Class 2 Permit Modification Request

Packaging-Specific Drum Age Criteria for New Approved Waste Containers

Waste Isolation Pilot Plant
Carlsbad, New Mexico

WIPP HWFP #NM4890139088-TSDF

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Acronyms and Abbreviations

CFR	Code of Federal Regulations
DAC	Drum Age Criteria
HWDU	Hazardous Waste Disposal Unit
HWFP	Hazardous Waste Facility Permit
NMAC	New Mexico Administrative Code
NMED	New Mexico Environment Department
PMR	Permit Modification Request
TDOP	Ten-Drum Overpack
VOC	Volatile Organic Compound
WIPP	Waste Isolation Pilot Plant

Overview of the Permit Modification Request

This document contains a Class 2 Permit Modification Request (**PMR**) for the Waste Isolation Pilot Plant (**WIPP**) Hazardous Waste Facility Permit (**HWFP**), Number NM4890139088-TSDF, hereinafter referred to as the WIPP HWFP.

This PMR is being submitted by the U.S. Department of Energy, Carlsbad Field Office and Washington TRU Solutions, LLC, collectively referred to as the Permittees, in accordance with the WIPP HWFP, Condition I.B.1 (20.4.1.900 New Mexico Administrative Code (**NMAC**) incorporating Title 40, Code of Federal Regulations (**CFR**), §270.42(b)). The modification will establish packaging-specific drum age criteria (**DAC**) values for waste containers that have recently been added to the WIPP HWFP. The proposed changes will not reduce the ability of the Permittees to provide continued protection to human health and the environment.

The purpose of the DAC is to ensure that samples of gaseous volatile organic compounds (**VOCs**) collected from within a waste container are representative. Samples are considered representative when the VOCs have reached concentrations that are at least 90 percent of the equilibrium steady-state concentrations, after which the collection of a representative headspace gas sample is ensured. As stated in Section B1-1a(3) of Attachment B1 of the WIPP HWFP, *drum age criteria are to ensure that the container contents have reached 90 percent of steady state concentration within each layer of confinement*. The DAC values are implemented on a container basis in terms of the number of days required to reach at least 90 percent of steady-state.

The requested modifications to the WIPP HWFP and supporting documents are provided in this PMR. The proposed modifications to the text of the WIPP HWFP have been identified using a double underline and a revision bar in the right hand margin for added information, and a ~~strikeout~~ font for deleted information. All direct quotations are indicated by italicized text. The following information specifically addresses how compliance has been achieved with the WIPP HWFP requirement, Permit Condition I.B.1 for submission of this Class 2 PMR.

1. 20.4.1.900 NMAC (incorporating 40 CFR §270.42(b)(1)(i)) requires the applicant to describe the exact change to be made to the permit conditions and supporting documents referenced by the permit.

This modification adds packaging-specific DAC values for 85-gallon and 100-gallon drums, and for ten-drum overpacks (**TDOPs**). The addition of these DAC values requires the revision of text in Attachment B1 of the WIPP HWFP, Sections B1-1a(1), B1-1a(2), and B1-1a(3) and Tables B1-5, B1-8, B1-9 and B1-10. Details of these revisions are summarized in Attachment A of this PMR and the proposed changes to the WIPP HWFP text are presented in Attachment B.

The proposed packaging-specific DAC values have been determined using the same methodology used to calculate the currently permitted DAC values. The methodology is in *Determination of Drum Age Criteria and Prediction Factors Based on Packaging Configurations,* INEEL/EXT-2000-01207, Bechtel BWXT Idaho, LLC, Idaho Falls, Idaho [BWXT (2000)]. This PMR has been prepared as directed by Section B1-1a(3) of Attachment B1 of the WIPP HWFP, which requires the following: *"If additional packaging configurations are identified, an appropriate Permit Modification will be submitted to incorporate the DAC using the methodology in BWXT (2000)*."

The determination of packaging-specific DAC values for specific packaging configurations using the BWXT (2000) methodology is described in a report entitled *Determination of Drum Age Criteria Values for Ten-Drum Overpacks, 85-Gallon Drums, and 100-Gallon Drums, Revision 1*. A copy of this report is provided as Attachment C of this PMR. The report documents how the BWXT (2000) methodology was used to determine the DAC values for 85-gallon drums, 100-gallon drums, and TDOPs that are proposed for addition to Tables B1-9 and B1-10 of Attachment B1 of the WIPP HWFP. This report is necessary because the separate packaging configurations proposed for 85-gallon, 100-gallon drums and TDOPs were not included in the BWXT (2000) report.

This PMR incorporates responses to applicable stakeholder and New Mexico Environment Department (**NMED**) comments on the previous Class 2 PMR, Packaging-Specific Drum Age Criteria for New Approved Waste Containers, submitted on May 13, 2003 and is a resubmittal of the May 13, 2003 PMR. Changes to the proposed WIPP HWFP text from the previous submittal are noted by italicized text in Attachment A, Table of Changes. Many of the stakeholder and NMED comments focused on one particular use of 100-gallon drums to package super compacted 55-gallon drums. Super compaction is a process that the U.S. Department of Energy will use at its Advanced Mixed Waste Treatment Facility at the Idaho National Engineering and Environmental Laboratory under a permit issued by the State of Idaho. These comments requested technical information related to super compacted waste and suggested the need to perform additional DAC modeling for this waste. The CBFO has fully addressed these comments in a companion document entitled Response to Stakeholder and NMED Comments on the May 13, 2003 DAC Submittal. The reason this information is a companion document is to emphasize that while the question and concerns expressed by stakeholders and the NMED regarding the super compaction process are valid, this PMR is only focused on simply establishing DAC values for specific packaging configurations using the accepted methodology.

2. 20.4.1.900 NMAC (incorporating 40 CFR §270.42(b)(1)(ii)) requires the applicant to identify that the modification is a Class 2 modification.

The proposed modification is classified as a Class 2 permit modification for the following reasons:

- It is considered an *other change* to waste sampling and analysis methods in accordance with 20.4.1.900 NMAC incorporating 40 CFR §270.42 Appendix I, Item B.1.d., because the methodology used for the determining the new DAC values is the same as that used to calculate the DAC values in the WIPP HWFP.

- The addition of new packaging configurations does not require that the BWXT (2000) methodology be changed. The additional DAC values are calculated by identifying additional input values for the model.

3. 20.4.1.900 NMAC (incorporating 40 CFR §270.42(b)(1)(iii)) requires the applicant to explain why the modification is needed.

This modification is needed so generator/storage sites can use 85-gallon and 100-gallon drums and direct loaded TDOPs in their waste management process for waste that is intended for disposal at the WIPP. The new DAC values assure that a representative headspace gas

sample is taken prior disposal at the WIPP. The 85-gallon drum, 100-gallon drum, and TDOP were previously added as permitted containers for waste management at the WIPP. Without the DAC values the approved containers cannot be disposed at the WIPP when directly loaded with waste.

4. 20.4.1.900 NMAC (incorporating 40 CFR §270.42 (b)(1)(iv)) requires the applicant to provide the applicable information required by 40 CFR §§270.13 through 270.21, 270.62, and 270.63.

The Regulatory Crosswalk Table on page 4 describes those portions of the WIPP HWFP that are affected by this PMR. Where applicable, regulatory citations in this modification reference Title 20, Chapter 4, Part 1, NMAC, revised June 14, 2000, incorporating the CFR, Title 40 (40 CFR Parts 264 and 270). 40 CFR §§270.16 through 270.22, 270.62, 270.63, and 270.66 are not applicable at WIPP. Consequently, they are not listed in the regulatory crosswalk table. 40 CFR §270.23 is applicable to the WIPP Hazardous Waste Disposal Units (**HWDUs**). This modification does not impact the conditions associated with the HWDUs.

5. 20.4.1.900 NMAC (incorporating 40 CFR §270.11(d)(1) and 40 CFR §270.30(k)) requires that any person signing under paragraph a and b must certify the document in accordance with 20.4.1.900 NMAC.

The transmittal letter for this PMR contains the signed certification statement in accordance with Module I.F of the WIPP HWFP.

Regulatory Crosswalk Table

Regulatory Citation(s) 20.4.1.900 NMAC (incorporating 40 CFR Part 270)	Regulatory Citation(s) 20.4.1.500 NMAC (incorporating 40 CFR Part 264)	Description of Requirement	Added or Clarified Information		
			Section of the HWFP	Yes	No
§270.13		Contents of Part A permit application	Attachment O, Part A		✓
§270.14(b)(1)		General facility description	Attachment A		✓
§270.14(b)(2)	§264.13(a)	Chemical and physical analyses	Attachment B	✓	
§270.14(b)(3)	§264.13(b)	Development and implementation of waste analysis plan	Attachment B	✓	
	§264.13(c)	Off-site waste analysis requirements	Attachment B	✓	
§270.14(b)(4)	§264.14(a-c)	Security procedures and equipment	Attachment C		✓
§270.14(b)(5)	§264.15(a-d)	General inspection requirements	Attachment D		✓
	§264.174	Container inspections	Attachment D		✓
§270.23(a)(2)	§264.602	Miscellaneous units inspections	Attachment D		✓
§270.14(b)(6)		Request for waiver from preparedness and prevention requirements of Part 264 Subpart C	NA		
§270.14(b)(7)	264 Subpart D	Contingency plan requirements	Attachment F		✓
	§264.51	Contingency plan design and implementation	Attachment F		✓
	§264.52 (a) & (c-f)	Contingency plan content	Attachment F		✓
	§264.53	Contingency plan copies	Attachment F		✓
	§264.54	Contingency plan amendment	Attachment F		✓
	§264.55	Emergency coordinator	Attachment F		✓
	§264.56	Emergency procedures	Attachment F		✓
§270.14(b)(8)		Description of procedures, structures or equipment for:	Attachment E		✓
§270.14(b)(8)(i)		Prevention of hazards in unloading operations (e.g., ramps and special forklifts)	Attachment E		✓
§270.14(b)(8)(ii)		Runoff or flood prevention (e.g., berms, trenches, and dikes)	Attachment E		✓
§270.14(b)(8)(iii)		Prevention of contamination of water supplies	Attachment E		✓
§270.14(b)(8)(iv)		Mitigation of effects of equipment failure and power outages	Attachment E		✓
§270.14(b)(8)(v)		Prevention of undue exposure of personnel (e.g., personal protective equipment)	Attachment E		✓
§270.14(b)(8)(vi) §270.23(a)(2)	§264.601	Prevention of releases to the atmosphere	Module II Module IV Attachment M2 Attachment N		✓
	264 Subpart C	Preparedness and Prevention	Attachment E		✓
	§264.31	Design and operation of facility	Attachment E		✓

Regulatory Citation(s) 20.4.1.900 NMAC (incorporating 40 CFR Part 270)	Regulatory Citation(s) 20.4.1.500 NMAC (incorporating 40 CFR Part 264)	Description of Requirement	Added or Clarified Information		
			Section of the HWFP	Yes	No
	§264.32	Required equipment	Attachment E Attachment F		✓
	§264.33	Testing and maintenance of equipment	Attachment D		✓
	§264.34	Access to communication/alarm system	Attachment E		✓
	§264.35	Required aisle space	Attachment E		✓
	§264.37	Arrangements with local authorities	Attachment F		✓
§270.14(b)(9)	§264.17(a-c)	Prevention of accidental ignition or reaction of ignitable, reactive, or incompatible wastes	Attachment E		✓
§270.14(b) (10)		Traffic pattern, volume, and controls, for example: Identification of turn lanes Identification of traffic/stacking lanes, if appropriate Description of access road surface Description of access road load-bearing capacity Identification of traffic controls	Attachment G		✓
§270.14(b) (11)(i) and (ii)	§264.18(a)	Seismic standard applicability and requirements	Part B, Rev. 6 Chapter B		✓
§270.14(b) (11)(iii-v)	§264.18(b)	100-year floodplain standard	Part B, Rev. 6 Chapter B		✓
	§264.18(c)	Other location standards	Part B, Rev. 6 Chapter B		✓
§270.14(b) (12)	§264.16(a-e)	Personnel training program	Permit Module II Attachment H		✓
§270.14(b) (13)	264 Subpart G	Closure and post-closure plans	Attachment I & J		✓
§270.14(b)(13)	§264.111	Closure performance standard	Attachment I		✓
§270.14(b)(13)	§264.112(a), (b)	Written content of closure plan	Attachment I		✓
§270.14(b)(13)	§264.112(c)	Amendment of closure plan	Attachment I		✓
§270.14(b)(13)	§264.112(d)	Notification of partial and final closure	Attachment I		✓
§270.14(b)(13)	§264.112(e)	Removal of wastes and decontamination/dismantling of equipment	Attachment I		✓
§270.14(b)(13)	§264.113	Time allowed for closure	Attachment I		✓
§270.14(b)(13)	§264.114	Disposal/decontamination	Attachment I		✓
§270.14(b)(13)	§264.115	Certification of closure	Attachment I		✓
§270.14(b)(13)	§264.116	Survey plat	Attachment I		✓
§270.14(b)(13)	§264.117	Post-closure care and use of property	Attachment J		✓
§270.14(b)(13)	§264.118	Post-closure plan; amendment of plan	Attachment J		✓

