (x). If the calculated x value is outside the time range for the data points used for the regression, repeat the above procedures. The data for the next regression analysis uses the same number of data points but the starting point is incremented by one.

6.3.1.5 Report the value of x determined in 6.3.1.4 as standardized breakthrough time for a closed-loop permeation test once the conditions are satisfied.

6.3.2 *Open-loop permeation test:*

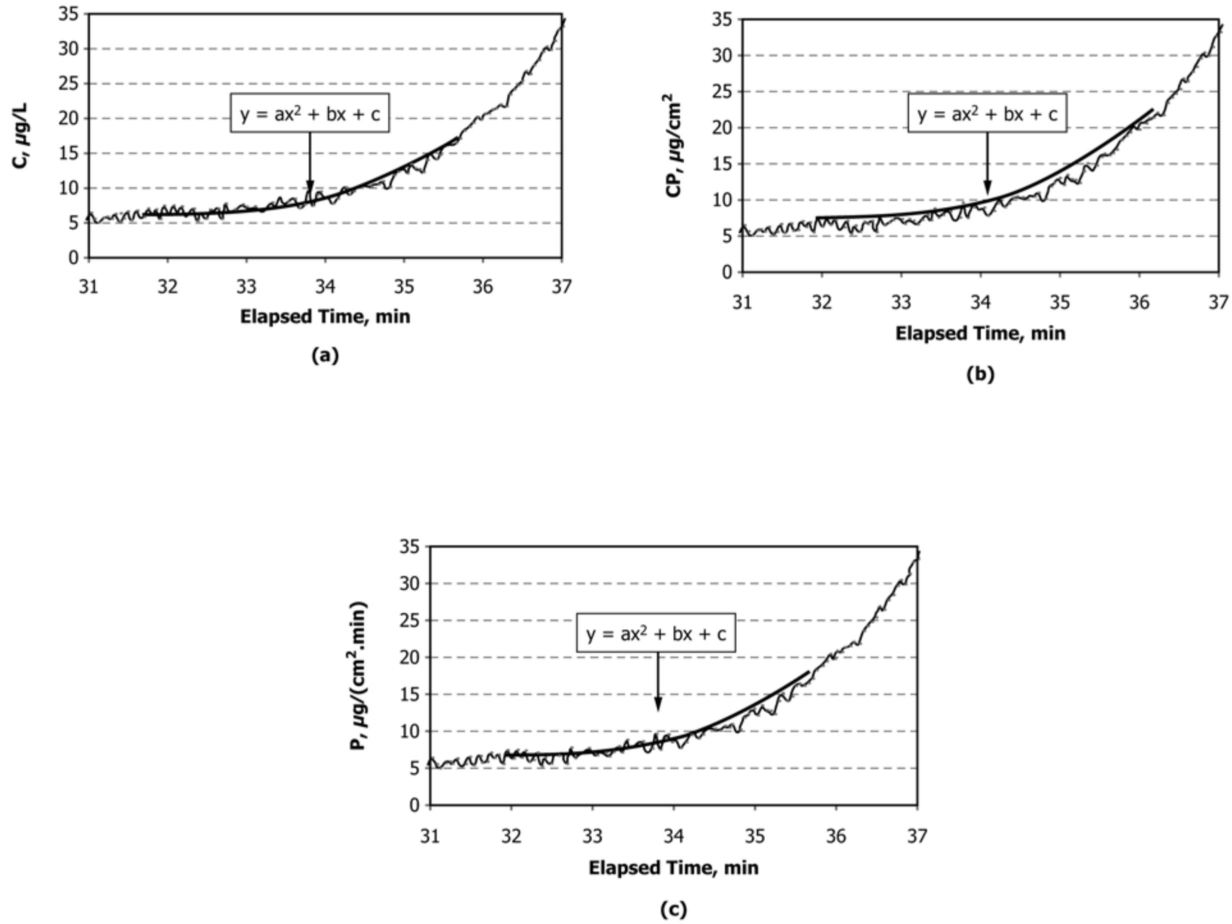


FIG. 1 Determination for Various Breakthrough Times

6.3.2.1 Find two consecutive points where the permeation rate at point i < 0.1 µg/(cm^2*min) and point i+1 ≥ 0.1 µg/(cm^2*min). Select the point with a permeation rate closest to 0.1 µg/(cm^2*min).

6.3.2.2 Perform a regression analysis using 11 data points centered on the selected point from Step 6.3.2.1 to obtain a polynomial equation (0.1 = ax^2+bx+c) as illustrated in Fig. 1(c).

6.3.2.3 Calculate the standardized breakthrough time by solving the polynomial equation. Take the root x1 or x2, whichever is closest to the time of the point determined in 6.3.2.1.

6.4 *Normalized breakthrough detection time:*

6.4.1 *Closed-loop permeation test with continuous sampling:*

6.4.1.1 Find two consecutive points where the cumulative permeation at point i < 2.5 µg/cm^2 and point i+1 ≥ 2.5 µg/cm^2. Select the point with a cumulative permeation closest to 2.5 µg/cm^2.

6.4.1.2 Perform a regression analysis using eleven data points centered on the selected point from Step 6.4.1.1 to obtain a polynomial equation (2.5 = ax^2+bx+c) as illustrated in Fig. 1(b).

6.4.1.3 Calculate normalized breakthrough detection time by solving the polynomial equation. Take the root x1 or x2, whichever is closest to the time of the point determined in 6.4.1.1.

6.4.2 *Open-loop permeation test:*

6.4.2.1 Find two consecutive points where the permeation rate at point i < 1.0 µg/(cm^2*min) and point i+1 ≥ 1.0 µg/(cm^2*min). Select the point with a permeation rate closest to 1.0 µg/(cm^2*min).

