

Modeling VOC Transport in Simulated Waste Drums

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Published June 1993

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Prepared for the
U.S. Department of Energy
Assistant Secretary for ER&WM
Under DOE Idaho Field Office
Contract DE-AC07-76ID01570

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Table C-3. Percent relative error for continuing calibration standard analytes for test period II.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	MeCl2	Freon	TCA	CCl4	TCE
Day 2	Conc. (ppm)	500.8	396.6	536.6	209.6	49.2	497.4	439.5	480.0	158.6	149.9
	%Rec	100.4	105.2	105.6	99.3	84.4	104.7	97.5	96.8	106.4	98.0
	Rel. % Error	0.4	5.2	5.6	-0.7	-15.6	4.7	-2.5	-3.2	6.4	-2.0
Day 5	Conc. (ppm)	519.5	383.9	520.2	219.9	55.4	507.6	436.0	480.9	158.7	146.5
	%Rec	104.1	101.8	102.4	104.2	95.0	106.9	96.7	97.0	106.5	95.8
	Rel. % Error	4.1	1.8	2.4	4.2	-5.0	6.9	-3.3	-3.0	6.5	-4.2
Day 7	Conc. (ppm)	515.0	382.6	520.1	211.7	52.7	513.4	451.2	497.2	162.3	158.0
	%Rec	103.2	101.5	102.4	100.3	90.4	108.1	100.0	100.2	108.9	103.3
	Rel. % Error	3.2	1.5	2.4	0.3	-9.6	8.1	0.0	0.2	8.9	3.3
Day 9	Conc. (ppm)	510.1	373.5	507.5	212.0	58.0	506.4	452.5	492.6	156.4	155.8
	%Rec	102.2	99.1	99.9	100.5	99.5	106.6	100.3	99.3	105.0	101.8
	Rel. % Error	2.2	-0.9	-0.1	0.5	-0.5	6.6	0.3	-0.7	5.0	1.8
Day 12	Conc. (ppm)	469.7	361.0	482.9	199.6	48.3	456.9	423.3	448.5	138.7	143.4
	%Rec	94.1	95.8	95.1	94.6	82.8	96.2	93.9	90.4	93.1	93.7
	Rel. % Error	-5.9	-4.2	-4.9	-5.4	-17.2	-3.8	-6.1	-9.6	-6.9	-6.3
Day 14	Conc. (ppm)	465.8	347.6	470.0	199.0	51.9	468.6	421.3	434.0	116.3	136.3
	%Rec	93.3	92.2	92.5	94.3	89.0	98.7	93.4	87.5	78.1	89.1
	Rel. % Error	-6.7	-7.8	-7.5	-5.7	-11.0	-1.3	-6.6	-12.5	-21.9	-10.9
Day 16	Conc. (ppm)	477.0	363.0	489.3	200.9	52.5	479.3	437.1	451.7	124.4	144.1
	%Rec	95.6	96.3	96.3	95.2	90.1	100.9	96.9	91.1	83.5	94.2
	Rel. % Error	-4.4	-3.7	-3.7	-4.8	-9.9	0.9	-3.1	-8.9	-16.5	-5.8
Day 19	Conc. (ppm)	472.2	363.0	491.7	198.3	49.8	486.6	436.2	460.4	129.7	144.1
	%Rec	94.6	96.3	96.8	94.0	85.4	102.4	96.7	92.8	87.0	94.2
	Rel. % Error	-5.4	-3.7	-3.2	-6.0	-14.6	2.4	-3.3	-7.2	-13.0	-5.8
Day 22	Conc. (ppm)	467.2	356.9	484.7	188.9	47.3	489.8	436.1	465.5	135.3	144.1
	%Rec	93.6	94.7	95.4	89.5	81.1	103.1	96.7	93.9	90.8	94.2
	Rel. % Error	-6.4	-5.3	-4.6	-10.5	-18.9	3.1	-3.3	-6.1	-9.2	-5.8
Mean % Error		-2.1	-1.9	-1.5	-3.1	-11.4	3.1	-3.1	-5.7	-4.5	-4.0
Std. Dev.		4.5	4.1	4.3	4.5	5.9	4.0	2.3	4.3	11.5	4.4