Regulatory Citation(s) 20.4.1.900 NMAC (incorporating 40 CFR Part 270)	Regulatory Citation(s) 20.4.1.500 NMAC (incorporating 40 CFR Part 264)	Description of Requirement	Added or Clarified Information		
			Section of the HWFP	Yes	No
§270.14(b)(13)	§264.178	Closure/ containers	Attachment I		✓
§270.14(b)(13)	§264.601	Environmental performance standards-Miscellaneous units	Attachment I		✓
§270.14(b)(13)	§264.603	Post-closure care	Attachment I		✓
§270.14(b)(14)	§264.119	Post-closure notices	Attachment J		✓
§270.14(b)(15)	§264.142	Closure cost estimate	NA		✓
	§264.143	Financial assurance	NA		✓
§270.14(b)(16)	§264.144	Post-closure cost estimate	NA		✓
	§264.145	Post-closure care financial assurance	NA		✓
§270.14(b)(17)	§264.147	Liability insurance	NA		✓
§270.14(b)(18)	§264.149-150	Proof of financial coverage	NA		✓
§270.14(b)(19)(i), (vi), (vii), and (x)		Topographic map requirements Map scale and date Map orientation Legal boundaries Buildings Treatment, storage, and disposal operations Run-on/run-off control systems Fire control facilities	Attachment O Part A		✓
§270.14(b)(19)(ii)	§264.18(b)	100-year floodplain	Attachment O Part A		✓
§270.14(b)(19)(iii)		Surface waters	Attachment O Part A		✓
§270.14(b)(19)(iv)		Surrounding Land use	Attachment O Part A		✓
§270.14(b)(19)(v)		Wind rose	Attachment O Part A		✓
§270.14(b)(19)(viii)	§264.14(b)	Access controls	Attachment O Part A		✓
§270.14(b)(19)(ix)		Injection and withdrawal wells	Attachment O Part A		✓
§270.14(b)(19)(xi)		Drainage on flood control barriers	Part B, Rev. 6 Chapter B, E, F		✓

Regulatory Citation(s) 20.4.1.900 NMAC (incorporating 40 CFR Part 270)	Regulatory Citation(s) 20.4.1.500 NMAC (incorporating 40 CFR Part 264)	Description of Requirement	Added or Clarified Information		
			Section of the HWFP	Yes	No
§270.14(b)(19)(xii)		Location of operational units	Part B, Rev. 6 Chapter B		✓
§270.14(b)(20)		Other federal laws Wild and Scenic Rivers Act National Historic Preservation Act Endangered Species Act Coastal Zone Management Act Fish and Wildlife Coordination Act Executive Orders	Part B, Rev. 6 Chapter K		✓
§270.15	§264 Subpart I	Containers	Attachment M1		✓
	§264.171	Condition of containers	Attachment M1		✓
	§264.172	Compatibility of waste with containers	Attachment M1		✓
	§264.173	Management of containers	Attachment M1		✓
	§264.174	Inspections	Attachment D Attachment M1		✓
§270.15(a)	§264.175	Containment systems	Attachment M1		✓
§270.15(c)	§264.176	Special requirements for ignitable or reactive waste	Attachment E Permit Module II		✓
§270..15(d)	§264.177	Special requirements for incompatible wastes	Attachment E Permit Module II		✓
	§264.178	Closure	Attachment I		✓
§270.15(e)	§264.179	Air emission standards	Attachment E Attachment N		✓
§270.23	264 Subpart X	Miscellaneous units	Attachment M2		✓
§270.23(a)	§264.601	Detailed unit description	Attachment M2		✓
§270.23(b)	§264.601	Hydrologic, geologic, and meteorologic assessments	Permit Module IV Attachment M2		✓
§270.23(c)	§264.601	Potential exposure pathways	Permit Module IV Attachment M2 Attachment N		✓
§270.23(d)		Demonstration of treatment effectiveness	Permit Module IV Attachment M2 Attachment N		✓
	§264.602	Monitoring, analysis, inspection, response, reporting, and corrective action	Permit Module IV Attachment M2 Attachment N		✓
	§264.603	Post-closure care	Attachment J Attachment J1		✓
	264 Subpart E	Manifest system, record keeping, and reporting	Permit Module I Permit Module II Permit Module IV Attachment B		✓

Attachment A

Table of Changes

Table of Changes

Affected Permit Section	Explanation for Change
a.1. Attachment B1, Section B1-1a(1)	**The reference to Table B1-10 for drums containing compacted 55 gallon drum with rigid liners that was in the previous submittal has been changed (corrected) to reference Table B1-9. This is in response to a public comment.*
a.1. Attachment B1, Section B1-1a(1) a.2. Attachment B1, Section B1-1a(2)	Text has been revised in Sections B1-1a(1) and B1-1a(2) as follows: • **To specify the default Packaging Configuration Group 6 for ten-drum overpacks (TDOPs) and 8 for 85-gallon and 100-gallon drums*. • *To indicate that Packaging Configuration Groups 7 and 8, which have been added for specific packaging configurations of 85- and 100-gallon drums, are not Summary Category Group dependent.* • To clarify that the new Packaging Configuration Group requirements apply when the 85-gallon drum, 100-gallon drum, or TDOP is used for the direct loading of waste. • *To specify that compacted 55-gallon drums in 100-gallon drums under Packaging Configuration Group 7 must have met the appropriate 55-gallon drum DAC (an assumption of the model).*
a.3. Attachment B1, Section B1-1a(3)	Text has been revised as follows: • **To specify the default Packaging Configuration Group 6 for TDOPs* and 8 for 85-gallon and 100-gallon drums. • To expand the statement pertaining to the applicability of the DAC to include 85-gallon drums, 100-gallon drums, and TDOPs. • **In response to NMED comments concerning layers of confinement (September 11, 2003 letter, Attachment 2, Item 1, bullet 3) inserted a new bullet which states "For supercompacted waste the absence of layers of confinement must be documented in the WWIS if Packaging Configuration Group 7 is used."*
a.4. Attachment B1, Table B1-5	Table B1-5 has been revised as follows: • To clarify that the descriptions for Scenarios 1 and 2 apply to 55-gallon drums. • To clarify that Scenario 3 applies to 55-gallon drums, 85-gallon drums, 100-gallon drums, and TDOPs.

Affected Permit Section	Explanation for Change
a.5. Attachment B1, Table B1-8	Table B1-8 has been revised as follows: • To add the TDOP configuration to Packaging Configuration Groups 5 and 6. • To add Packaging Configuration Group 7 to describe specific packaging configurations for 85- and 100-gallon drums that are directly loaded with waste. • **To add Packaging Configuration Group 8 to provide DAC default values for 85-gallon and 100-gallon drums. This is a change from the previous submittal in response to a NMED comment (September 11, 2003, Attachment 2, Item 1, bullet 1).* • **To specify (in Footnote "a") the default Packaging Configuration Group 6 for TDOPs and 8 for 85-gallon and 100-gallon drums. This is a change from the previous submittal in response to a NMED comment (September 11, 2003, Attachment 2, Item 1, bullet 1).* • **The strikeout of SWB in both Packaging Configurations 5 and 6 that was in the previous submittal has been removed. The same liner bags are used for both SWBs and TDOPs. This is in response to an NMED comment (September, 2003, Attachment 2, Item 1, bullet 1).* • **The definition of liner bags was revised to indicate that TDOPs use SWB liner bags. This is in response to an NMED comment (September, 2003, Attachment 2, Item 1, bullet 1).* • *Added a note to indicate that rigid liners are not used in 85-gallon or 100-gallon drums. This is in response to an NMED comment (September, 2003, Attachment 2, Item 1, bullet 1).*
a.6. Attachment B1, Table B1-9 a.7. Attachment B1, Table B1-10	Tables B1-9 and B1-10 have been revised as follows: • **To specify TDOP DAC values for Packaging Configuration Groups 5 and 6 and 85- and 100-gallon drum DAC values for Packaging Configuration Group 7 and 8. The addition of a DAC for Packaging Configuration Group 8 is a change from the previous submittal in response to a NMED comment (September 11, 2003, Attachment 2, Item 1, bullet 1).* • To clarify (in Footnote "c") that, similar to the standard waste box, the filter H_2 diffusivity specified for a TDOP is the sum of the diffusivities for all of the filters on the container. • To add a new Footnote "d" for Packaging Configuration Group 7 (85- and 100-gallon drums) to clarify that the DAC values apply when the headspace gas sample is taken between the inner and outer drum lids. Footnote "d" specifies a DAC value of 2 days for an 85- or 100-gallon drum in which the headspace gas sample is taken inside the filtered inner drum lid. • **Footnote "d" has been revised from the previous submittal to include the following; "Packaging Configuration Group 7 DAC values apply to drums with up to two lids."* • **To add a new Footnote "e" to clarify that while a DAC value of 2 days may be determined, containers must also comply with the equilibrium requirements in Section B1-1a (i.e., 72 hours at 18°C or higher) and to clarify that the equilibrium requirement for headspace gas sampling shall be met separately. This is in response to public comment 5.12.*

* = Indicates changes from the previous DAC Class 2 Submitted May 13, 2003.

Attachment B

Proposed Revised Permit Text

Proposed Revised Permit Text:

a.1. Attachment B1, Section B1-1a(1)

B1-1a(1) Summary Category S5000 Requirements

All waste containers or randomly selected containers from waste streams that meet the conditions for reduced headspace gas sampling listed in Permit Attachment B, Section B-3a(1), designated as summary category S5000 (Debris waste) shall be categorized under one of the sampling scenarios shown in Table B1-5 and depicted in Figure B1-1. If the container is categorized under Scenario 1, the applicable drum age criteria (**DAC**) from Table B1-6 must be met prior to headspace gas sampling. If the container is categorized under Scenario 2, the applicable Scenario 1 DAC from Table B1-6 must be met prior to venting the container and then the applicable Scenario 2 DAC from Table B1-7 must be met after venting the container. The DAC for Scenario 2 containers that contain filters or rigid liner vent holes other than those listed in Table B1-7 shall be determined using footnotes "a" and "b" in Table B1-7. Containers that have not met the Scenario 1 DAC at the time of venting must be categorized under Scenario 3. Containers categorized under Scenario 3 must be placed into one of the Packaging Configuration Groups listed in Table B1-8. If a specific packaging configuration cannot be determined based on the data collected during packaging and/or repackaging (Attachment B, Section B-3(d)1), a conservative default Packaging Configuration Group of 3 for 55-gallon drums, 6 for Standard Waste Boxes (**SWBs**) and ten-drum overpacks (**TDOPs**), and 8 for 85-gallon and 100-gallon drums must be assigned, provided the drums do not contain pipe component packaging. If a container is designated as Packaging Configuration Group 4 (i.e., a pipe component), the headspace gas sample must be taken from the pipe component headspace. If a 100-gallon drum in Packaging Configuration Group 7 contains a compacted 55-gallon drum containing a rigid liner, the 55-gallon drum must meet the appropriate 55-gallon drum DAC listed in Table B1-6, B1-7 or B1-9 to ensure that VOC solubility associated with the presence of the 55-gallon rigid drum liner does not impact the specification of a representative DAC for the 100-gallon drum. The DAC for Scenario 3 containers that contain rigid liner vent holes that are undocumented during packaging (Attachment B, Section B-3(d)1), repackaging (Attachment B, Section B-3(d)1), and/or venting (Section B1-1a[6][ii]) shall be determined using the default conditions in footnote "b" in Table B1-9.The DAC for Scenario 3 containers that contain filters that are either undocumented or are other than those listed in Table B1-9 shall be determined using footnote 'a' in Table B1-9. Each of the Scenario 3 containers shall be sampled for headspace gas after waiting the DAC in Table B1-9 based on its packaging configuration (note: Packaging Configuration Groups 4, 5, ~~and~~ 6, 7, and 8 are not summary category group dependent, and 85-gallon drum, 100-gallon drum, SWB, and TDOP requirements apply when the 85-gallon drum, 100-gallon drum, SWB, or TDOP ~~itself~~ is used for the direct loading of waste).

a.2. Attachment B1, Section B1-1a(2)

B1-1a(2) Summary Category S3000/S4000 Requirements

All waste containers or randomly selected containers from waste streams that meet the conditions for reduced headspace gas sampling listed in Permit Attachment B, Section B-3a(1), designated as summary categories S3000 (Homogenous solids) and S4000 (Soil/gravel) shall be categorized under one of the sampling scenarios shown in Table B1-5 and depicted in Figure B1-1. If the container is categorized under Scenario 1, the applicable DAC from Table B1-6 must be met prior to headspace gas sampling. If the container is categorized under Scenario 2, the applicable Scenario 1 DAC from Table B1-6 must be met prior to venting the container and then the applicable Scenario 2 DAC from Table B1-7 must be met after venting the container. The DAC for Scenario 2 containers that contain filters or rigid liner vent holes other than those listed in Table B1-7 shall be determined using footnotes “a” and “b” in Table B1-7. Containers that have not met the Scenario 1 DAC at the time of venting must be categorized under Scenario 3. Containers categorized under Scenario 3 must be placed into one of the Packaging Configuration Groups listed in Table B1-8. If a specific packaging configuration cannot be determined based on the data collected during packaging and/or repackaging (Attachment B, Section B-3(d)1), a conservative default Packaging Configuration Group of 3 for 55-gallon drums, 6 for SWBs and TDOPs,and 8 for 85-gallon and 100-gallon drums must be assigned, provided the drums do not contain pipe component packaging. If a container is designated as Packaging Configuration Group 4 (i.e., a pipe component), the headspace gas sample must be taken from the pipe component headspace. If a 100-gallon drum in Packaging Configuration Group 7 contains a compacted 55-gallon drum containing a rigid liner, the 55-gallon drum must meet the appropriate 55-gallon drum DAC listed in Table B1-6, B1-7 or B1-10 to ensure that VOC solubility associated with the presence of the 55-gallon rigid drum liner does not impact the specification of a representative DAC for the 100-gallon drum. The DAC for Scenario 3 containers that contain rigid liner vent holes that are undocumented during packaging (Attachment B, Section B-3(d)1), repackaging (Attachment B, Section B-3(d)1), and/or venting (Section B1-1a[6][ii]) shall be determined using the default conditions in footnote “b” in Table B1-10. The DAC for Scenario 3 containers that contain filters that are either undocumented or are other than those listed in Table B1-10 shall be determined using footnote ‘a’ in Table B1-10. Each of the Scenario 3 containers shall be sampled after waiting the DAC in Table B1-10 based on its packaging configuration (note: Packaging Configuration Groups 4, 5, ~~and~~ 6, 7, and 8 are not summary category group dependent, and 85-gallon drum, 100-gallon drum, SWB, and TDOP requirements apply when the 85-gallon drum, 100-gallon drum, SWB, or TDOP ~~itself~~ is used for the direct loading of waste).