6.4.2.2 Perform a regression analysis using eleven data points centered on the selected point from Step 6.4.2.1 to obtain a polynomial equation (1.0 = ax^2+bx+c) as shown in Fig. 1(c).

6.4.2.3 Calculate normalized breakthrough detection time by solving the polynomial equation. Take the root x1 or x2, whichever is closest to the time of the point determined in 6.4.2.1.

6.5 *Steady-state permeation rate (SSPR):*

6.5.1 *Closed-loop permeation test with continuous sampling:*

6.5.1.1 For a permeation curve of *y* (µg/L) against *x* (min), determine the slope of the steady-state region by taking a linear regression of the data points between 65 % and 85 % of the maximum concentration point to obtain the slope. Calculate the SSPR based on Eq 4:

$$SSPR = \frac{Slope * V_t}{A} \tag{4}$$

where slope is in µg/(L*min), V_t is total volume of the collection medium in *L*, and *A* is area of the material specimen contacted in cm^2.

As shown for the example in Fig. 2, the slope for this case is 205.11 µg/(L*min).

6.5.2 *Open-loop permeation test:*

6.5.2.1 Find three data points with the three highest concentrations located in the steady-state region (Fig. 3).

6.5.2.2 Take the average of the three concentrations.

6.5.2.3 Calculate SSPR based on Eq 5:

$$SSPR = \frac{\bar{C} * F}{A} \tag{5}$$

where $\bar{C}$ is the average concentration of test chemical in collection medium in µg/L, *F* is flow rate of fresh collection medium through the permeation cell in L/min, and *A* is area of the material specimen contacted in cm^2.

NOTE 3—In order for the user to determine the SSPR using more data points or remove any outliers, the program not only reports value calculated based on Eq 5 as the SSPR, but also reports the seven highest individual permeation rates.

6.6 *Cumulative permeation (CP_a) at a given elapsed time a:*

6.6.1 *Closed-loop permeation test with continuous sampling:*

6.6.1.1 For the permeation curve of *y* (µg/cm^2) against *x* (min), identify the data point (*i*) immediately before the given elapsed time (*a*), and the next data point (i+1). Add the cumulative permeation (CP) of the first point (*i*) to the resultant of the difference in cumulative permeation for these two points multiplied by the ratio of the difference between the given elapsed time (*a*) and the time (i+1), and divided by the difference in time (i) and time (i+1).

$$CP_a = CP_i + \frac{(CP_{i+1} - CP_i)(T_a - T_i)}{T_{i+1} - T_i} \tag{6}$$

6.6.2 *Open-loop permeation test:*

6.6.2.1 As shown in Fig. 4, the shaded area under the permeation curve of y (µg/(cm^2*min)) against *x* (min) from t_0 to t_a is the cumulative permeation, which is the product of *y* (µg/(cm^2 *min)) and *x* (min) with an unit of µg/cm^2 for cumulative permeation.

6.6.2.2 Calculate the area under the permeation curve (Fig. 4) from time 0 to the point immediately before the given elapsed time (T_a) by adding the area of trapezoids under the curve between consecutive points, using the mean permeation rate between points ([P(m) + P(m+1)]/2) multiplied by the difference in time between points (T(m+1) - T(m)). For the final interval, the proportion of the area of the trapezoid between points i and i+1 is added: (T(a)-T(i))/(T(i+1)-T(i)).

$$CP_a = \sum_{m=0}^{i-1}\left[\frac{1}{2}(P_m + P_{m+1})(T_{m+1} - T_m)\right] + \frac{1}{2}(P_i + P_{i+1}) * (T_{i+1} - T_i) * \frac{(T_a - T_i)}{(T_{i+1} - T_i)}$$

which can be reduced to:

$$CP_a = \sum_{m=0}^{i-1}\left[\frac{1}{2}(P_m + P_{m+1})(T_{m+1} - T_m)\right] + \frac{1}{2}(P_i + P_{i+1}) * (T_a - T_i) \tag{7}$$

NOTE 4—For any intervals with a constant permeation rate, the trapezoid become a rectangular or square where P(m) = P(m+1) but the formula for calculating the areas remains the same.

6.7 *Elapsed time (T_a) at a given cumulative permeation:*

6.7.1 *Closed-loop permeation test with continuous sampling:*

6.7.1.1 For a given cumulative permeation CP_a, rearranging Eq 6, T_a can be expressed as:

$$T_a = T_i + \frac{[T_{i+1} - T_i] * [CP_a - CP_i]}{CP_{i+1} - CP_i} \tag{8}$$

6.7.2 *Open-loop permeation test:*

6.7.2.1 For a given cumulative permeation CP_a, rearranging Eq 7, T_a can be expressed as:

$$T_a = T_i + \frac{2\left\{CP_a - \sum_{m=0}^{i-1}\left[\frac{1}{2}(P_m + P_{m+1})(T_{m+1} - T_m)\right]\right\}}{P_i + P_{i+1}} \tag{9}$$