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl2 - Methylene Chloride
 Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
 % Rec - Percent Recovery, Rel. % Error - Relative Percent Error

Table C-4. Percent relative error for continuing calibration standard analytes for test period III.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	MeCl ₂	Freon	TCA	CCl ₄	TCE
Day 2	Conc. (ppm)	525.2	394.3	522.4	212.4	57.0	511.9	463.8	503.7	157.1	161.0
	%Rec	105.3	104.6	102.8	100.7	97.8	107.8	102.8	101.6	105.4	105.2
	Rel. % Error	5.3	4.6	2.8	0.7	-2.2	7.8	2.8	1.6	5.4	5.2
Day 3	Conc. (ppm)	531.3	378.8	507.8	200.2	58.7	505.7	457.7	498.2	160.7	158.5
	%Rec	106.5	100.5	100.0	94.9	100.7	106.5	101.5	100.4	107.9	103.6
	Rel. % Error	6.5	0.5	0.0	-5.1	0.7	6.5	1.5	0.4	7.9	3.6
Day 5	Conc. (ppm)	519.6	369.9	497.4	193.0	54.7	494.5	444.1	482.2	151.3	152.8
	%Rec	104.1	98.1	97.9	91.5	93.8	104.1	98.5	97.2	101.5	99.9
	Rel. % Error	4.1	-1.9	-2.1	-8.5	-6.2	4.1	-1.5	-2.8	1.5	-0.1
Day 8	Conc. (ppm)	527.4	326.2	439.5	187.2	56.8	461.9	425.0	455.0	142.6	145.4
	%Rec	105.7	86.5	86.5	88.7	97.4	97.2	94.2	91.7	95.7	95.0
	Rel. % Error	5.7	-13.5	-13.5	-11.3	-2.6	-2.8	-5.8	-8.3	-4.3	-5.0
Day 10	Conc. (ppm)	514.7	342.6	456.4	202.4	61.8	459.2	422.8	453.7	142.1	144.6
	%Rec	103.1	90.9	89.8	95.9	106.0	96.7	93.7	91.5	95.4	94.5
	Rel. % Error	3.1	-9.1	-10.2	-4.1	6.0	-3.3	-6.3	-8.5	-4.6	-5.5
Day 12	Conc. (ppm)	510.5	364.5	484.7	194.2	53.9	463.9	424.6	459.1	146.0	145.3
	%Rec	102.3	96.7	95.4	92.0	92.5	97.7	94.1	92.6	98.0	95.0
	Rel. % Error	2.3	-3.3	-4.6	-8.0	-7.5	-2.3	-5.9	-7.4	-2.0	-5.0
Day 16	Conc. (ppm)	514.8	362.5	483.1	196.3	57.0	464.5	422.0	455.9	148.4	142.9
	%Rec	103.2	96.2	95.1	93.0	97.8	97.8	93.6	91.9	99.6	93.4
	Rel. % Error	3.2	-3.8	-4.9	-7.0	-2.2	-2.2	-6.4	-8.1	-0.4	-6.6
Day 19	Conc. (ppm)	494.1	353.9	468.4	194.1	53.9	441.9	409.6	439.6	139.7	140.9
	%Rec	99.0	93.9	92.2	92.0	92.5	93.0	90.8	88.6	93.8	92.1
	Rel. % Error	-1.0	-6.1	-7.8	-8.0	-7.5	-7.0	-9.2	-11.4	-6.2	-7.9
Day 22	Conc. (ppm)	515.3	367.7	484.4	212.9	62.3	450.3	419.3	452.4	155.9	144.6
	%Rec	103.3	97.5	95.4	100.9	106.9	94.8	93.0	91.2	104.6	94.5
	Rel. % Error	3.3	-2.5	-4.6	0.9	6.9	-5.2	-7.0	-8.8	4.6	-5.5
Mean % Error		3.6	-3.9	-5.0	-5.6	-1.6	-0.5	-4.2	-5.9	0.2	-3.0
Standard Deviation		2.2	5.3	5.0	4.2	5.3	5.3	4.1	4.5	5.0	4.7

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl₂ - Methylene Chloride
 Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl₄ - Carbon Tetrachloride, TCE - Trichloroethylene
 % Rec - Percent Recovery, Rel. % Error - Relative Percent Error

Table C-5. Percent relative error for continuing calibration standard analytes for test period IV.