a.3. Attachment B1, Section B1-1a(3)

B1-1a(3) General Requirements

The determination of packaging configuration consists of identifying the number of confinement layers and the identification of rigid poly liners when present. Generator/storage sites shall use either the default conditions specified in Tables B1-7 through B1-10 for retrievably stored waste or the data documented during packaging (Attachment B, Section B-3(d)1), repackaging (Attachment B, Section B-3(d)1), and/or venting (Section B1-1a[6][ii]) for determining the appropriate DAC for each container from which a headspace gas sample is collected. These drum age criteria are to ensure that the container contents have reached 90 percent of steady state concentration within each layer of confinement (Lockheed, 1995; BWXT, 2000). The following information must be reported in the headspace gas sampling documents for each container from which a headspace gas sample is collected:

- sampling scenario from Table B1-5 and associated information from Tables B1-6 and/or Table B1-7;
- the packaging configuration from Table B1-8 and associated information from Tables B1-9 or B1-10, including the diameter of the rigid liner vent hole, the number of inner bags, the number of liner bags, the presence/absence of drum liner, and the filter hydrogen diffusivity,
- the permit-required equilibrium time~~, and~~
- the drum age, and
- for supercompacted waste the absence of layers of confinement must be documented in the WWIS if Packaging Configuration Group 7 is used.

For all retrievably stored waste containers, the rigid liner vent hole diameter must be assumed to be 0.3 inches unless a different size is documented during drum venting or repackaging. For all retrievably store waste containers, the filter hydrogen diffusivity must be assumed to be the most restrictive unless container-specific information clearly identifies a filter model and/or diffusivity characteristic that is less restrictive. For all retrievably stored waste containers that have not been repackaged, acceptable knowledge shall not be used to justify any packaging configuration less conservative than the default (i.e., Packaging Configuration Group 3 for 55-gallon drums, 6 for SWBs and TDOPs, and 8 for 85-gallon and 100-gallon drums). For information reporting purposes listed above, sites may report the default packaging configuration for retrievably stored waste without further confirmation.

All waste containers with unvented rigid containers greater than 4 liters (exclusive of rigid poly liners) shall be subject to innermost layer of containment sampling or shall be vented prior to initiating drum age and equilibrium criteria. When sampling the rigid poly liner under Scenario 1, the sampling device must form an airtight seal with the rigid poly liner to ensure that a representative sample is collected (using a sampling needle connected to the sampling head to pierce the rigid poly liner, and that allows for the collection of a representative sample, satisfies this requirement). The configuration of the containment area and remote-handling equipment at each sampling facility are expected to differ. Headspace-gas samples will be analyzed for the analytes listed in Table B3-2 of Permit

Attachment B3. If additional packaging configurations are identified, an appropriate Permit Modification will be submitted to incorporate the DAC using the methodology in BWXT (2000). Consistent with footnote “a” in Table B1-8, any waste container that cannot be assigned a packaging configuration specified in Table B1-8 shall not be shipped to or accepted for disposal at WIPP.

Drum age criteria apply only to 55-gallon drums, 85-gallon drums, 100-gallon drums, ~~and~~ standard waste boxes, and TDOPs. Drum age criteria for all other container types must be established through permit modification prior to acceptance of these containers at WIPP.

a.4. Attachment B1, Table B1-5

TABLE B1-5
HEADSPACE GAS DRUM AGE CRITERIA SAMPLING SCENARIOS

Scenario	Description
1	A. Unvented 55-gallon drums without rigid poly liners are sampled through the drum lid at the time of venting. B1. Unvented 55-gallon drums with unvented rigid poly liners are sampled through the rigid poly liner at the time of venting or prior to venting. B2. Vented 55-gallon drums with unvented rigid poly liners are sampled through the rigid poly liner at the time of venting or prior to venting. C. Unvented 55-gallon drums with vented rigid poly liners are sampled through the drum lid at the time of venting.
2	55-gallon dDrums that have met the criteria for Scenario 1 and then are vented, but not sampled at the time of venting. [a]
3	Containers (i.e., 55-gallon drums, 85-gallon drums, 100-gallon drums, SWBs, TDOPs, and pipe components) that are initially packaged in a vented condition and sampled in the container headspace and containers that are not sampled under Scenario 1 or 2.

[a] Containers that have not met the Scenario 1 DAC at the time of venting must be categorized under Scenario 3. This requires the additional information required of each container in Scenario 3 (i.e., determination of packaging configuration), and such containers can only be sampled after meeting the appropriate Scenario 3 DAC.

a.5. Attachment B1, Table B1-8

TABLE B1-8
SCENARIO 3 PACKAGING CONFIGURATION GROUPS

Packaging Configuration Group	Covered S3000/S4000 Packaging Configuration Groups	Covered S5000 Packaging Configuration Groups
Packaging Configuration Group 1, 55 gal. drums [a]	• No layers of confinement, filtered inner lid [b] • No inner bags, no liner bags (bounding case)	• No layers of confinement, filtered inner lid [b] • No inner bags, no liner bags (bounding case)
Packaging Configuration Group 2, 55 gal. drums [a]	• 1 inner bag • 1 filtered inner bag • 1 liner bag (bounding case) • 1 filtered liner bag	• 1 inner bag • 1 filtered inner bag • 1 liner bag • 1 filtered liner bag • 1 inner bag, 1 liner bag • 1 filtered inner bag, 1 filtered liner bag • 2 inner bags • 2 filtered inner bags • 2 inner bags, 1 liner bag • 2 filtered inner bags, 1 filtered liner bag • 3 inner bags • 3 filtered inner bags • 3 filtered inner bags, 1 filtered liner bag • 3 inner bags, 1 liner bag (bounding case)
Packaging Configuration Group 3, 55 gal. drums [a]	• 1 inner bag, 1 liner bag • 1 filtered inner bag, 1 filtered liner bag • 2 inner bags • 2 filtered inner bags • 2 liner bags (bounding case) • 2 filtered liner bags	• 2 liner bags • 2 filtered liner bags • 1 inner bag, 2 liner bags • 1 filtered inner bag, 2 filtered liner bags • 2 inner bags, 2 liner bags • 2 filtered inner bags, 2 filtered liner bags • 3 filtered inner bags, 2 filtered liner bags • 4 inner bags • 3 inner bags, 2 liner bags • 4 inner bags, 2 liner bags (bounding case)

Packaging Configuration Group	Covered S3000/S4000 Packaging Configuration Groups	Covered S5000 Packaging Configuration Groups
Packaging Configuration Group 4, pipe components	• No layers of confinement inside a pipe component • 1 filtered inner bag, 1 filtered metal can inside a pipe component • 2 inner bags inside a pipe component • 2 filtered inner bags inside a pipe component • 2 filtered inner bags, 1 filtered metal can inside a pipe component • 2 inner bags, 1 filtered metal can inside a pipe component (bounding case)	• No layers of confinement inside a pipe component • 1 filtered inner bag, 1 filtered metal can inside a pipe component • 2 inner bags inside a pipe component • 2 filtered inner bags inside a pipe component • 2 filtered inner bags, 1 filtered metal can inside a pipe component • 2 inner bags, 1 filtered metal can inside a pipe component (bounding case)
Packaging Configuration Group 5, Standard Waste Box or Ten-Drum Overpack [a]	• No layers of confinement • 1 SWB liner bag (bounding case)	• No layers of confinement • 1 SWB liner bag (bounding case)
Packaging Configuration Group 6, Standard Waste Box or Ten-Drum Overpack [a]	• any combination of inner and/or liner bags that is less than or equal to 6 • 5 inner bags, 1 SWB liner bag (bounding case)	• any combination of inner and/or liner bags that is less than or equal to 6 • 5 inner bags, 1 SWB liner bag (bounding case)
Packaging Configuration Group 7, 85-gal. drums and 100-gal. drums [a]	• No inner bags, no liner bags, no rigid liner, filtered inner lid (bounding case) [b] • No inner bags, no liner bags, no rigid liner	• No inner bags, no liner bags, no rigid liner, filtered inner lid (bounding case) [b] • No inner bags, no liner bags, no rigid liner
Packaging Configuration Group 8, 85-gal. drums and 100-gal. drums [a]	• 4 inner bags and 2 liner bags, no rigid liner, filtered inner lid (bounding case) [b]	• 4 inner bags and 2 liner bags, no rigid liner, filtered inner lid (bounding case) [b]

[a] If a specific Packaging Configuration Groups cannot be determined based on the data collected during packaging (Attachment B, Section B-3(d)1) and/or repackaging (Attachment B, Section B-3(d)1), a conservative default Packaging Configuration Group of 3 for 55-gallon drums, 6 for SWBs and TDOPs, and 8 for 85-gallon and 100-gallon drums must be assigned provided the drums do not contain pipe component packaging. If pipe components are present as packaging in the drums, the pipe components must be sampled following the requirements for Packaging Configuration Group 4.

[b] A “filtered inner lid” is the inner lid on a double lid drum that contains a filter.

Definitions:

Liner Bags: One or more optional plastic bags that are used to control radiological contamination. Liner bags for drums have a thickness of approximately 11 mils. ~~SWB liner bags have a thickness of approximately 14 mils.~~ Liner bags are typically similar in size to the container. SWB liner bags have a thickness of approximately 14 mils. TDOPs use SWB liner bags.

Inner Bags: One or more optional plastic bags that are used to control radiological contamination. Inner bags have a thickness of approximately 5 mils and are typically smaller than liner bags.

Note: Rigid liners are not used in 85-gallon or 100-gallon drums.

a.6. Attachment B1, Table B1-9

TABLE B1-9
SCENARIO 3 DRUM AGE CRITERIA (in days) MATRIX FOR S5000 WASTE
BY PACKAGING CONFIGURATION GROUP

Packaging Configuration Group 1						
	Rigid Liner Vent Hole Diameter [b]					
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	0.3-inch Diameter Hole	0.375-inch Diameter Hole	0.75-inch Diameter Hole	1-inch Diameter Hole	No Liner Lid	No Liner
1.9×10^{-6}	131	95	37	24	4	4
3.7×10^{-6}	111	85	36	24	4	4
3.7×10^{-5}	28	28	23	19	4	4

Packaging Configuration Group 2						
	Rigid Liner Vent Hole Diameter [b]					
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	0.3-inch Diameter Hole	0.375-inch Diameter Hole	0.75-inch Diameter Hole	1-inch Diameter Hole	No Liner Lid	No Liner
1.9×10^{-6}	175	138	75	60	30	11
3.7×10^{-6}	152	126	73	59	30	11
3.7×10^{-5}	58	57	52	47	28	8

Packaging Configuration Group 3						
	Rigid Liner Vent Hole Diameter [b]					
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	0.3-inch Diameter Hole	0.375-inch Diameter Hole	0.75-inch Diameter Hole	1-inch Diameter Hole	No Liner Lid	No Liner
1.9×10^{-6}	199	161	96	80	46	16
3.7×10^{-6}	175	148	93	79	46	16
3.7×10^{-5}	72	72	67	62	42	10

Packaging Configuration Group 4	
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	Headspace Sample Taken Inside Pipe Component
$> 1.9 \times 10^{-6}$	152

Packaging Configuration Group 5	
Filter H_2 Diffusivity [a, c] (mol/s/mol fraction)	**Headspace Sample Taken Inside SWB/TDOP**
> 7.4 x 10^{-6} (SWB)	15
3.33 x 10^{-5} (TDOP)	15

Packaging Configuration Group 6	
Filter H_2 Diffusivity [a, c] (mol/s/mol fraction)	**Headspace Sample Taken Inside SWB/TDOP**
> 7.4 x 10^{-6} (SWB)	56
3.33 x 10^{-5} (TDOP)	56

Packaging Configuration Group 7 [d]			
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	**Inner Lid Filter Vent Minimum H_2 Diffusivity (mol/s/mol fraction) [a]**		
	7.4 x 10^{-6}	**1.85 x 10^{-5}**	**9.25 x 10^{-5} [e]**
3.7 x 10^{-6}	13	7	2
7.4 x 10^{-6}	10	6	2
1.85 x 10^{-5}	6	4	2

Packaging Configuration Group 8	
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	**Inner Lid Filter Vent Minimum H_2 Diffusivity (mol/s/mol fraction)**
	7.4 x 10^{-6}
3.7 x 10^{-6}	21

[a] The documented filter H_2 diffusivity must be greater than or equal to the listed value to use the DAC for the listed filter H_2 diffusivity (e.g., a container with a filter H_2 diffusivity of 4.2 x 10^{-6} must use a DAC for a filter with a 3.7 x 10^{-6} filter H_2 diffusivity). If a filter H_2 diffusivity for a container is undocumented or unknown or is less than 1.9 x 10^{-6} filter H_2 diffusivity, a filter of known H_2 diffusivity that is greater than or equal to 1.9 x 10^{-6} filter H_2 diffusivity must be installed prior to initiation of the relevant DAC period.