6.8 *Average permeation rate ($\bar{P}$):*

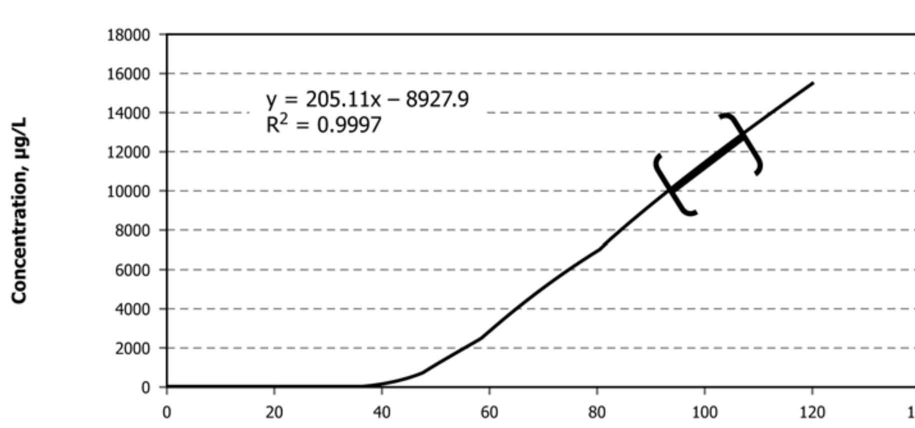


FIG. 2 Determination of Slope for a Closed-Loop Permeation Test

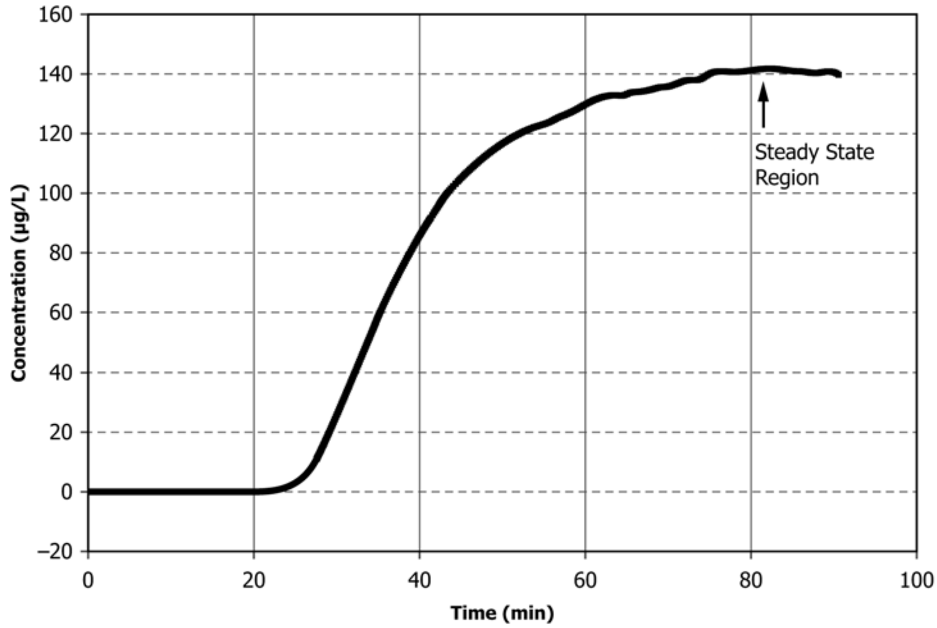


FIG. 3 Calculation of SSPR for an Open-Loop Permeation Test

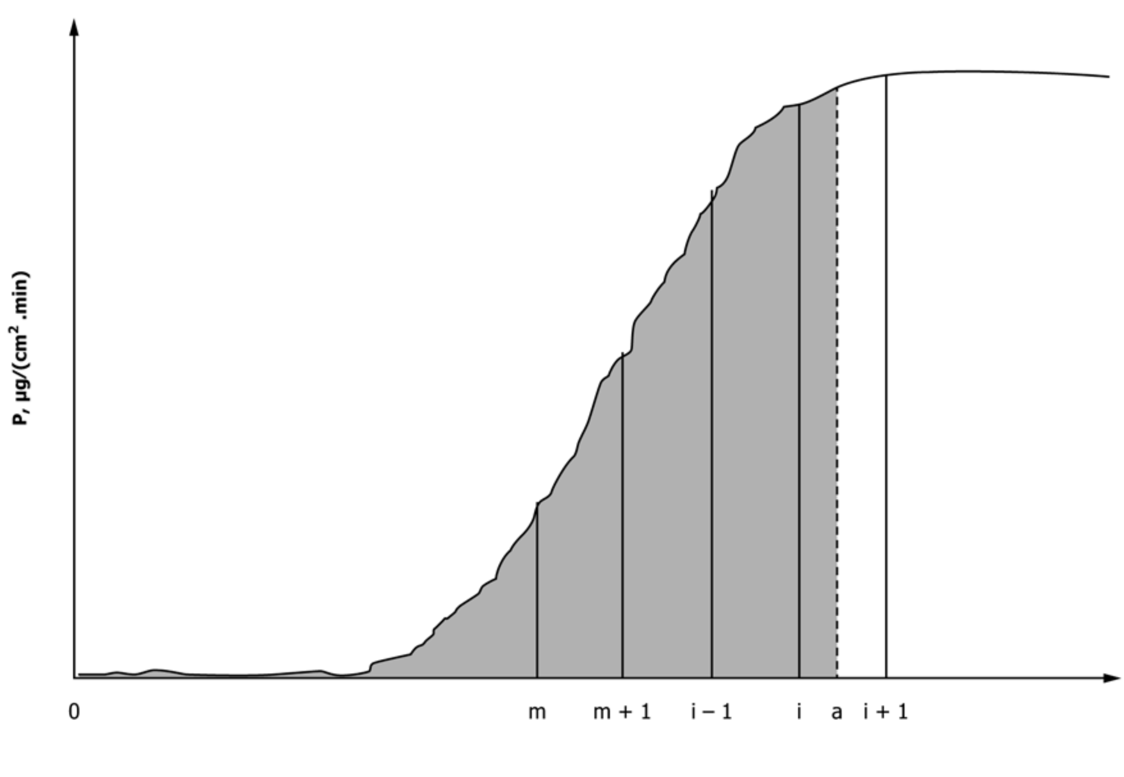


FIG. 4 A Diagram for Calculating the Cumulative Permeation for an Open-Loop Test

6.8.1 *Closed-loop permeation test with continuous sampling:*

6.8.1.1 First, calculate cumulative permeations (CP_a) and (CP_b) using Eq 6 for time *a* (T_a) and time *b* (T_b), respectively. The average permeation rate ($\bar{P}$) between time *a* (T_a) and time *b* (T_b) is obtained:

$$\bar{P} = \frac{CP_b - CP_a}{T_b - T_a} \tag{10}$$

6.8.2 *Open-loop permeation test:*

6.8.2.1 Calculate cumulative permeations (CP_a) and (CP_b) using Eq 7 for time *a* (T_a) and time *b* (T_b), respectively. The average permeation rate ($\bar{P}$) between time a (T_a) and time b (T_b) can be calculated using Eq 10.