CCS Day		MeOH	Hexane	TCA	Toluene	Xylene	MeCl2	Freon	TCA	CCl4	TCE
Day 2	Conc. (ppm)	447.6	405.1	504.5	214.3	52.8	362.1	446.2	531.3	264.2	166.5
	%Rec	89.7	107.5	99.3	101.6	90.6	76.2	98.9	107.1	177.3	108.8
	Rel. % Error	-10.3	7.5	-0.7	1.6	-9.4	-23.8	-1.1	7.1	77.3	8.8
Day 3	Conc. (ppm)	417.6	350.6	463.8	197.9	56.7	387.9	447.9	457.3	136.3	140.2
	%Rec	83.7	93.0	91.3	93.8	97.3	81.7	99.3	92.2	91.5	91.6
	Rel. % Error	-16.3	-7.0	-8.7	-6.2	-2.7	-18.3	-0.7	-7.8	-8.5	-8.4
Day 5	Conc. (ppm)	444.1	375.9	503.0	205.5	59.1	418.6	485.8	509.6	155.1	155.4
	%Rec	89.0	99.7	99.0	97.4	101.4	88.1	107.7	102.7	104.1	101.6
	Rel. % Error	-11.0	-0.3	-1.0	-2.6	1.4	-11.9	7.7	2.7	4.1	1.6
Day 8	Conc. (ppm)	451.4	379.1	504.9	214.9	63.2	416.5	484.6	508.6	152.1	155.2
	%Rec	90.5	100.6	99.4	101.8	108.4	87.7	107.5	102.5	102.1	101.4
	Rel. % Error	-9.5	0.6	-0.6	1.8	8.4	-12.3	7.5	2.5	2.1	1.4
Day 10	Conc. (ppm)	473.2	380.4	509.4	213.3	65.0	420.8	495.1	525.7	160.1	162.9
	%Rec	94.8	100.9	100.3	101.1	111.5	88.6	109.8	106.0	107.4	106.5
	Rel. % Error	-5.2	0.9	0.3	1.1	11.5	-11.4	9.8	6.0	7.4	6.5
Day 12	Conc. (ppm)	473.8	381.4	507.3	217.7	66.8	420.1	495.2	527.9	164.3	162.4
	%Rec	94.9	101.2	99.9	103.2	114.6	88.4	109.8	106.4	110.3	106.1
	Rel. % Error	-5.1	1.2	-0.1	3.2	14.6	-11.6	9.8	6.4	10.3	6.1
Day 16	Conc. (ppm)	488.0	404.7	546.0	231.9	68.7	447.0	522.4	543.0	155.7	164.8
	%Rec	97.8	107.3	107.5	109.9	117.8	94.1	115.8	109.5	104.5	107.7
	Rel. % Error	-2.2	7.3	7.5	9.9	17.8	-5.9	15.8	9.5	4.5	7.7
Day 19	Conc. (ppm)	473.1	388.4	527.2	226.0	67.9	445.2	516.9	536.7	162.4	164.0
	%Rec	94.8	103.0	103.8	107.1	116.5	93.7	114.6	108.2	109.0	107.2
	Rel. % Error	-5.2	3.0	3.8	7.1	16.5	-6.3	14.6	8.2	9.0	7.2
Day 22	Conc. (ppm)	476.3	395.7	530.9	229.9	67.3	434.3	511.0	531.7	153.1	165.1
	%Rec	95.5	105.0	104.5	109.0	115.4	91.4	113.3	107.2	102.8	107.9
	Rel. % Error	-4.5	5.0	4.5	9.0	15.4	-8.6	13.3	7.2	2.8	7.9
Mean % Error		-7.7	2.0	0.5	2.8	8.2	-12.2	8.5	4.7	4.0	4.3
Std. Dev.		4.4	4.5	4.5	5.3	9.6	5.7	6.1	5.2	5.8	5.5