[b] The documented rigid liner vent hole diameter must be greater than or equal to the listed value to use the DAC for the listed rigid liner vent hole diameter (e.g., a container with a rigid liner vent hole of 0.5 in. must use a DAC for a rigid liner vent hole of 0.375 in.). If the rigid liner vent hole diameter for a container is undocumented during packaging (Attachment B, Section B-3(d)1), repackaging (Attachment B, Section B-3(d)1), and/or venting (Section B1-1a[6][ii]), that container must use a DAC for a rigid liner vent hole diameter of 0.30 in.

[c] The filter H_2 diffusivity for SWBs or TDOPs is the sum of the diffusivities for all of the filters on the container because SWBs and TDOPs have more than 1 filter.

[d] Headspace sample taken between inner and outer drum lids. If headspace sample is taken inside the filtered inner drum lid prior to placement of the outer drum lid, then a DAC value of 2 days may be used. Footnote e is also applicable. Packaging Configuration Group 7 DAC values apply to drums with up to two lids.

[e] While a DAC value of 2 days may be determined, containers must comply with the equilibrium requirements specified in Section B1-1a (i.e., 72 hours at 18°C or higher). The equilibrium requirement for headspace gas sampling shall be met separately.

a.7. Attachment B1, Table B1-10

TABLE B1-10
SCENARIO 3 DRUM AGE CRITERIA (in days) MATRIX FOR S3000 AND S4000 WASTE BY PACKAGING CONFIGURATION GROUP

Packaging Configuration Group 1						
	Rigid Liner Vent Hole Diameter [b]					
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	0.3-inch Diameter Hole	0.375-inch Diameter Hole	0.75-inch Diameter Hole	1-inch Diameter Hole	No Liner Lid	No Liner
1.9×10^{-6}	131	95	37	24	4	4
3.7×10^{-6}	111	85	36	24	4	4
3.7×10^{-5}	28	28	23	19	4	4

Packaging Configuration Group 2						
	Rigid Liner Vent Hole Diameter [b]					
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	0.3-inch Diameter Hole	0.375-inch Diameter Hole	0.75-inch Diameter Hole	1-inch Diameter Hole	No Liner Lid	No Liner
1.9×10^{-6}	213	175	108	92	56	18
3.7×10^{-6}	188	161	105	90	56	17
3.7×10^{-5}	80	80	75	71	49	10

Packaging Configuration Group 3						
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	Rigid Liner Vent Hole Diameter [b]				No Liner Lid	No Liner
	0.3-inch Diameter Hole	0.375-inch Diameter Hole	0.75-inch Diameter Hole	1-inch Diameter Hole		
1.9×10^{-6}	283	243	171	154	107	34
3.7×10^{-6}	253	225	166	151	106	31
3.7×10^{-5}	121	121	115	110	84	13

Packaging Configuration Group 4	
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	Headspace Sample Taken Inside Pipe Component
$> 1.9 \times 10^{-6}$	152

Packaging Configuration Group 5	
Filter H_2 Diffusivity [a, c] (mol/s/mol fraction)	Headspace Sample Taken Inside SWBS/TDOP
$> 7.4 \times 10^{-6}$ (SWB)	15
3.33×10^{-5} (TDOP)	15

Packaging Configuration Group 6	
Filter H_2 Diffusivity [a, c] (mol/s/mol fraction)	Headspace Sample Taken Inside SWBS/TDOP
$> 7.4 \times 10^{-6}$ (SWB)	56
3.33×10^{-5} (TDOP)	56

Packaging Configuration Group 7 [d]			
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	Inner Lid Filter Vent Minimum H_2 Diffusivity (mol/s/mol fraction) [a]		
	7.4×10^{-6}	1.85×10^{-5}	9.25×10^{-5} [e]
3.7×10^{-6}	13	7	2
7.4×10^{-6}	10	6	2
1.85×10^{-5}	6	4	2

Packaging Configuration Group 8	
Filter H_2 Diffusivity [a] (mol/s/mol fraction)	Inner Lid Filter Vent Minimum H_2 Diffusivity (mol/s/mol fraction)
	7.4×10^{-6}
3.7×10^{-6}	21

[a] The documented filter H_2 diffusivity must be greater than or equal to the listed value to use the DAC for the listed filter H_2 diffusivity (e.g., a container with a filter H_2 diffusivity of 4.2×10^{-6} must use a DAC for a filter with a 3.7×10^{-6} filter H_2 diffusivity). If a filter H_2 diffusivity for a container is undocumented or unknown or is less than 1.9×10^{-6} filter H_2 diffusivity, a filter of known H_2 diffusivity that is greater than or equal to 1.9×10^{-6} filter H_2 diffusivity must be installed prior to initiation of the relevant DAC period.

[b] The documented rigid liner vent hole diameter must be greater than or equal to the listed value to use the DAC for the listed rigid liner vent hole diameter (e.g., a container with a rigid liner vent hole of 0.5. in must use a DAC for a rigid liner vent hole of 0.375 in.). If the rigid liner vent hole diameter for a container is undocumented during packaging (Attachment B, Section B-3(d)1), repackaging (Attachment B, Section B-3(d)1), and/or venting (Section B1-1a[6][ii]), that container must use a DAC for a rigid liner vent hole diameter of 0.30 in.

[C] The filter H_2 diffusivity for SWBs or TDOPs is the sum of the diffusivities for all of the filters on the container because SWBs and TDOPs have more than 1 filter.

[d] Headspace sample taken between inner and outer drum lids. If headspace sample is taken inside the filtered inner drum lid prior to placement of the outer drum lid, then a DAC value of 2 days may be used. Footnote e is also applicable. Packaging Configuration Group 7 DAC values apply to drums with up to two lids.

[e] While a DAC value of 2 days may be determined, containers must comply with the equilibrium requirements specified in Section B1-1a (i.e., 72 hours at 18°C or higher). The equilibrium requirement for headspace gas sampling shall be met separately.

Attachment C

Determination of Drum Age Criteria Values for Ten-Drum Overpacks, 85-Gallon Drums, and 100-Gallon Drums, Revision 1

DETERMINATION OF DRUM AGE CRITERIA VALUES FOR TEN-DRUM OVERPACKS, 85-GALLON DRUMS, AND 100-GALLON DRUMS

REVISION 1

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December 2003

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Background and Purpose

Containers of transuranic (TRU) waste must meet a minimum age criterion before a gas sample collected from the waste container headspace is considered representative of the gas within the container. The drum age criterion (DAC) is the time required after container closure, or after container closure and container venting, before a headspace gas sample can be collected. The methodology described in "Determination of Drum Age Criteria and Prediction Factors Based on Packaging Configurations" (Bechtel BWXT Idaho, LLC [BWXT], 2000) [1] is the basis for the packaging-specific DAC values currently approved in the Hazardous Waste Facility Permit for the Waste Isolation Pilot Plant (WIPP) ("Permit") [2].

The following three new waste containers have been proposed for disposal at the WIPP: direct-loaded ten-drum overpack (TDOP), 100-gallon drum, and direct-loaded 85-gallon drum.

The purpose of this report is to document packaging-specific DAC values for the TDOP, 100-gallon drum, and 85-gallon drum as determined using the BWXT (2000) methodology [1]. The application of the BWXT (2000) methodology [1] to the TDOP, 100-gallon drum, and 85-gallon drum is consistent with the direction provided by Section B1-1a (3) of Attachment B1 of the Permit [2], which requires the following: "If additional packaging configurations are identified, an appropriate Permit Modification will be submitted to incorporate the DAC using the methodology in BWXT (2000)." Model parameters and assumptions used in determining the DAC values are also documented in this report.

In Revision 1 of this document, for clarity the methodology for expressing the filter vent hydrogen diffusivity on the inner lid of a 100- or 85-gallon waste drum as an opening in a confinement layer defined by an equivalent surface area is presented with an example calculation. In addition, a bounding case for a 100-gallon drum was also evaluated in which waste is contained inside four consecutive inner bags inside two liner bags and the drum has inner and outer lid filter vents.

Assumptions

The BWXT (2000) report documents all parameters and assumptions used in previous DAC calculations [1]. Parameter values specific to the TDOP, 100-gallon drum, and 85-gallon drum are listed in the input and output files included in Appendix A. Additional assumptions used in determining the DAC values for the TDOP, 100-gallon drum, and 85-gallon drum are presented in this section.

TDOP

The TDOP packaging configurations consist of (1) up to one standard waste box (SWB) liner bag and (2) up to six bag layers total, up to one of which may be an SWB liner bag. The TDOP has nine filter vents with minimum hydrogen diffusivity values of 3.7E-6 moles per second per mole fraction (mol/s/mol fraction). All other configuration parameters for the TDOP are assumed to be the same as those used for determining the packaging-specific DAC values for the

SWB [1]. The inner bags and SWB liner bags used in the TDOP packaging configurations are of the same dimensions as those used in an SWB.

100-Gallon Drum

The modeled 100-gallon drum packaging configuration includes one filtered non-polymeric (e.g., steel) inner drum lid, no layers of confinement, and no rigid drum liner. The DAC values are calculated for the case in which the headspace gas sample is collected between the inner and outer drum lids, as well as for the case in which the headspace gas sample is collected inside the inner drum lid. The DAC values for this 100-gallon drum packaging configuration were determined for three hydrogen diffusion values for the inner drum lid filter vent (i.e., 7.4E-6 mol/s/mol fraction, 1.85E-5 mol/s/mol fraction, and 9.25E-5 mol/s/mol fraction) in combination with three hydrogen diffusion values for the outer drum lid filter vent (i.e., 3.7E-6 mol/s/mol fraction, 7.4E-6 mol/s/mol fraction, and 1.85E-5 mol/s/mol fraction).

In order to model this configuration using VDRUM in which the confinement layer beneath the outer drum is a drum liner with an opening in the lid, the hydrogen diffusion value of the inner lid filter vent is expressed as an equivalent surface area of the opening in the liner lid. If the transport rate of a volatile organic compound (VOC) across a filter vent and an opening in a drum liner are set equal to each other [3], then an equivalent opening surface area can be defined in terms of the VOC diffusivity across the filter vent:

$$D^*_{VOC}\Delta y = \frac{D_{VOC} A_d c}{x_d}\Delta y \qquad (1)$$

where

D^*_{VOC}	VOC diffusivity across filter vent, mole (mol) [second (s)]$^{-1}$
D_{VOC}	VOC diffusivity in air, [centimeter (cm)]^2 s^{-1}
A_d	surface area of opening in confinement layer, cm^2
c	gas concentration, mol cm^{-3}
x_d	thickness of confinement layer at opening, cm
Δy	VOC mole fraction difference across confinement layer

Rearranging Equation (1) yields an equation defining the equivalent opening surface area:

$$A_d = \frac{D^*_{VOC} x_d}{D_{VOC} c} \qquad (2)$$

The ratio of VOC diffusivity across a filter vent to that in air is assumed to equal the same ratio for hydrogen:

$$\frac{D^*_{VOC}}{D_{VOC}} = \frac{D^*_{H_2}}{D_{H_2}} \qquad (3)$$

Therefore, the equivalent surface area of an opening in a confinement layer can be expressed in terms of hydrogen diffusivity across the filter vent in the confinement layer assuming a confinement layer thickness:

$$A_d = \frac{D^*_{H_2} x_d}{D_{H_2} c} \quad (4)$$

The ideal gas law estimates the gas concentration:

$$c = \frac{P_{atm}}{RT} \quad (5)$$

where

P_{atm}	pressure, atmosphere (atm)
T	temperature, Kelvin (K)
R	gas constant = 82.06 cm^3 atm/(mol) K

Hydrogen (H_2) diffusivity in air is estimated using the Slattery equation [4]:

$$D_{H_2} = 2.745\times10^{-4}\left[\frac{T}{\sqrt{\left(T_{c,air}T_{c,H_2}\right)}}\right]^{1.823}\left(p_{c,air}p_{c,H_2}\right)^{1/3}\left(T_{c,air}T_{c,H_2}\right)^{5/12}\left(\frac{1}{M_{air}}+\frac{1}{M_{H_2}}\right)^{1/2} \quad (6)$$

The key compound parameters (critical temperature, T_c; critical pressure, p_c; molecular weight, M) are [4]:

Hydrogen:	T_c = 33.3 K;	p_c =12.8 atm;	M = 2.016 [grams (g)]/mol
Air:	T_c = 132 K;	p_c =36.4 atm;	M = 28.97 g/mol

The total gas concentration and hydrogen diffusivity were both calculated at standard temperature (273.2 K) and pressure (1 atm), and since both terms appear in the denominator of Equation (4) they are rounded up.

$$c = \frac{P_{atm}}{RT} = \frac{1}{(82.06)(273.2)} = 4.46\times10^{-5} \approx 4.5\times10^{-5}\ \text{mol/cm}^3$$

$$D_{H_2} = 2.745\times10^{-4}\left[\frac{273.2}{\sqrt{132(33.3)}}\right]^{1.823}\left(36.4(12.8)\right)^{1/3}\left(33.3(132)\right)^{5/12}\left(\frac{1}{2.016}+\frac{1}{28.97}\right)^{1/2} \approx 0.68\text{cm}^2\text{s}^{-1}$$

Equivalent surface area:

A_d = (7.4e-6)(1)/[(0.68)(4.5e-5)] = 0.2418 cm^2 ≈ 0.241 cm^2

For other inner lid filter vents:

D* = 1.85 x 10^{-5} mol s^{-1}; A_d ≈ 0.603 cm^2

D* = 9.25 x 10^{-5} mol s^{-1}; A_d ≈ 3.01 cm^2

The calculated equivalent area terms were conservatively truncated or rounded down.