6.9 *Maximum permeation rate for open-loop permeation testing:*

6.9.1 The program reports the highest permeation rate as the maximum permeation rate.

NOTE 5—This option is applicable to the open-loop permeation test only. It can be utilized for decision making to see if the permeation rate ever reaches the threshold maximum.

6.10 *Perform all the permeation calculations for variable sampling flow rate for open-loop permeation testing:*

6.10.1 For variable sampling flow rate, an additional column in the data file is needed (refer to X1.2.3 in Appendix X1).

6.10.2 The program first takes the product of the sampling flow rate (*F*) and the concentration (*C*) to calculate permeation rate, that is, P = C*F/A. Then it calculates all of the permeation parameters in the same manner as those for a constant sampling flow.

NOTE 6—Because the value of (C*F) is independent of changes in the sampling flow rate, concentration is inversely proportional to flow rate.

6.11 *Perform all the permeation calculations for closed-loop permeation testing with discrete sampling:*

6.11.1 Convert the cumulative permeation from discrete sampling to a continuous sampling mode and then calculate all the permeation parameters as the manner for continuous sampling.

6.11.2 To obtain the continuous sampling mode *y* values for the permeation curve of *y* (µg/cm^2) against *x* (min), the following equations are used based on whether the sample volume is or is not replaced.

$$CP_a = \frac{C_i V_i}{A} + \frac{\sum_{n=0}^{i-1} C_n V_s}{A} \tag{11}$$

where V_s is volume of discrete sample removed from the collection medium.

6.11.2.1 *Close-loop with discrete sampling and the sample volume is not replaced:*

Assuming that V_i is the remaining medium volume at t_i, that is,

$$V_i = V_t - (i-1)V_s \tag{12}$$

Note that V_t is the total medium volume at the beginning of the permeation testing, that is, t_0. Therefore, Eq 11 can be unambiguously expressed as the following:

$$CP_a = \frac{C_i[V_t - (i-1)V_s]}{A} + \frac{\sum_{n=0}^{i-1} C_n V_s}{A} \tag{13}$$

6.11.2.2 *Closed-loop with discrete sampling and the sample volume is replaced:*

Since sample volume is replaced, V_i is equal to V_t so Eq 11 becomes:

$$CP_a = \frac{C_i V_t}{A} + \frac{\sum_{n=0}^{i-1} C_n V_s}{A} \tag{14}$$

6.12 *Minimum breakthrough detection time:*

6.12.1 Because the Practice D6978 standard specifies a closed-loop permeation testing with discrete sampling and when volume is replaced to determine the minimum breakthrough detection time, cumulative permeation from discrete sampling is first converted into a continuous sampling mode using Eq 14.

6.12.2 Minimum breakthrough detection time is then calculated using the procedure described in 6.3.1, but using Eq 15 instead of Eq 3 since minimum breakthrough detection time is defined as the time at which the permeation rate reaches 0.01 µg/cm^2/min rather than 0.1 µg/cm^2/min.

$$2ax + b = 0.01 \tag{15}$$

7. Computer Program

7.1 *General:*

7.1.1 The computer program, referred to as "Permeation Calculator" to perform the calculations for this practice was created using Microsoft Visual C++ and compiled to an executable file "PermCalc.exe."

7.1.2 The Permeation Calculator will run on the following 32-bit or 64-bit operating systems: Microsoft Windows 95, Windows 98SE, Windows NT, Windows 2000, and Windows XP. It will be modified to be compatible with future versions of Microsoft Windows if needed.

7.2 *Detailed:*

7.2.1 A flow chart for the program is given in Fig. 5. The program starts by importing permeation testing data located in a Microsoft Excel PC formatted file, which contains data points in time vs. concentration.

7.2.2 Next, the program allows the user to enter variables under the "Choice of Variable" window, as shown in Fig. 6.

7.2.3 Specify the concentration format: "Option 1: use concentration (in µg/L)", "Option 2: use concentration (in ppm)" or "Option 3: use other analyzer output reading."

7.2.4 Enter the molecular weight for the test chemical if Option 2 is selected.

7.2.5 Enter the equation for converting the output reading to a concentration reading in µg/L if Option 3 is selected. A linear or polynomial (2nd to 9th order) can be entered.

7.2.6 In the next step, the program allows the user to select the "Time Format" either in minutes, YYYY/MM/DD HH:MM:SS, or MM/DD/YYYY HH:MM:SS ##.

7.2.7 The program then asks the user to select either "Open Loop System" or "Closed Loop System" for the "Choose System Type" section.

7.2.8 *For an "Open-Loop System":*

7.2.8.1 The program first requires specifying if the permeation test was based on Constant Flow Rate or Variable Flow Rate.