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl2 - Methylene Chloride
 Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene
 % Rec - Percent Recovery, Rel. % Error - Relative Percent Error

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Table C-6. Relative percent difference (RPD) for duplicate sample analyses during test period I.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	MeCl2	Freon	TCA	CCl4	TCE
102-3SB4						774.6	228.9	303.2	68.0	49.0
102-3SB4D						758.7	225.2	291.7	65.1	48.4
RPD						2.07	1.63	3.87	4.36	1.23
103-3SB2						615.4	195.0	206.6	48.6	42.6
103-3SB2D						601.7	192.2	202.9	47.9	42.1
RPD						2.25	1.45	1.81	1.45	1.18
105-1SB2						248.7	162.9	156.7	39.3	34.4
105-1SB2D						247.0	162.7	163.3	41.3	37.5
RPD						0.69	0.12	-4.13	-4.96	-8.62
108-2SB2	No Data	No Data	No Data	No Data	No Data					
108-2SB2D	No Data	No Data	No Data	No Data	No Data					
RPD										
110-4SB2	108.3 *	65.7	101.5 *	18.6 *	6.4					
110-4SB2D	108.4 *	65.5	101.1 *	18.5 *	6.4					
RPD	-0.09	0.30	0.39	0.54	0.00					
112-2SB3	* 83.7 *	62.1	93.5 *	19.8 *	6.7					
112-2SB3D	* 83.3 *	70.4	101.3 *	24.3 *	7.6					
RPD	0.48	-12.53	-8.01	-20.41	-12.59					
116-1SB4						102.3 *	67.3 *	79.9 *	19.5 *	14.7
116-1SB4D						104.5 *	68.7 *	88.2 *	22.7 *	17.6
RPD						-2.13	-2.06	-9.88	-15.17	-17.96
119-4SB3	* 79.6 *	57.0 *	86.0 *	16.7 *	6.1					
119-4SB3D	* 79.5 *	57.1 *	86.1 *	16.6 *	6.1					
RPD	0.13	-0.18	-0.12	0.60	0.00					
122-3SB3						110.6 *	65.4 *	82.0 *	20.2 *	13.5
122-3SB3D						111.0 *	65.3 *	81.9 *	19.4 *	13.6
RPD						-0.36	0.15	0.12	4.04	-0.74

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl2 - Methylene Chloride

Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene

RPD - Relative Percent Difference, * - Outside Linear Dynamic Range

Table C-7. Relative percent difference (RPD) for duplicate sample analyses during test period II.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	MeCl2	Freon	TCA	CCl4	TCE
202-3SB4						579.2	180.4	203.3	48.3	35.5
202-3SB4D						568.0	179.0	198.8	48.2	35.2
RPD						1.95	0.78	2.24	0.21	0.85
203-3SB2						389.0	161.5	160.6	41.1 *	32.0
203-3SB2D						380.3	160.1	159.0	40.3 *	31.7
RPD						2.26	0.87	1.00	1.97	0.94
205-1SB2						240.3	138.7	143.7	36.9 *	29.6
205-1SB2D						213.4	127.7	135.5	36.5 *	29.8
RPD						11.86	8.26	5.87	1.09	-0.67
208-2SB2	106.7 *	59.3	96.8 *	16.5 *	4.9					
208-2SB2D	106.0	75.5	112.8 *	16.4 *	7.4					
RPD	0.66	-24.04	-15.27	0.61	-40.65					
210-4SB2	107.4 *	61.8	100.7 *	14.9 *	4.8					
210-4SB2D	107.6 *	61.8	100.7 *	14.9 *	4.8					
RPD	-0.19	0.00	0.00	0.00	0.00					
212-2SB3	* 73.0	* 47.8	* 77.1	* 15.0	* 5.0					
212-2SB3D	* 74.1	* 56.9	* 86.4	* 19.4	* 5.8					
RPD	-1.50	-17.38	-11.38	-25.58	-14.81					
216-1SB4						* 89.0	* 64.3	* 76.6	* 19.9	* 17.4
216-1SB4D						* 78.8	* 58.2	* 74.3	* 19.7	* 18.5
RPD						12.16	9.96	3.05	1.01	-6.13
219-4SB3	* 74.2	* 46.0	* 76.6	* 10.9	* 4.3					
219-4SB3D	* 74.2	* 46.0	* 76.6	* 10.9	* 4.3					
RPD	0.00	0.00	0.00	0.00	0.00					
222-3SB3						95.9	* 65.1	* 75.2	* 20.3	* 15.4
222-3SB3D						95.3	* 64.6	* 75.1	* 20.6	* 15.4
RPD						0.63	0.77	0.13	-1.47	0.00