In some cases, 55-gallon drums may be supercompacted and packaged as “pucks” directly into 100-gallon drums. Compacted 55-gallon drums containing rigid drum liners placed inside the 100-gallon drum must meet the appropriate 55-gallon drum DAC value established by the Permit [2] prior to compaction. This ensures that VOC solubility associated with the presence of the 55-gallon rigid drum liner does not impact the calculated DAC for a 100-gallon drum.

85-Gallon Drum
The packaging configuration and possible sampling locations with respect to the inner and outer drum lids for the 85-gallon drum are assumed to be the same as the 100-gallon drum.

Defining DAC Values for TDOP, 100-Gallon Drum, and 85-Gallon Drum

The DAC values calculated using the methodology described in BWXT (2000) [1] for the TDOP, 100-gallon drum, and 85-gallon drum packaging configurations are documented in the output files included in Appendix A. In some cases, a more conservative DAC value than that shown in the output files was selected to simplify and facilitate implementation at the generator sites. These differences are summarized, with explanations as needed, in Table A-1 of Appendix A. Table 1 presents the DAC values applicable to the TDOP, 100-gallon drum, and 85-gallon drum packaging configurations. As shown in Table 1, the DAC values for the TDOP are the same as those determined for the SWB [1]. Except for the total hydrogen diffusivity of the TDOP filters, all input parameters are the same as the SWB. The minimum total hydrogen diffusivity of the TDOP filters (nine filters, each with a hydrogen diffusivity value of 3.7E-6 mol/s/mol fraction) is 4.5 times greater than the minimum total hydrogen diffusivity of the SWB filters (two filters, each with a hydrogen diffusivity value of 3.7E-6 mol/s/mol fraction). As shown in the output files in Appendix A, the difference in the total hydrogen diffusivity values between the TDOP and the SWB filters results in the calculation of shorter DAC values for the TDOP. The SWB DAC values bound the modeled TDOP packaging configurations DAC values.

The DAC values calculated for 85-gallon drums are less than the DAC values for the 100-gallon drum as shown in the output files included in Appendix A due to the smaller void volume in the 85-gallon drum. As documented in Table A-1 of Appendix A, the 100-gallon drum DAC values bound the DAC values for the 85-gallon drum packaging configurations (with one or two vented lids) that were modeled.

For the case in which the 100-gallon drum or 85-gallon drum headspace gas sample is taken inside the inner drum lid, the highest DAC value determined was one day for a drum with an inner drum lid filter vent with a hydrogen diffusivity value equal to or greater than 7.4E-6 mol/s/mol fraction. As documented in Appendix A, a 2-day DAC value bounds the 100-gallon drum and 85-gallon drum packaging configurations sampled inside the inner drum lid.

In addition, DAC values for 100-gallon and 85-gallon drums were considered in which waste is contained within four consecutive inner bags inside two liner bags and the drum had filter vents with the lowest hydrogen diffusivity values as listed in Table 1. The bounding DAC value of 21 days listed in Table 1 applies to both 100-gallon and 85-gallon drums that have waste packaged inside six or less layers of polymer bags. The input and output files for these cases are listed in Appendix A.

Table 1. DAC Values (in days) for Summary Category Groups S3000, S4000, and S5000

TDOP with Up to One Liner Bag	
TDOP Minimum Total Filter Diffusivity[a] (mol/s/mol fraction)	Headspace Sample Taken Inside Direct Load TDOP
3.33E-5	15

TDOP with Up to Five Inner Bags and One Liner Bag	
TDOP Minimum Total Filter Diffusivity[a] (mol/s/mol fraction)	Headspace Sample Taken Inside Direct Load TDOP
3.33E-5	56

100-Gallon Drum and 85-Gallon Drum with Headspace Samples Taken between Inner and Outer Drum Lids[b]			
Outer Lid Minimum Filter Diffusivity (mol/s/mol fraction)	Inner Lid Filter Minimum Diffusivity (mol/s/mol fraction)		
	7.4E-6	1.85E-5	9.25E-5
3.7E-6	13	7	2
7.4E-6	10	6	2
1.85E-5	6	4	2

100-Gallon Drum and 85-Gallon Drum (with four inner bags and two liner bags) with Headspace Samples Taken between Inner and Outer Drum Lids	
Outer Lid Minimum Filter Diffusivity: 3.7E-6 mol/s/mol fraction	Inner Lid Filter Minimum Diffusivity: 7.4E-6 mol/s/mol fraction
	21

[a] Sum of all filters in the lid of the TDOP.

[b] If headspace sample is taken inside the non-polymeric (e.g., steel) inner drum lid with a filter vent of hydrogen diffusivity value equal to or greater than 7.4E-6 mol/s/mol fraction prior to placement of the outer drum lid, then a DAC value of 2 days is applicable.

References

1 Liekhus, K.J., Djordjevic, S.M., Devarakonda, M., and Connolly, M.J., October 2000, "Determination of Drum Age Criteria and Prediction Factors Based on Packaging Configurations," INEEL/EXT-2000-01207, Bechtel BWXT Idaho, LLC, Idaho Falls, Idaho.

2 New Mexico Environment Department, "Waste Isolation Pilot Plant Hazardous Waste Facility Permit," NM4890139088-TSDF, New Mexico Environment Department, Santa Fe, New Mexico.

3 Connolly M. J. et al., June 1998, "Position for Determining Gas Phase Volatile Organic Compound Concentrations in Transuranic Waste Containers," INEEL-95/0109, Rev. 2, Idaho National Engineering Laboratory, Idaho Falls, Idaho.

4 Bird R. B., Stewart W. E., and Lightfoot E. N., 1960, *Transport Phenomena*, John Wiley, New York.

Appendix A
Input and Output Files Associated with DAC Value Determination for the TDOP, 85-Gallon Drum, and 100-Gallon Drum

This appendix includes the input and output files for the TDOP, 85-gallon drum, and 100-gallon drum that document the calculation of DAC values using the methodology described in BWXT (2000) [1]. In some cases, a more conservative DAC value than that shown in the output files was selected to simplify and facilitate implementation at the generator sites. These differences are summarized, with explanations as needed, in Table A-1.

Table A-1
Correlation between Calculated DAC Values and DAC Values Selected for Use for the TDOP, 100-Gallon Drum, and 85-Gallon Drum

Input/Output Filename	Waste Container Type and Packaging	DAC Value Calculated by VDRUM	DAC Value Selected for Use	Justification for Difference (if applicable)
TDOP				
tdop02/ tdop02.out	TDOP with one SWB liner bag and nine 3.7E-06 mol/s/mf filters	13	15	Bounded by DAC value for SWB configuration with one SWB liner bag [1]
tdop01/ tdop01.out	TDOP with five inner bags and one SWB liner bag and nine 3.7E-06 mol/s/mf filters	40	56	Bounded by DAC value for SWB configuration with five inner bags and one SWB liner bag [1]
100-Gallon Drum – Headspace Sample Taken between Inner and Outer Drum Lids				
t7037074/ t7037074.out	100-gallon drum outer lid filter = 3.7E-06 mol/s/mf inner lid filter = 7.4E-06 mol/s/mf	13	13	NA
t7037185/ t7037185.out	100-gallon drum outer lid filter = 3.7E-06 mol/s/mf inner lid filter = 1.85E-05 mol/s/mf	7	7	NA
t7037925/ t7037925.out	100-gallon drum outer lid filter = 3.7E-06 mol/s/mf inner lid filter = 9.25E-05 mol/s/mf	2	2	NA
t7074074/ t7074074.out	100-gallon drum outer lid filter = 7.4E-06 mol/s/mf inner lid filter = 7.4E-06 mol/s/mf	10	10	NA
t7074185/ t7074185.out	100-gallon drum outer lid filter = 7.4E-06 mol/s/mf inner lid filter = 1.85E-05 mol/s/mf	6	6	NA
t7074925/ t7074925.out	100-gallon drum outer lid filter = 7.4E-06 mol/s/mf inner lid filter = 9.25E-05 mol/s/mf	2	2	NA
t7185074/ t7185074.out	100-gallon drum outer lid filter = 1.85E-05 mol/s/mf inner lid filter = 7.4E-06 mol/s/mf	6	6	NA
t7185185/ t7185185.out	100-gallon drum outer lid filter = 1.85E-05 mol/s/mf inner lid filter = 1.85E-05 mol/s/mf	4	4	NA

Table A-1
Correlation between Calculated DAC Values and DAC Values Selected for Use for the TDOP, 100-Gallon Drum, and 85-Gallon Drum (continued)

Input/Output Filename	Waste Container Type and Packaging	DAC Value Calculated by VDRUM	DAC Value Selected for Use	Justification for Difference (if applicable)
t7185925/ t7185925.out	100-gallon drum outer lid filter = 1.85E-05 mol/s/mf inner lid filter = 9.25E-05 mol/s/mf	2	2	NA
100-Gallon Drum – Headspace Sample Taken Inside Inner Drum Lid				
t7000074/ t7000074.out	100-gallon drum inner lid filter = 7.4E-6 mol/s/mf	1	2	Bounded by DAC value for 100-gallon drum with two lids (t7185925/t7185925.out)
t7000185/ t7000185.out	100-gallon drum inner lid filter = 1.85E-5 mol/s/mf	1	2	Bounded by DAC value for 100-gallon drum with two lids (t7185925/t7185925.out)
t7000925/ t7000925.out	100-gallon drum inner lid filter = 9.25E-5 mol/s/mf	1	2	Bounded by DAC value for 100-gallon drum with two lids (t7185925/t7185925.out)
100-Gallon Drum – Headspace Sample Taken between Drum Lids, w/4 Inner Bags and 2 Liner Bags				
u7037074/ u7037074.out	100-gallon drum outer lid filter = 3.7E-06 mol/s/mf inner lid filter = 7.4E-06 mol/s/mf Four (4) polymer inner bags Two (2) polymer liner bags	21	21	NA
85-Gallon Drum – Headspace Sample Taken between Inner and Outer Drum Lids				
t8037074/ t8037074.out	85-gallon drum outer lid filter = 3.7E-6 mol/s/mf inner lid filter = 7.4E-6 mol/s/mf	9	13	Bounded by DAC value for corresponding 100-gallon drum configuration
t8037185/ t8037185.out	85-gallon drum outer lid filter = 3.7E-6 mol/s/mf inner lid filter = 1.85E-5 mol/s/mf	5	7	Bounded by DAC value for corresponding 100-gallon drum configuration
t8037925/ t8037925.out	85-gallon drum outer lid filter = 3.7E-6 mol/s/mf inner lid filter = 9.25E-5 mol/s/mf	2	2	Bounded by DAC value for corresponding 100-gallon drum configuration
t8074074/ t8074074.out	85-gallon drum outer lid filter = 7.4E-6 mol/s/mf inner lid filter = 7.4E-6 mol/s/mf	7	10	Bounded by DAC value for corresponding 100-gallon drum configuration
t8074185/ t8074185.out	85-gallon drum outer lid filter = 7.4E-6 mol/s/mf inner lid filter = 1.85E-5 mol/s/mf	4	6	Bounded by DAC value for corresponding 100-gallon drum configuration
t8074925/ t8074925.out	85-gallon drum outer lid filter = 7.4E-6 mol/s/mf inner lid filter = 9.25E-5 mol/s/mf	2	2	Bounded by DAC value for corresponding 100-gallon drum configuration
t8185074/ t8185074.out	85-gallon drum outer lid filter = 1.85E-5 mol/s/mf inner lid filter = 7.4E-6 mol/s/mf	4	6	Bounded by DAC value for corresponding 100-gallon drum configuration
t8185185/ t8185185.out	85-gallon drum outer lid filter = 1.85E-5 mol/s/mf inner lid filter = 1.85E-5 mol/s/mf	3	4	Bounded by DAC value for corresponding 100-gallon drum configuration

Table A-1
Correlation between Calculated DAC Values and DAC Values Selected for Use for the TDOP, 100-Gallon Drum, and 85-Gallon Drum (continued)

Input/Output Filename	Waste Container Type and Packaging	DAC Value Calculated by VDRUM	DAC Value Selected for Use	Justification for Difference (if applicable)
t8185925/ t8185925.out	85-gallon drum outer lid filter = 1.85E-5 mol/s/mf inner lid filter = 9.25E-5 mol/s/mf	1	2	Bounded by DAC value for corresponding 100-gallon drum configuration
85-Gallon Drum – Headspace Sample Taken Inside Inner Drum Lid				
t8000074/ t8000074.out	85-gallon drum No outer lid inner lid filter = 7.4E-6 mol/s/mf	1	2	Bounded by DAC value for corresponding 100-gallon drum configuration
t8000185/ t8000185.out	85-gallon drum No outer lid inner lid filter = 1.85E-5 mol/s/mf	1	2	Bounded by DAC value for corresponding 100-gallon drum configuration
t8000925/ t8000925.out	85-gallon drum No outer lid inner lid filter = 9.25E-5 mol/s/mf	1	2	Bounded by DAC value for corresponding 100-gallon drum configuration
85-Gallon Drum – Headspace Sample Taken between Drum Lids, w/4 Inner Bags and 2 Liner Bags				
u8037074/ u8037074.out	85-gallon drum outer lid filter = 3.7E-06 mol/s/mf inner lid filter = 7.4E-06 mol/s/mf Four (4) polymer inner bags Two (2) polymer liner bags	16	21	Bounded by DAC value for corresponding 100-gallon drum configuration

mol/s/mf = mole per second per mole fraction
NA = Not applicable

The computer program VDRUM used for deriving DAC values in BWXT (2000) [1] employs input files of required data and reports the time for volatile organic compounds (VOCs) to reach at least 90 percent of their steady state concentrations. The input file for each packaging configuration includes the same data structure beginning with the input and output file names and the number of VOCs evaluated. Each VOC included in the analysis has two lines of input data, the initial concentrations in the layers of confinement and the physical and chemical properties. The physical characteristics, such as thickness and surface area, of each type of confinement layer are entered. Specific information about data input includes the following:

- For the 100-gallon drum in which the headspace sample is taken between the filtered inner and outer drum lids, the configuration modeled by VDRUM includes one filtered non-polymeric (e.g., steel) inner drum lid and one filtered outer lid. The hydrogen release rate across the inner drum lid is defined by the hydrogen diffusivity of the filter vent. The DAC value was calculated for three hydrogen diffusivity values for the inner drum lid (i.e., 7.4E-6 mol/s/mol fraction, 1.85E-5 mol/s/mol fraction, and 9.25E-5 mol/s/mol fraction). The packaging configuration has no rigid drum liner but may or may not have plastic layers of confinement (i.e., inner bags and no liner bags).
- For the 100-gallon drum in which the headspace sample is taken inside the filtered non-polymeric (e.g., steel) inner drum lid prior to placement of the outer drum lid, VDRUM models this packaging configuration with a hypothetical innermost layer that is very thin. By making the innermost layers very thin, their resistance to the release of hydrogen is removed from the analysis.
- T_c, P_c are required if $D = 0$. (See input file format for parameter definitions.)
- T_c, P_c, D_v* are required if $D^* = 0$ and drum is vented.
- If $D > 0$ and $D^* > 0$, T_c and P_c can equal zero.
- In case of VOCs, gas generation does not occur ($g = 0$) at all times.
- Only gas permeation across bags is considered, so $A_d = x_d = 0$ (for bags only).
- Although gas permeation across drum liner is not considered, specification of A_p and x_p is required to estimate the volume of liner material. x_p is set to a small, non-zero value as shown in the input files.
- TDOP packaging configuration parameter values are assumed to be the same as those for the SWB [1] given the normal packaging of large items (e.g., gloveboxes) directly in the TDOP. These values are shown in the corresponding input files.
- 100-gallon drum and 85-gallon drum headspace void volumes are assumed to be 20% of the empty void volume below the lid. Assumptions for the void volumes between the drum lids (if two lids are used) are determined based on 100-gallon drum dimensions and by scaling the 100-gallon drum dimensions for the 85-gallon drum.
- When the headspace sample is taken between inner and outer drum lids, D_v^*, the release rate of the outermost layer of confinement, is set to the diffusivity of the outer lid filter. Because VDRUM only allows entry of one filtered layer of confinement, the filter on the inner lid can be accounted for by adjusting the parameter values for the rigid liner. The dimensions of the drum liner are adjusted so the effective release rate equals the inner lid filter vent (Given $A_d = (D^*)(x_d)/(Dc_0)$, where D^* = diffusivity of the inner lid filter vent, $x_d = 1.0$, and D = hydrogen diffusivity and c_0 = total gas

concentration at standard temperature and pressure). The resulting drum liner dimensions are shown in the corresponding input files.

- When headspace sample is taken inside inner drum lid, D_v^*, the release rate of the outermost layer of confinement, is set to the diffusivity of the inner lid filter.

To determine the drum age criteria from each analysis, the greatest time in days is selected from the VOCs (shown in bold in the output data listing). The data structures for the input and output files are shown in the following sections.

Input File Format

Line 1: Input file name, output file name, number of VOCs evaluated

Line 2: Name of VOC #1, $[IB]_0$, $[LB]_0$, $[LHS]_0$, $[DHS]_0$

Where:

$[IB]_0$ – Initial VOC concentration (ppmv) in inner bags
$[LB]_0$ – Initial VOC concentration (ppmv) in liner bags
$[LHS]_0$ – Initial VOC concentration (ppmv) in drum liner headspace
$[DHS]_0$ – Initial VOC concentration (ppmv) in drum headspace

Line 3: MW, ρ, D, T_c, P_c, D*, H, k, G (see Reference 1 for VOC-specific values)

Where:

MW – VOC molecular weight (g/gmol)
ρ – VOC permeability in polyethylene @ 25ºC, Ba x (1.e-10)
D – VOC diffusivity in air @ 25ºC, $cm^2\ s^{-1}$
T_c – VOC critical temperature, K
P_c – VOC critical pressure, atm
D* – VOC diffusivity across filter vent, mol/s/mol fraction
H – VOC Henrys constant for polyethylene drum liner, (cm3 polymer) atm/(cm3 (STP) gas)
k – VOC mass transfer coefficient at drum liner surface, s^{-1}
G – VOC generate rate (always set to 0 (zero)).

Lines (2n, 2n+1): Information for n^{th} (last) VOC

Line (2n+2): $A_p(1)$, $A_d(1)$, V(1), $x_p(1)$, $x_d(1)$
Line (2n+3): $A_p(2)$, $A_d(2)$, V(2), $x_p(2)$, $x_d(2)$
Line (2n+4): $A_p(3)$, $A_d(3)$, V(3), $x_p(3)$, $x_d(3)$
Line (2n+5): $A_p(4)$, $A_d(4)$, V(4), $x_p(4)$, $x_d(4)$

Where:

A_p – permeable surface area, cm^2
A_d – diffusional cross-sectional area, cm^2
V – void volume inside layer of confinement, cm^3
x_p – layer thickness, cm
x_d – length of diffusional path length, cm
1 – inner bag
2 – drum liner bag
3 – drum liner headspace
4 – drum headspace

Line (2n+6): T, P, D_v*

Where:

T – gas temperature = 25°C
P – gas pressure = 76 cm Hg
D_v* – hydrogen diffusion characteristic across drum filter vent, mol/s/mol fraction

Output File Format

Line 1: Input file name

Lines 2, n+1: VOC, DAC, [DAC], [SS]

Where:

VOC – name of VOC
DAC – drum age criterion, days
[DAC] – VOC concentration at the time of the DAC value, ppmv
[SS] – VOC concentration at steady-state conditions, ppmv

TDOP with Up to One SWB Liner Bag

TDOP02 Input File

```
'tdop02','tdop02.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
1.4e4,0.,0.,0.036,0.
1.4e4,150.,1.e5,0.0001,1.4
0.,0.,1.e5,0.,0.
25.,76.,333.e-7

c     Case 02: Ten-drum overpack (TDOP)
c     One liner bag (xp=0.036 cm)
c     No rigid liner (estimated by Ad=150 cm2, xp = 0.0001, xd=1.4 cm)
c     Void volume in layers of confinement same as in case of SWB
c     Void volume in headspace = 100000 cm3
c     D*H2 = total H2 diffusivity characteristic across (9) TDOP vents = 333.e-7 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

TDOP02 Output File

tdop02

carbon tetrachloride	8	793.7534	873.4544
methanol	10	694.2427	760.2239
dichloromethane	6	804.3660	883.2648
toluene	3	889.4951	954.5489
trichloroethylene	3	860.2493	947.2747
butanol	6	843.0952	906.8333
chloroform	6	807.2958	892.3996
1,1-dichloroethene	**13**	**720.5433**	**785.3380**
methyl ethyl ketone	9	768.9844	847.1186
methyl isobutyl ketone	11	755.0751	836.7894
1,1,2,2-tetrachloroethane	1	891.8437	979.1128
chlorobenzene	3	865.7315	950.6065

TDOP with up to Five Inner Bags and One SWB Liner Bag

TDOP01 Input File

```
'tdop01','tdop01.out',12
'carbon tetrachloride',1000.,0.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',1000.,0.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',1000.,0.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',1000.,0.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',1000.,0.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',1000.,0.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',1000.,0.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',1000.,0.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',1000.,0.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',1000.,0.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',1000.,0.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',1000.,0.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
1.4e4,0.,0.,0.063,0.
1.4e4,0.,1.9e5,0.036,0.
1.4e4,150.,1.e5,0.0001,1.4
0.,0.,1.e5,0.,0.
25.,76.,333.e-7

c     Case 01: Ten-drum overpack (TDOP)
c     Small bags, 5 polymer bags, xp=0.063 cm, Asb=Alb=14,000 cm2
c     One liner bag (xp=0.036 cm)
c     No rigid liner (estimated by Ad=150 cm2, xp=0.0001 cm, xd=1.4 cm)
c     Assume same void volumes between layers of confinement as in SWB
c     Void volume in headspace = 100000 cm3
c     D*H2 = total H2 diffusivity characteristic across 9 TDOP vents = 333.e-7 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

TDOP01 Output File

```
tdop01
carbon tetrachloride        28      656.5827        723.6465
methanol                    31      489.2478        539.6707
dichloromethane             21      673.3795        742.2752
toluene                     10      815.8182        896.8104
trichloroethylene           11      795.8295        879.5875
butanol                     19      712.1110        790.4583
chloroform                  22      692.4474        760.9515
1,1-dichloroethene          40      521.8710        576.6337
methyl ethyl ketone         30      608.8997        676.2224
methyl isobutyl ketone      38      596.2039        658.3813
1,1,2,2-tetrachloroethane    4      912.9481        960.4730
chlorobenzene               11      807.3900        888.5585
```

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids

T7037074: Input File

```
't7037074','t7037074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.241,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,3.7e-6
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c           Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids: 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.241 cm2
c     so effectiveH2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 3.7e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7037074: Output File

t7037074

carbon tetrachloride	12	604.5770	668.3834
methanol	8	611.4951	668.0692
dichloromethane	10	609.0457	668.4044
toluene	12	603.0229	668.4935
trichloroethylene	12	610.1760	668.4959
butanol	12	613.8976	668.4516
chloroform	11	605.9961	668.4244
1,1-dichloroethene	11	605.9680	668.1514
methyl ethyl ketone	11	602.2529	668.3221
methyl isobutyl ketone	**13**	**603.7643**	**668.2958**
1,1,2,2-tetrachloroethane	12	603.9773	668.2681
chlorobenzene	13	611.3399	668.4954

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7037185: Input File

```
't7037185','t7037185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.603,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,3.7e-6
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids: 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.603 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=1.85e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 3.7e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7037185: Output File

t7037185

carbon tetrachloride	6	753.7844	834.2632
methanol	4	760.9191	833.7641
dichloromethane	5	759.5344	834.2980
toluene	6	752.7831	834.4780
trichloroethylene	6	761.6633	834.4718
butanol	6	765.9401	834.3775
chloroform	6	771.1051	834.3312
1,1-dichloroethene	6	769.8293	833.8936
methyl ethyl ketone	6	766.4401	834.1641
methyl isobutyl ketone	**7**	**765.7963**	**834.1223**
1,1,2,2-tetrachloroethane	6	754.2537	834.3008
chlorobenzene	7	775.4692	834.4761

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7037925: Input File

```
't7037925','t7037925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,3.01,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,3.7e-6
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids = 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 3.01 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=9.25e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 3.7e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7037925: Output File

t7037925

carbon tetrachloride	2	924.4605	961.2931
methanol	1	871.2048	960.6116
dichloromethane	2	944.9376	961.3426
toluene	2	927.0502	961.6615
trichloroethylene	2	932.1554	961.6351
butanol	2	933.4634	961.4602
chloroform	2	935.8391	961.3906
1,1-dichloroethene	**2**	**930.6243**	**960.7859**
methyl ethyl ketone	2	931.3690	961.1545
methyl isobutyl ketone	2	910.1282	961.0969
1,1,2,2-tetrachloroethane	2	928.7170	961.7114
chlorobenzene	2	924.0621	961.6506

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7074074: Input File

```
't7074074','t7074074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.241,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,7.4e-6
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids: 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.241 cm2
c     so effectiveH2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 7.4e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7074074: Output File

```
t7074074
carbon tetrachloride          9        453.6972        501.9455
methanol                      6        458.6211        501.5847
dichloromethane               8        463.8039        501.9705
toluene                       9        452.7043        502.0988
trichloroethylene             9        458.0820        502.0949
butanol                       9        460.8127        502.0279
chloroform                    9        463.9797        501.9944
1,1-dichloroethene            9        463.7275        501.6783
methyl ethyl ketone           9        461.3951        501.8739
methyl isobutyl ketone       10        455.8464        501.8437
1,1,2,2-tetrachloroethane     9        453.4766        501.9493
chlorobenzene                10        461.6004        502.0977
```

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7074185: Input File

```
't7074185','t7074185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.603,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,7.4e-6
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids: 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.603 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=1.85e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 7.4e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7074185: Output File

t7074185

carbon tetrachloride	6	668.8000	715.6856
methanol	4	673.2346	714.9333
dichloromethane	5	672.7111	715.7399
toluene	6	668.3233	716.0817
trichloroethylene	5	648.8851	716.0544
butanol	5	652.5829	715.8685
chloroform	5	657.1573	715.7926
1,1-dichloroethene	5	655.5094	715.1261
methyl ethyl ketone	5	652.7585	715.5331
methyl isobutyl ketone	**6**	**656.4354**	**715.4695**
1,1,2,2-tetrachloroethane	6	669.3817	716.0912
chlorobenzene	6	665.1900	716.0702

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7074925: Input File