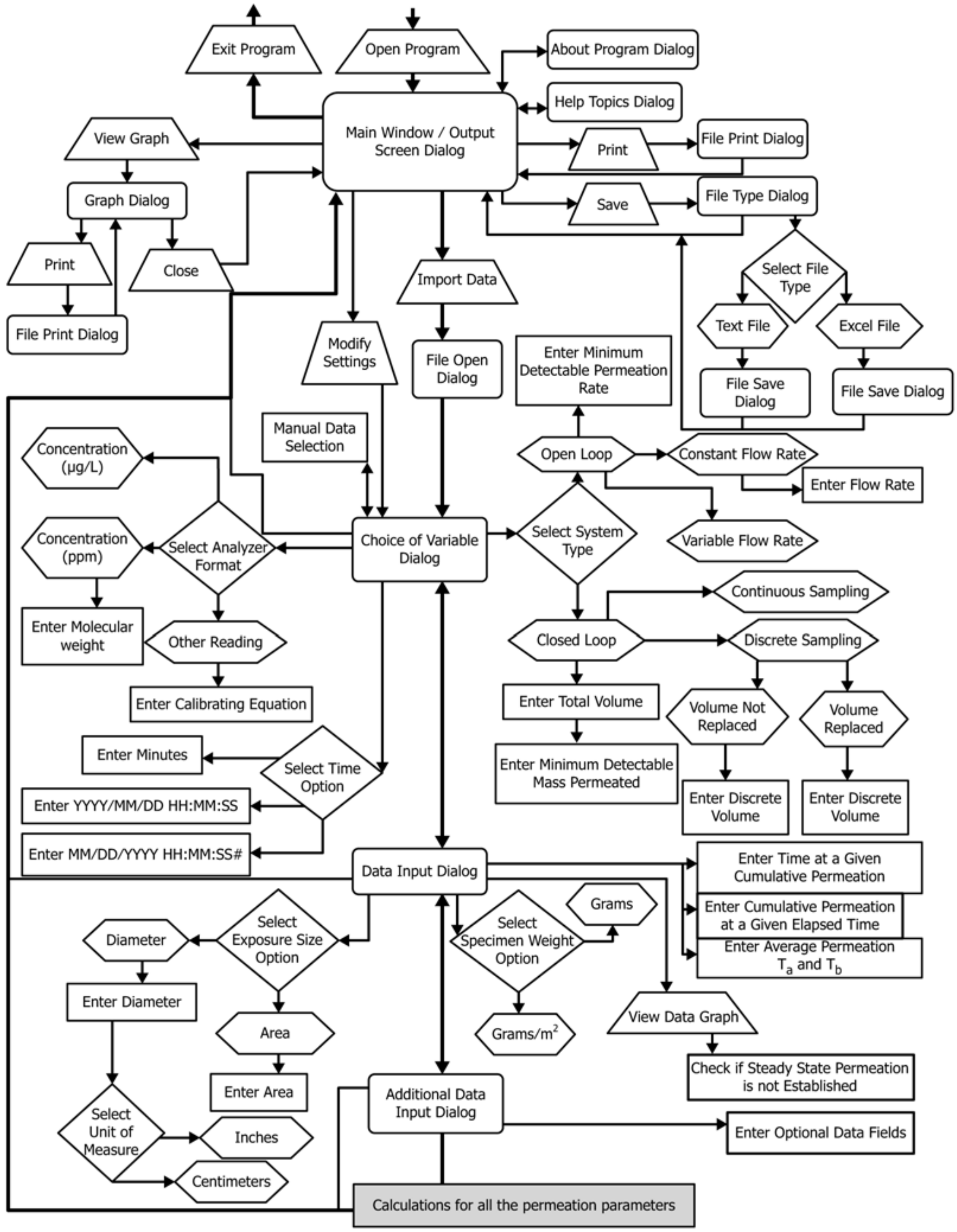


FIG. 5 Flow Chart for the Computer Program

7.2.8.2 Enter the value for the flow rate in L/min, if it was based on "Constant Flow Rate."

7.2.8.3 Enter the value for the Analytical Method Detection Limit (optional) if selected "Constant Flow Rate of Fresh Collection Medium."

NOTE 7—This value is used to calculate the Minimum Detectable Permeation Rate. The Minimum Detectable Permeation Rate will only be reported if a value is entered.

7.2.8.4 Enter the "Minimum detectable permeation rate" in µg/(cm^2*min).

7.2.9 *For a "Closed-Loop System":*

7.2.9.1 The program first requires entering the value for the "Total Volume of the Collection Medium" in litre (L), and then requires specifying if the test was "Continuous Sampling" or "Discrete Sampling."

7.2.9.2 For "Discrete Sampling", the program then asks whether or not the sample volume was being replaced. Enter the "Sample Volume."