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl2 - Methylene Chloride

Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl4 - Carbon Tetrachloride, TCE - Trichloroethylene

RPD - Relative Percent Difference, * - Outside Linear Dynamic Range

Table C-8. Relative percent difference (RPD) for duplicate sample analyses during test period III.
(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	MeCl ₂	Freon	TCA	CCl ₄	TCE
302-3SB4	286.5	128.5	229.0 *	26.6 *	9.6					
302-3SB4D	271.1	123.6	219.5 *	26.2 *	9.5					
RPD	5.52	3.89	4.24	1.52	1.05					
305-3SB2	149.7	80.5	129.8 *	18.6 *	8.7					
305-3SB2D	144.3	78.5	126.5 *	18.3 *	8.6					
RPD	3.67	2.52	2.58	1.63	1.16					
307-1SB2						168.5	112.2	118.0 *	28.9 *	22.4
307-1SB2D						* 86.6 *	* 65.3 *	* 72.8 *	* 17.8 *	16.3
RPD						64.21	52.85	47.38	47.54	31.52
309-2SB2	108.9 *	67.5	103.3 *	16.2 *	8.5					
309-2SB2D	104.4	74.7	109.7 *	21.5 *	9.6					
RPD	4.22	-10.13	-6.01	-28.12	-12.15					
312-4SB2						119.6 *	70.8 *	80.4 *	17.6 *	14.0
312-4SB2D						119.1 *	71.2 *	80.4 *	17.7 *	14.0
RPD						0.42	-0.56	0.00	-0.57	0.00
314-2SB3	* 51.9 *	* 35.2 *	* 49.4 *	* 11.4	9.1					
314-2SB3D	No Data	No Data	No Data	No Data	No Data					
RPD										
316-1SB4						No Data	No Data	No Data	No Data	No Data
316-1SB4D						* 83.7 *	* 59.4	71.1 *	* 14.7 *	16.1
RPD										
319-4SB3						* 76.5 *	* 52.4 *	* 62.5 *	* 11.5 *	10.9
319-4SB3D						* 48.8 *	* 38.5 *	* 45.6 *	* 7.8 *	8.7
RPD						44.21	30.58	31.27	38.34	22.45
322-3SB3	* 59.3 *	* 41.3 *	* 67.3 *	* 8.0 *	7.9					
322-3SB3D	* 57.4 *	* 41.2 *	* 67.2 *	* 8.0 *	7.6					
RPD	3.26	0.24	0.15	0.00	3.87					

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl₂ - Methylene Chloride
 Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl₄ - Carbon Tetrachloride, TCE - Trichloroethylene
 RPD - Relative Percent Difference, * - Outside Linear Dynamic Range

Table C-9. Relative percent difference (RPD) for duplicate sample analyses during test period IV.