```
't7074925','t7074925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,3.01,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,7.4e-6
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids = 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 3.01 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=9.25e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 7.4e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7074925: Output File

t7074925

carbon tetrachloride	2	894.2050	925.4778
methanol	1	845.7206	924.2118
dichloromethane	2	912.0676	925.5702
toluene	2	896.8283	926.1776
trichloroethylene	2	901.2860	926.1241
butanol	2	902.2644	925.7906
chloroform	2	904.2629	925.6602
1,1-dichloroethene	**2**	**899.1498**	**924.5353**
methyl ethyl ketone	2	900.1448	925.2198
methyl isobutyl ketone	2	881.3079	925.1124
1,1,2,2-tetrachloroethane	2	898.3928	926.3226
chlorobenzene	2	894.1815	926.1549

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7185074: Input File

```
't7185074','t7185074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.241,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,1.85e-5
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids: 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.241 cm2
c     so effectiveH2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 1.85e-5 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7185074: Output File

```
t7185074
carbon tetrachloride        6       268.3586        287.3175
methanol                    4       270.2604        287.0151
dichloromethane             5       269.9278        287.3393
toluene                     6       268.0994        287.4739
trichloroethylene           5       260.2567        287.4636
butanol                     5       261.7852        287.3906
chloroform                  5       263.6452        287.3604
1,1-dichloroethene          5       263.1042        287.0927
methyl ethyl ketone         5       261.9208        287.2563
methyl isobutyl ketone      6       263.4129        287.2308
1,1,2,2-tetrachloroethane   6       268.5070        287.4666
chlorobenzene               6       266.8367        287.4695
```

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7185185: Input File

```
't7185185','t7185185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.603,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,1.85e-5
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids: 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.603 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=1.85e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 1.85e-5 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7185185: Output File

```
t7185185
carbon tetrachloride        4        463.6586        501.7245
methanol                    3        476.3261        500.7971
dichloromethane             3        455.9167        501.7920
toluene                     4        463.7949        502.2289
trichloroethylene           4        468.3401        502.1913
butanol                     4        470.2715        501.9525
chloroform                  4        472.7728        501.8576
1,1-dichloroethene          4        471.1799        501.0342
methyl ethyl ketone         4        470.0128        501.5358
methyl isobutyl ketone      4        453.8768        501.4572
1,1,2,2-tetrachloroethane   4        464.7393        502.2992
chlorobenzene               4        461.3665        502.2127
```

100-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T7185925: Input File

```
't7185925','t7185925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,3.01,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,1.85e-5
c     100-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 380 L (100 gal) – 12.4 L (void above lid)
c          Approximate void volume = 0.2 (368) = 73.6 L ⇔ 75,000 cm3
c     Void volume between lids = 12,400 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 3.01 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=9.25e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 1.85e-5 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T7185925: Output File

t7185925

carbon tetrachloride	2	813.1340	832.4349
methanol	1	776.2728	829.8742
dichloromethane	2	825.0309	832.6224
toluene	2	815.8369	833.8713
trichloroethylene	2	818.7859	833.7578
butanol	2	819.0015	833.0712
chloroform	2	820.1381	832.8055
1,1-dichloroethene	**2**	**815.2557**	**830.5270**
methyl ethyl ketone	2	816.8259	831.9116
methyl isobutyl ketone	2	803.6511	831.6942
1,1,2,2-tetrachloroethane	2	817.1591	834.2287
chlorobenzene	2	813.9915	833.8227

100-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid

T7000074: Input File

```
't7000074','t7000074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
3000.,0.,20000.,0.0005,0.
12800.,150.,40000.,0.00005,1.4
0.,0.,40000.,0.,0.
25.,76.,74.e-7

c     100-gallon drum w/inner lid only w/ filter vent
c     No plastic liner bag (xp=0.0005 cm)
c     No liner (estimated by Ad=150 cm2, xd=1.4 cm, xp=0.00005)
c     Void volume under inner lid = 80,000 cm3, equally divided between
c     "liner" and outer headspace
c     H2 diffusion characteristic across drum filter vent = 74.e-7 mol/s/mol fr
```

T7000074: Output File

t7000074

carbon tetrachloride	1	995.4536	995.9554
methanol	1	992.2009	993.7885
dichloromethane	1	996.1278	996.1657
toluene	1	997.3411	997.4221
trichloroethylene	1	997.2678	997.2731
butanol	1	996.3918	996.4465
chloroform	1	996.1041	996.1917
1,1-dichloroethene	**1**	**987.1293**	**994.0134**
methyl ethyl ketone	1	994.2435	995.3361
methyl isobutyl ketone	1	990.8757	995.1285
1,1,2,2-tetrachloroethane	1	997.5544	997.6054
chlorobenzene	1	997.1347	997.1719

100-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid (continued)

T7000185: Input File

't7000185','t7000185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
3000.,0.,20000.,0.0005,0.
12800.,150.,40000.,0.00005,1.4
0.,0.,40000.,0.,0.
25.,76.,1.85e-5

c 100-gallon drum w/inner lid only w/ filter vent
c No plastic liner bag (xp=0.0005 cm)
c No liner (estimated by Ad=150 cm2, xd=1.4 cm, xp=0.00005)
c Void volume under inner lid = 80,000 cm3, equally divided between
c fictional "liner" and outer headspace
c H2 diffusion characteristic across drum filter vent = 1.85e-5 mol/s/mol fr

T7000185: Output File

t7000185

carbon tetrachloride	1	989.4744	989.9521
methanol	1	983.1256	984.6177
dichloromethane	1	990.4398	990.4753
toluene	1	993.5066	993.5869
trichloroethylene	1	993.2097	993.2147
butanol	1	991.1147	991.1666
chloroform	1	990.4536	990.5367
1,1-dichloroethene	**1**	**978.6265**	**985.1689**
methyl ethyl ketone	1	987.3871	988.4250
methyl isobutyl ketone	1	983.8448	987.9128
1,1,2,2-tetrachloroethane	1	993.9983	994.0485
chlorobenzene	1	992.9288	992.9655

100-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid (continued)

T7000925: Input File

't7000925','t7000925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
3000.,0.,20000.,0.0005,0.
12800.,150.,40000.,0.00005,1.4
0.,0.,40000.,0.,0.
25.,76.,9.25e-5

c 100-gallon drum w/inner lid only w/ filter vent
c No plastic liner bag (xp=0.0005 cm)
c No liner (estimated by Ad=150 cm2, xd=1.4 cm, xp=0.00005)
c Void volume under inner lid = 80,000 cm3, equally divided between
c fictional "liner" and outer headspace
c H2 diffusion characteristic across drum filter vent = 9.25e-5 mol/s/mol fr

T7000925: Output File

t7000925

carbon tetrachloride	1	951.3634	951.7078
methanol	1	926.5816	927.5541
dichloromethane	1	954.1159	954.1395
toluene	1	968.6768	968.7536
trichloroethylene	1	966.9766	966.9810
butanol	1	957.3126	957.3516
chloroform	1	954.3596	954.4175
1,1-dichloroethene	**1**	**925.3331**	**930.0065**
methyl ethyl ketone	1	943.9569	944.6948
methyl isobutyl ketone	1	939.3307	942.3590
1,1,2,2-tetrachloroethane	1	970.9238	970.9720
chlorobenzene	1	965.7707	965.8041

100-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid (continued)

U7037074: Input File (Bounding Case: 100-gallon drum with four (4) inner polymer bags and two (2) liner bags)

```
 'u7037074','u7037074.out',12
'carbon tetrachloride',1000.,0.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',1000.,0.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',1000.,0.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',1000.,0.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',1000.,0.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',1000.,0.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',1000.,0.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',1000.,0.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',1000.,0.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',1000.,0.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',1000.,0.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',1000.,0.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
20000.,0.,0.,0.050,0.
20000.,0.,20000.,0.056,0.
1.e3,0.241,75000.,0.0001,1.0
0.,0.,12400.,0.,0.
25.,76.,3.7e-6
c   100-gallon, w/inner and outer lids, each w/ filter vent, 4 inner bags, 2 liner bags
c   Value for volume within innermost bags not required.
c   Void volume between bags: 20,000 cm3
c   Bag thickness same as in Scenario 3
c   Void volume beneath inner lid is approx. 20% of total empty volume
c     Total volume beneath lid = 380 L (100 gal) - 12.4 L (void above lid)
c     Approximate void volume = 0.2 (367) = 73.4 L <=> 75,000 cm3
c   Void volume between lids: 12,400 cm3
c   Inner lid exhibits no solubility for VOCs (thus,thin "liner thickness" xp =0.0001 cm)
c   Effective surface area across liner (assuming xd= 1.0 cm): Ad = 0.241 cm2
c    so effective H2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c   D*H2 = total H2 diff. char. across outer filter vent = 3.7e-6 mol/s/mol fr
c   VOC diff. char. estimated knowing D*H2, VOC Tc, VOC Pc
```

U7037074: Output File

```
 u7037074
 carbon tetrachloride      17  594.1344    655.0419
 methanol                  16  581.8834    638.6003
 dichloromethane           13  590.8961    656.2762
 toluene                   14  609.3403    664.6276
 trichloroethylene         13  601.7316    663.8490
 butanol                   14  594.4874    659.2490
 chloroform                15  602.4097    657.4854
 1,1-dichloroethene        21  585.7845    642.7220
 methyl ethyl ketone       17  588.2260    651.6213
 methyl isobutyl ketone    21  590.6235    650.2089
 1,1,2,2-tetrachloroethane 13  610.9872    667.1132
 chlorobenzene             14  604.2247    664.2889
```

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids

T8037074: Input File

't8037074','t8037074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.241,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,3.7e-6
c 85-gallon, w/inner and outer lids, each w/ filter vent
c Only two void volumes: Below inner lid and between inner and outer lids
c System modeled as inner bag-liner-drum
c Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c Void volume beneath inner lid is approx. 20% of total empty volume
c Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c Void volume between lids: 8600 cm3
c Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c Effective surface area across liner (xd= 1.0 cm): Ad = 0.241 cm2
c so effective release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c D*H2 = total H2 diffusivity characteristic across outer filter vent = 3.7e-6 mol/s/mol fr
c VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc

T8037074: Output File

t8037074

carbon tetrachloride	9	615.5707	668.3928
methanol	6	621.5620	668.0734
dichloromethane	7	610.2208	668.4149
toluene	9	614.2779	668.5266
trichloroethylene	8	604.3128	668.5236
butanol	8	608.1995	668.4655
chloroform	8	612.6898	668.4360
1,1-dichloroethene	8	612.4759	668.1564
methyl ethyl ketone	8	609.0936	668.3295
methyl isobutyl ketone	**9**	**603.2180**	**668.3029**
1,1,2,2-tetrachloroethane	9	615.1697	668.3894
chlorobenzene	9	611.0323	668.5259

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8037185: Input File

```
't8037185','t8037185.out',12
'carbon tetachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.603,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,3.7e-6
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids: 8600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad=0.603 cm2
c     so effective release rate equals inner lid filter vent, D*(H2)=1.85e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 3.7e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8037185: Output File

```
t8037185
carbon tetrachloride        5        783.9326        834.2728
methanol                    3        773.3948        833.7684
dichloromethane             4        782.5410        834.3085
toluene                     5        783.3315        834.5110
trichloroethylene           4        754.2708        834.4995
butanol                     4        758.6446        834.3913
chloroform                  4        764.0444        834.3427
1,1-dichloroethene          4        762.1296        833.8985
methyl ethyl ketone         4        758.8429        834.1717
methyl isobutyl ketone      5        770.2270        834.1293
1,1,2,2-tetrachloroethane   5        784.4841        834.4132
chlorobenzene               5        779.8882        834.5066
```

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8037925: Input File

```
't8037925','t8037925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,3.01,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,3.7e-6
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids = 8600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 3.01 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=9.25e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 3.7e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8037925: Output File

```
t8037925
carbon tetrachloride          2        952.6547        961.2953
methanol                      1        929.7321        960.6126
dichloromethane               1        907.5975        961.3450
toluene                       1        872.9199        961.6689
trichloroethylene             1        882.3066        961.6415
butanol                       1        883.6639        961.4632
chloroform                    1        887.8140        961.3934
1,1-dichloroethene            1        871.9528        960.7872
methyl ethyl ketone           1        876.8266        961.1564
methyl isobutyl ketone        2        947.3242        961.0986
1,1,2,2-tetrachloroethane     1        876.6570        961.7367
chlorobenzene                 1        867.2034        961.6577
```

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8074074: Input File

```
't8074074','t8074074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.241,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,7.4e-6
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids: 8,600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.241 cm2
c     so effectiveH2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 7.4e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8074074: Output File

```
t8074074
carbon tetrachloride        7       465.5561        501.9527
methanol                    4       453.8141        501.5878
dichloromethane             5       452.4838        501.9785
toluene                     7       464.8130        502.1236
trichloroethylene           6       453.6494        502.1157
butanol                     6       456.4865        502.0382
chloroform                  6       459.8274        502.0032
1,1-dichloroethene          6       459.3513        501.6820
methyl ethyl ketone         6       456.9875        501.8796
methyl isobutyl ketone      7       456.6086        501.8490
1,1,2,2-tetrachloroethane   7       465.4999        502.0477
chlorobenzene               7       462.4960        502.1206
```

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8074185: Input File

```
't8074185','t8074185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.603,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,7.4e-6
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids: 8,600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.603 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=1.85e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 7.4e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8074185: Output File

t8074185

carbon tetrachloride	4	663.1346	715.6897
methanol	3	681.4182	714.9351
dichloromethane	3	652.2636	715.7444
toluene	4	662.9108	716.0959
trichloroethylene	4	669.3142	716.0663
butanol	4	672.1841	715.8744
chloroform	4	675.7382	715.7976
1,1-dichloroethene	**4**	**674.1207**	**715.1282**
methyl ethyl ketone	4	672.1323	715.5364
methyl isobutyl ketone	4	649.6943	715.4725
1,1,2,2-tetrachloroethane	4	664.1242	716.1395
chlorobenzene	4	659.5460	716.0833

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8074925: Input File