7.2.9.3 Enter the "Minimum detectable mass permeated" in µg/cm^2.

7.2.10 Next, the program calls for more variables under the "Data Input" window, as shown in Fig. 7. These include the

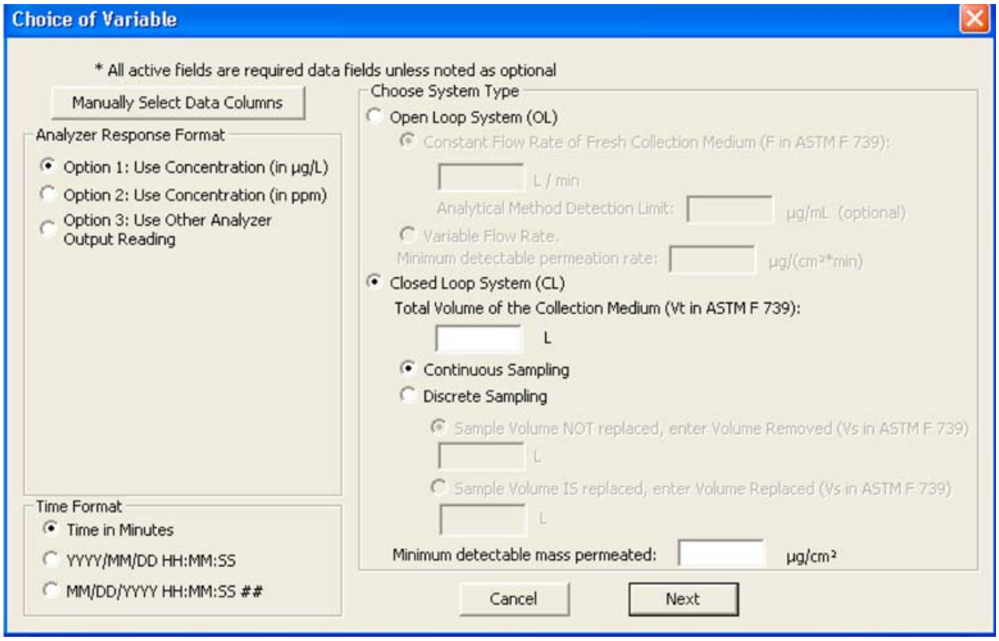


FIG. 6 Screen Shot for Choice of Variable Window

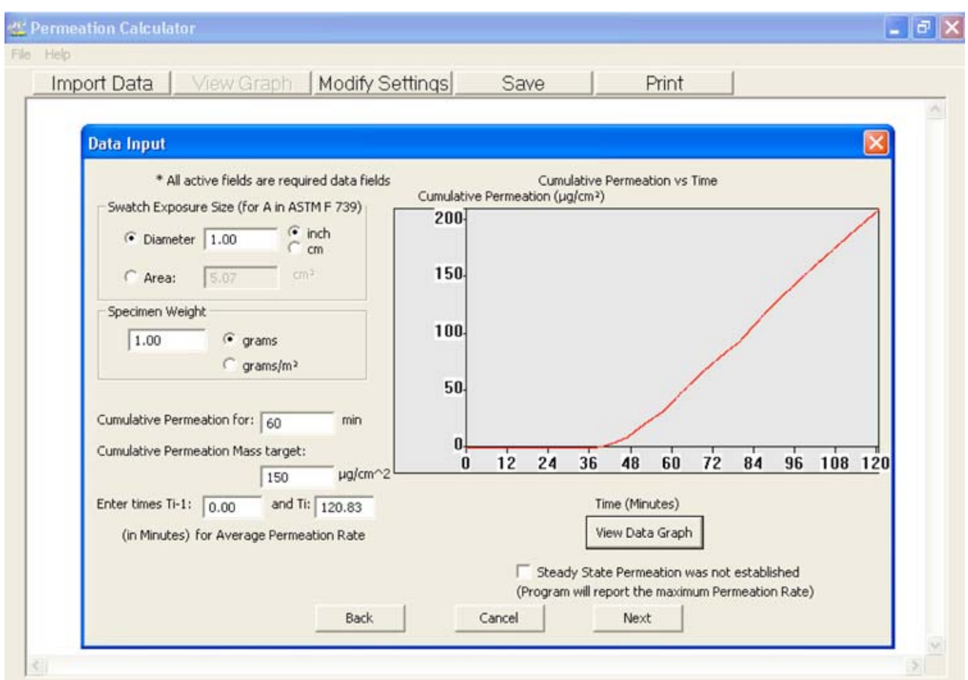


FIG. 7 Screen Shot for Data Input Window (The values in the fields are default values and the permeation curve is for a closed-loop test as an example.)

diameter of the swatch contacted, specimen weight, the time value to be used to calculate the cumulative permeation, the value of "mass/area" for the cumulative permeation mass target section, and the time values to be used to calculate the average permeation rate.

7.2.11 The program then converts the data points into time versus cumulative permeation for a closed-loop test, or time versus permeation rate for an open-loop test. The permeation curve can be viewed by clicking on "View Data Graph."

7.2.12 Finally, the program allows the user to enter additional information under the "Additional Data Input" window, as shown in Fig. 8. Although the information is not required for the calculations, it will be incorporated into the final report file. These include report title, project number, operator, date, material type, average material thickness, test chemical name, physical state of the test chemical, CAS #, manufacturer, lot/batch #, expiration date, collection medium, analytical instrument used, data sampling interval, and test temperature

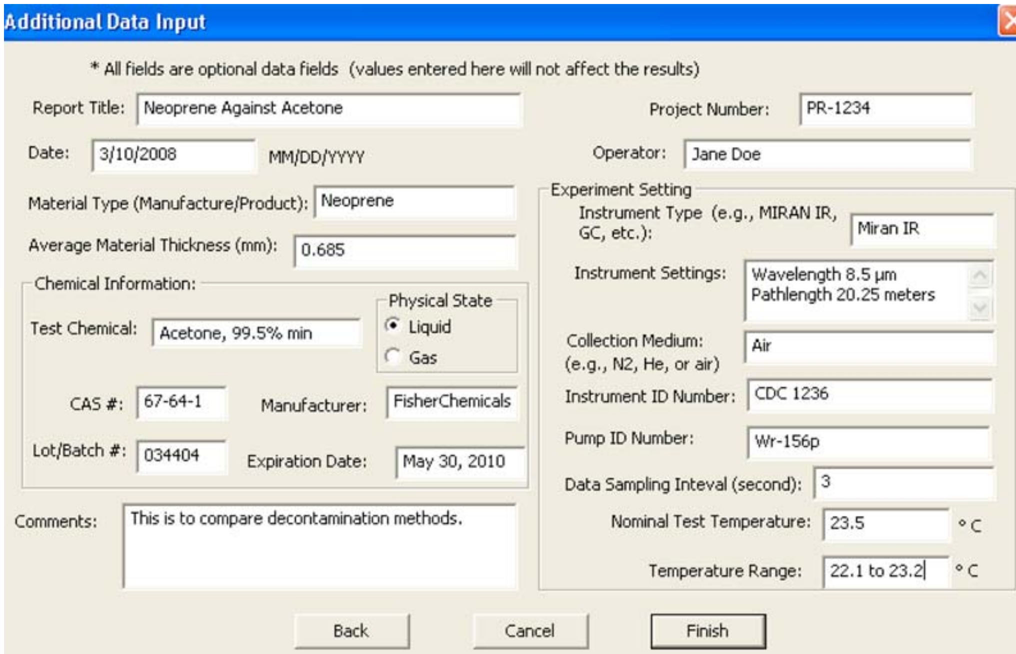


FIG. 8 Screen Shot of Window to Input Additional Information

when conducting the permeation testing. The user can enter part or all of the information in the fields, or leave all the fields blank.

7.2.13 At this point, all the information and the quantities for the calculations are available. The program calculates the permeation parameters and then displays a report file immediately after the user clicks on "Finish" as shown in Fig. 8.

8. Report

8.1 As stated in 7.2.13, the results of calculations performed in accordance with this practice, together with the input relevant information is displayed as a report file. The program allows the user to select the report file in either a Text file (Fig. 9) or a Microsoft Excel format (Fig. 10).

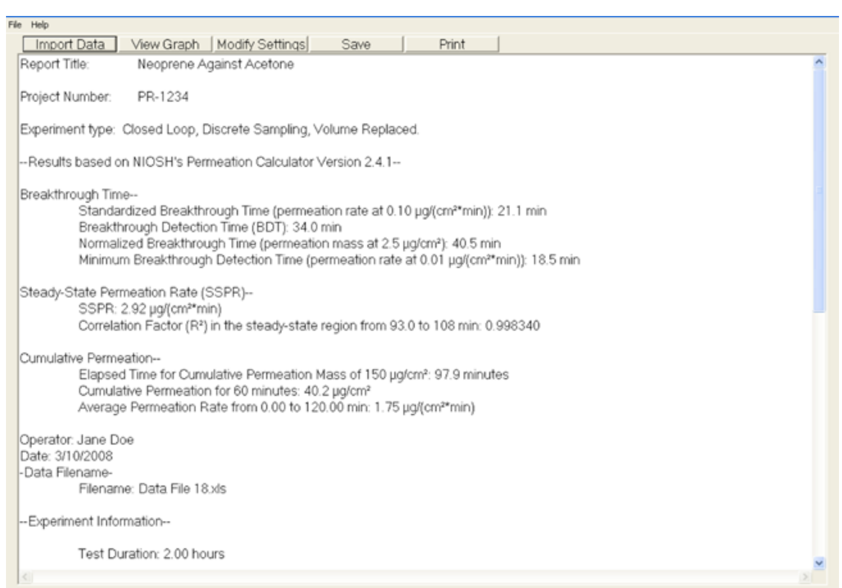
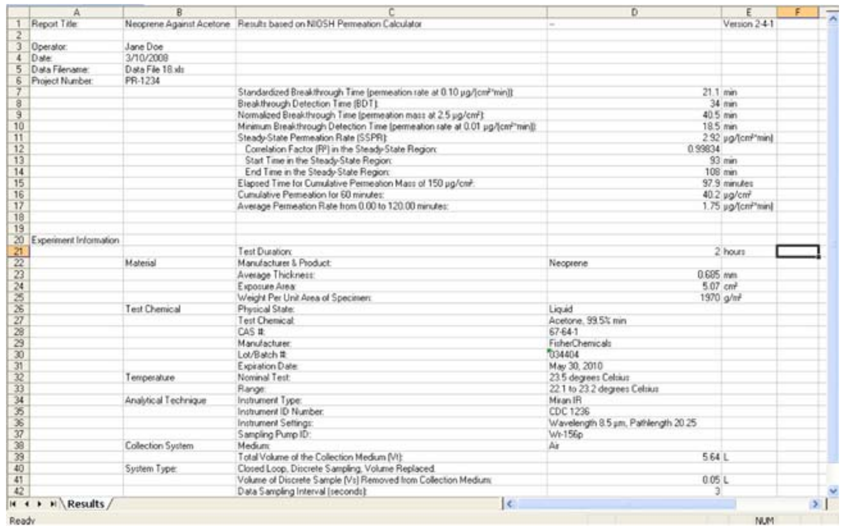


FIG. 9 Report File in a Text File Format for a Closed-Loop Test with Discrete Sampling and When Volume is Replaced as an Example