```
't8074925','t8074925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,3.01,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,7.4e-6
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids = 8,600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 3.01 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=9.25e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 7.4e-6 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8074925: Output File

```
t8074925
carbon tetrachloride        1        840.2238        925.4800
methanol                    1        898.1680        924.2128
dichloromethane             1        879.2485        925.5725
toluene                     1        848.1656        926.1848
trichloroethylene           1        856.6945        926.1303
butanol                     1        857.7880        925.7936
chloroform                  1        861.4701        925.6628
1,1-dichloroethene          1        846.4914        924.5364
methyl ethyl ketone         1        851.2829        925.2216
methyl isobutyl ketone      2        913.8542        925.1141
1,1,2,2-tetrachloroethane   1        851.6446        926.3470
chlorobenzene               1        842.9221        926.1617
```

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8185074: Input File

```
't8185074','t8185074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.241,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,1.85e-5
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids: 8600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.241 cm2
c     so effectiveH2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 1.85e-5 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8185074: Output File

```
t8185074
```

carbon tetrachloride	4	266.0744	287.3196
methanol	3	273.5497	287.0161
dichloromethane	3	261.6819	287.3415
toluene	4	265.9120	287.4810
trichloroethylene	4	268.5045	287.4695
butanol	4	269.6956	287.3936
chloroform	4	271.1426	287.3628
1,1-dichloroethene	**4**	**270.5892**	**287.0938**
methyl ethyl ketone	4	269.7270	287.2580
methyl isobutyl ketone	4	260.7000	287.2323
1,1,2,2-tetrachloroethane	4	266.3810	287.4908
chlorobenzene	4	264.5522	287.4761

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8185185: Input File

```
't8185185','t8185185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,0.603,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,1.85e-5
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids: 8,600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 0.603 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=1.85e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 1.85e-5 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8185185: Output File

t8185185

carbon tetrachloride	3	470.6234	501.7274
methanol	2	472.4922	500.7984
dichloromethane	3	485.9264	501.7951
toluene	3	470.9908	502.2386
trichloroethylene	3	474.9670	502.1997
butanol	3	476.5443	501.9566
chloroform	3	478.6462	501.8611
1,1-dichloroethene	**3**	**476.9117**	**501.0356**
methyl ethyl ketone	3	476.1206	501.5381
methyl isobutyl ketone	3	461.7566	501.4593
1,1,2,2-tetrachloroethane	3	471.8790	502.3331
chlorobenzene	3	468.8463	502.2219

85-Gallon Drum with Headspace Sample Taken between Inner and Outer Drum Lids (continued)

T8185925: Input File

```
't8185925','t8185925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
0.,0.,0.,0.,0.
1.e4,150.,0.,0.001,0.3
1.e3,3.01,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,1.85e-5
c     85-gallon, w/inner and outer lids, each w/ filter vent
c     Only two void volumes: Below inner lid and between inner and outer lids
c     System modeled as inner bag-liner-drum
c     Inner bag has ultrathin walls (xd = 0.001 cm) and is porous (openings w/ area, Ad=150 cm2)
c     Void volume beneath inner lid is approx. 20% of total empty volume
c          Total volume beneath lid = 320 L (85 gal) – 8.6 L (void above lid)
c          Approximate void volume = 0.2 (310) = 62 L ⇔ 65,000 cm3
c     Void volume between lids = 8600 cm3
c     Inner lid exhibits no solubility for VOCs (thus, thin "liner thickness" xp=0.0001 cm)
c     Effective surface area across liner (xd= 1.0 cm): Ad = 3.01 cm2
c     so effective H2 release rate equals inner lid filter vent, D*(H2)=9.25e-5 mol/s/mol fraction
c     D*H2 = total H2 diffusivity characteristic across outer filter vent = 1.85e-5 mol/s/mol fr
c     VOC diffusivity characteristic estimated knowing D*H2, VOC Tc, VOC Pc
```

T8185925: Output File

```
t8185925
carbon tetrachloride          1          773.5464          832.4368
methanol                      1          814.0908          829.8752
dichloromethane               1          802.7208          832.6246
toluene                       1          780.4547          833.8783
trichloroethylene             1          786.8436          833.7634
butanol                       1          787.2900          833.0738
chloroform                    1          789.8329          832.8079
1,1-dichloroethene            1          777.1080          830.5281
methyl ethyl ketone           1          781.6499          831.9131
methyl isobutyl ketone        1          752.5953          831.6956
1,1,2,2-tetrachloroethane     1          783.3111          834.2515
chlorobenzene                 1          776.4089          833.8287
```

85-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid

T8000074: Input File

't8000074','t8000074.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
3000.,0.,20000.,0.0005,0.
12800.,150.,32500.,0.00005,1.4
0.,0.,32500.,0.,0.
25.,76.,74.e-7

c 85-gallon drum w/inner lid only w/ filter vent
c No plastic liner bag (xp=0.0005 cm)
c No liner (estimated by Ad=150 cm2, xd=1.4 cm, xp=0.00005)
c Void volume under inner lid = 65,000 cm3, equally divided between
c "liner" and outer headspace
c H2 diffusion characteristic across drum filter vent = 74.e-7 mol/s/mol fr

T8000074: Output File

t8000074

carbon tetrachloride	1	995.8677	995.9557
methanol	1	993.4168	993.7886
dichloromethane	1	996.1627	996.1661
toluene	1	997.3427	997.4229
trichloroethylene	1	997.2693	997.2736
butanol	1	996.4285	996.4465
chloroform	1	996.1760	996.1920
1,1-dichloroethene	**1**	**991.8830**	**994.0137**
methyl ethyl ketone	1	995.1074	995.3364
methyl isobutyl ketone	1	993.9341	995.1288
1,1,2,2-tetrachloroethane	1	997.5565	997.6067
chlorobenzene	1	997.1373	997.1726

85-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid (continued)

T8000185: Input File

```
't8000185','t8000185.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
3000.,0.,20000.,0.0005,0.
12800.,150.,32500.,0.00005,1.4
0.,0.,32500.,0.,0.
25.,76.,1.85e-5

c    85-gallon drum w/inner lid only w/ filter vent
c    No plastic liner bag (xp=0.0005 cm)
c    No liner (estimated by Ad=150 cm2, xd=1.4 cm, xp=0.00005)
c    Void volume under inner lid = 65,000 cm3, equally divided between
c    fictional "liner" and outer headspace
c    H2 diffusion characteristic across drum filter vent = 1.85e-5 mol/s/mol fr
```

T8000185: Output File

t8000185

carbon tetrachloride	1	989.8693	989.9524
methanol	1	984.2750	984.6179
dichloromethane	1	990.4725	990.4758
toluene	1	993.5079	993.5881
trichloroethylene	1	993.2111	993.2153
butanol	1	991.1495	991.1669
chloroform	1	990.5217	990.5371
1,1-dichloroethene	**1**	**983.1649**	**985.1692**
methyl ethyl ketone	1	988.2098	988.4253
methyl isobutyl ketone	1	986.7792	987.9132
1,1,2,2-tetrachloroethane	1	994.0003	994.0502
chlorobenzene	1	992.9312	992.9661

85-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid (continued)

T8000925: Input File

```
't8000925','t8000925.out',12
'carbon tetrachloride',0.,1000.,0.,0.
153.82,193.e-10,0.0828,556.4,45.0,0.,0.0217,6.e-5,0.
'methanol',0.,1000.,0.,0.
32.0,135.e-10,0.152,513.2,78.5,0.,0.0272,2.4e-7,0.
'dichloromethane',0.,1000.,0.,0.
84.9,263.e-10,0.104,510.,62.2,0.,0.0431,2.e-6,0.
'toluene',0.,1000.,0.,0.
92.1,669.e-10,0.0849,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',0.,1000.,0.,0.
131.4,583.e-10,0.0875,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',0.,1000.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',0.,1000.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,8.e-6,0.
'1,1-dichloroethene',0.,1000.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,8.e-6,0.
'methyl ethyl ketone',0.,1000.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,8.e-6,0.
'methyl isobutyl ketone',0.,1000.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,8.e-6,0.
'1,1,2,2-tetrachloroethane',0.,1000.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,8.e-6,0.
'chlorobenzene',0.,1000.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,8.e-6,0.
0.,0.,0.,0.,0.
3000.,0.,20000.,0.0005,0.
12800.,150.,32500.,0.00005,1.4
0.,0.,32500.,0.,0.
25.,76.,9.25e-5

c    85-gallon drum w/inner lid only w/ filter vent
c    No plastic liner bag (xp=0.0005 cm)
c    No liner (estimated by Ad=150 cm2, xd=1.4 cm, xp=0.00005)
c    Void volume under inner lid = 65,000 cm3, equally divided between
c    fictional "liner" and outer headspace
c    H2 diffusion characteristic across drum filter vent = 9.25e-5 mol/s/mol fr
```

T8000925: Output File

t8000925

carbon tetrachloride	1	951.6512	951.7082
methanol	1	927.3497	927.5541
dichloromethane	1	954.1380	954.1399
toluene	1	968.6779	968.7537
trichloroethylene	1	966.9775	966.9815
butanol	1	957.3364	957.3524
chloroform	1	954.4067	954.4180
1,1-dichloroethene	**1**	**928.6652**	**930.0061**
methyl ethyl ketone	1	944.5496	944.6951
methyl isobutyl ketone	1	941.5576	942.3600
1,1,2,2-tetrachloroethane	1	970.9257	970.9733
chlorobenzene	1	965.7715	965.8041

85-Gallon Drum with Headspace Sample Taken Inside Inner Drum Lid (continued)

U8037074: Input File (Bounding Case: 85-gallon drum with four (4) inner polymer bags and two (2) liner bags)

```
'u8037074','u8037074.out',12
'carbon tetrachloride',1000.,0.,0.,0.
153.82,193.e-10,0.0,556.4,45.0,0.,0.0217,0.,0.
'methanol',1000.,0.,0.,0.
32.0,135.e-10,0.,513.2,78.5,0.,0.0272,0.,0.
'dichloromethane',1000.,0.,0.,0.
84.9,263.e-10,0.,510.,62.2,0.,0.0431,0.,0.
'toluene',1000.,0.,0.,0.
92.1,669.e-10,0.0,591.8,40.5,0.,0.002857,7.e-6,0.
'trichloroethylene',1000.,0.,0.,0.
131.4,583.e-10,0.0,572.0,49.8,0.,0.00640,6.e-5,0.
'butanol',1000.,0.,0.,0.
74.1,300.e-10,0.,563.1,43.6,0.,0.02273,8.e-6,0.
'chloroform',1000.,0.,0.,0.
119.4,260.e-10,0.,536.4,53.0,0.,0.04545,0.,0.
'1,1-dichloroethene',1000.,0.,0.,0.
96.9,110.e-10,0.,513.0,47.5,0.,0.09091,0.,0.
'methyl ethyl ketone',1000.,0.,0.,0.
72.1,165.e-10,0.,536.8,41.5,0.,0.03704,0.,0.
'methyl isobutyl ketone',1000.,0.,0.,0.
100.2,130.e-10,0.,571.0,32.3,0.,0.01724,0.,0.
'1,1,2,2-tetrachloroethane',1000.,0.,0.,0.
167.9,2300.e-10,0.,661.2,57.6,0.,0.003846,0.,0.
'chlorobenzene',1000.,0.,0.,0.
112.6,600.e-10,0.,632.4,44.6,0.,0.007692,0.,0.
20000.,0.,0.,0.050,0.
20000.,0.,20000.,0.056,0.
1.e3,0.241,65000.,0.0001,1.0
0.,0.,8600.,0.,0.
25.,76.,3.7e-6
c  85-gallon, w/inner and outer lids, each w/ filter vent, 4 inner bags, 2 liner bags
c   Value for volume within innermost bags not required.
c   Void volume between bags: 20,000 cm3
c   Bag thickness same as in Scenario 3
c   Void volume beneath inner lid is approx. 20% of total empty volume
c      Total volume beneath lid = 320 L (85 gal) - 8.6 L (void above lid)
c      Approximate void volume = 0.2 (310) = 62 L <=> 65,000 cm3
c   Void volume between lids: 8,600 cm3
c   Inner lid exhibits no solubility for VOCs (thus,thin "liner thickness" xp =0.0001 cm)
c   Effective surface area across liner (assuming xd= 1.0 cm): Ad = 0.241 cm2
c    so effective H2 release rate equals inner lid filter vent, D*(H2)=7.4e-6 mol/s/mol fraction
c   D*H2 = total H2 diff. char. across outer filter vent = 3.7e-6 mol/s/mol fr
c   VOC diff. char. estimated knowing D*H2, VOC Tc, VOC Pc
```

U8037074: Output File

```
  u8037074
 carbon tetrachloride        13   596.4114     655.0548
 methanol                    13   584.4387     638.6078
 dichloromethane             10   595.5059     656.2900
 toluene                     10   610.4662     664.6641
 trichloroethylene           10   613.4802     663.8801
 butanol                     11   605.7879     659.2662
 chloroform                  11   599.8601     657.5004
 1,1-dichloroethene          16   578.6065     642.7302
 methyl ethyl ketone         13   587.3387     651.6319
 methyl isobutyl ketone      16   588.0140     650.2192
 1,1,2,2-tetrachloroethane    9   609.8720     667.2350
 chlorobenzene               10   604.9708     664.3227
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