	A	B	C	D	E	F
1	Report Title:	Neoprene Against Acetone	Results based on NIOSH Permeation Calculator	–	Version 2-4-1	
2						
3	Operator:	Jane Doe				
4	Date:	3/10/2008				
5	Data Filename:	Data File 18.xls				
6	Project Number:	PR-1234				
7			Standardized Breakthrough Time (permeation rate at 0.10 µg/(cm²*min)):	21.1	min	
8			Breakthrough Detection Time (BDT):	34	min	
9			Normalized Breakthrough Time (permeation mass at 2.5 µg/cm²):	40.5	min	
10			Minimum Breakthrough Detection Time (permeation rate at 0.01 µg/(cm²*min)):	18.5	min	
11			Steady-State Permeation Rate (SSPR):	2.92	µg/(cm²*min)	
12			Correlation Factor (R²) in the Steady-State Region:	0.99834		
13			Start Time in the Steady-State Region:	93	min	
14			End Time in the Steady-State Region:	108	min	
15			Elapsed Time for Cumulative Permeation Mass of 150 µg/cm²:	97.9	minutes	
16			Cumulative Permeation for 60 minutes:	40.2	µg/cm²	
17			Average Permeation Rate from 0.00 to 120.00 minutes:	1.75	µg/(cm²*min)	
18						
19						
20	Experiment Information					
21			Test Duration:	2	hours	
22		Material	Manufacturer & Product:	Neoprene		
23			Average Thickness:	0.685	mm	
24			Exposure Area:	5.07	cm²	
25			Weight Per Unit Area of Specimen:	1970	g/m²	
26		Test Chemical	Physical State:	Liquid		
27			Test Chemical:	Acetone, 99.5% min		
28			CAS #:	67-64-1		
29			Manufacturer:	FisherChemicals		
30			Lot/Batch #:	034404		
31			Expiration Date:	May 30, 2010		
32		Temperature	Nominal Test:	23.5 degrees Celsius		
33			Range:	22.1 to 23.2 degrees Celsius		
34		Analytical Technique	Instrument Type:	Miran IR		
35			Instrument ID Number:	CDC 1236		
36			Instrument Settings:	Wavelength 8.5 µm, Pathlength 20.25		
37			Sampling Pump ID:	Wt-156p		
38		Collection System	Medium:	Air		
39			Total Volume of the Collection Medium (Vt):	5.64	L	
40		System Type:	Closed Loop, Discrete Sampling, Volume Replaced			
41			Volume of Discrete Sample (Vs) Removed from Collection Medium:	0.05	L	
42			Data Sampling Interval (seconds):	3		

FIG. 10 Report File in a Microsoft Excel Format for a Closed-Loop Test with Discrete Sampling and When Volume is Replaced as an Example

8.2 The report file contains all the items that are specified in the Report section of Test Method F739, the Report section of ISO 6529, the Report section of Practice D6978, if applicable. However, some items may be omitted in the report if the permeation data file does not contain enough information for the calculations. For instance, not enough data points before the breakthrough may result in no breakthrough detection time showing up in the report file.

9. Precision and Bias

9.1 The precision of this practice is a function of the program's code used to calculate the results. The computer program is written to calculate significant figures based on a combination of addition/subtraction and multiplication/division operations. The number of significant figures for each calculated value is determined based on the input values used in the calculations and is limited in precision to the least precise of these input values.

9.2 The reliability of the calculated permeation parameters is dependent on the data quality of the permeation testing data file. The smaller the data sampling interval in a data file, the more precise the results will be. Fewer data points before the breakthrough may result in the inability to correctly determine the various breakthrough times. Larger data sampling intervals over the permeation testing may result in imprecise determinations of cumulative permeation at a given elapsed time, elapsed time at a given cumulative permeation, and average permeation rate.

9.3 In addition to the data sampling interval, several factors also influence accurately determining the various breakthrough times. These factors include the accuracy of analytical method used to generate the data points, the background noise level of the analyzer, and the use of the second-order polynomial equation ($y=ax^2+bx+c$). A higher order of polynomial equation may be better but it will result in a more complicated computer program and a longer computing time.

9.4 From a standardization point of view, this practice uses data points ranging from 65 % to 85 % of the maximum concentration point for the linear regression in order to obtain the slope for a closed-loop system (Fig. 2). Switching the range up or down (or enlarging the range) may be able to improve the accuracy of the calculation for the slope. However, starting at a lower percentage may include data points from the transition region, resulting in a smaller slope, thus a smaller steady-state permeation rate; while extending the range to higher than 85 % may also result in a smaller slope because the calibration curve usually bends down at high concentrations. In addition, the values specified in 6.2.2 and 6.2.3 may have a similar effect on the reliability of determination of the breakthrough detection time.

9.5 This practice calculates the steady-state permeation rate for an open-loop test by averaging the concentration for the three highest data points. The reliability depends on the variance of the three data points.

NOTE 8—The report file includes the seven highest individual values so the user can remove any outliers before taking the mean.

10. Keywords

10.1 breakthrough detection times; chemical protective clothing; computer programs; cumulative permeations; minimum breakthrough detection times; normalized breakthrough detection times; permeation calculators; permeation testing; standardized breakthrough times; steady-state permeation rates

APPENDIX

(Nonmandatory Information)

X1. PERMEATION TESTING DATA FILE REQUIREMENTS

X1.1 The data must be in an Excel file. The number of data points can not exceed 5000. The number of significant figures used for the input data will affect the number of significant figures reported for the permeation parameters. Therefore, appropriate significant figures should be used when inputting the data.

X1.1.1 For Excel 2002, Excel 2003, and Excel 97-2003 and 5.0/95 workbooks, the worksheet containing the data must be named either "Sheet1" or the same as the data file's name. If the data file's name is changed, this worksheet must be renamed to the new data file's name or to "Sheet1." Otherwise the program will not run.

X1.2 The fields for the data files must be formatted as described below:

X1.2.1 The header for the column containing the time data must be "time," or "timestamp." The time format must be in minutes, YYYY/MM/DD HH:MM:SS, or MM/DD/YYYY HH:MM:SS ##.

X1.2.2 The header for the column containing the analyzer response data must be "analyzer output," "concentration," "voltage," "volt," "GC peak height," or "GC peak area." The program accepts concentration in μg/L, concentration in ppm, or entering an equation to convert the analyzer response to μg/L.

X1.2.3 If variable sampling flow rate is used for an open loop, an additional column is needed for the various sampling flow rates in L/min. The header for this column must be "flowrate" or "flow rate."

X1.2.4 The headers are not case sensitive. They must be located at the top of the appropriate column.

X1.2.5 If the data fields are manually selected, a data field must be assigned to Column A. The program will function more slowly if the data fields are not grouped consecutively.

X1.2.6 If the program is to automatically search for the data columns, the first column must contain the time; the second column must contain the analyzer response; and the third column must contain the sampling flow rates if it is an open loop test with variable sampling flow rate option.