(Concentrations in ppm)

Sample Location	MeOH	Hexane	TCA	Toluene	Xylene	MeCl ₂	Freon	TCA	CCl ₄	TCE
402-3SB4						562.8	142.3	226.9	88.3 *	33.7
402-3SB4D						554.8	140.0	219.5	84.5 *	33.3
RPD						1.43	1.63	3.32	4.40	1.19
403-3SB2						447.0	120.7	132.8	35.8 *	24.9
403-3SB2D						439.2	119.3	130.6	34.8 *	24.7
RPD						1.76	1.17	1.67	2.83	0.81
405-1SB2						337.9	130.8	142.1	40.2 *	29.9
405-1SB2D						326.7	130.9	150.1	43.9	35.2
RPD						3.37	-0.08	-5.48	-8.80	-16.28
408-2SB2	* 81.0	* 64.2	105.8	* 3.3	ND					
408-2SB2D	* 79.9	74.8	116.9	* 10.6	ND					
RPD	1.37	-15.25	-9.97	-105.04						
410-4SB2	* 72.2	* 66.3	108.7	* 3.4	ND					
410-4SB2D	* 72.4	* 66.0	108.2	* 3.3	ND					
RPD	-0.28	0.45	0.46	2.99						
412-2SB3	* 65.3	* 53.3	88.1	* 0.7	ND					
412-2SB3D	* 65.0	* 60.8	95.5	* 6.1	ND					
RPD	0.46	-13.15	-8.06	-158.82						
416-1SB4						193.1 *	56.4 *	81.7 *	25.0 *	20.0
416-1SB4D						195.0 *	57.7 *	89.8 *	27.7 *	23.1
RPD						-0.98	-2.28	-9.45	-10.25	-14.39
419-4SB3	* 46.7	* 42.3	* 71.9	ND	ND					
419-4SB3D	* 46.8	* 42.2	* 71.9	ND	ND					
RPD	-0.21	0.24	0.00							
422-3SB3						186.1 *	40.8 *	67.7 *	19.1 *	13.5
422-3SB3D						185.7 *	40.8 *	67.9 *	19.1 *	13.6
RPD						0.22	0.00	-0.29	0.00	-0.74

MeOH - Methanol, Hexane - Cyclohexane, TCA - 1,1,1-Trichloroethane, Xylene - para Xylene, MeCl₂ - Methylene Chloride

Freon - Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane), CCl₄ - Carbon Tetrachloride, TCE - Trichloroethylene

RPD - Relative Percent Difference, * - Outside Linear Dynamic Range, ND - Not Detected

Appendix D

Computer Program of VOC Transport Model for Lab-Scale Simulated Waste Drums


```

c
c program calculates the VOC concentration as a function of time
c in a simulated waste drum. The drum contains small poly bags initially
c filled with VOC-containing air. These bags were placed in a large poly
c bag inside a 90-mil rigid polyethylene liner, inside a vented metal drum.
c-----
c allows user to specify different model parameters for one small bag
c the parameters for other three small bags are the same. this allows user
c to describe situations where one bag may be smaller, have a leak, etc.
c-----
c model accounts for VOC accumulation in poly bags and liner
c-----
c model allows user to specify if drum temperature is constant or variable
c-----
c The program utilizes an IMSL routine to solve a series of first-order
c ordinary differential equations.
c
character*32 test,ifname,ofname,vocid(9)
real aa(1,1),yy(5,5),yz(9),sb1(5,21),sb2(5,21),lb(5,21),dh(5,21)
real param(50),p,d,ap(5),ad(5),v(5),xp(5),xd(5),mw
integer ivoc(5)
common/qq/p,d,ap,ad,v,xp,xd,pi,patm,pHg,dfh,c0,mw,temp0,
#vpb,vpc,y0,s0c0,nft,thr1
common/ss/s6,s7,s8,s9
external fcn,ivpag,sset
c-----
c input
c-----
write(*,9)
9 format(1x,'Enter name of input data file ')
read(*,*)ifname
open(unit=3,file=ifname,status='unknown')
c-----
c User provided input
c nvoc - number of VOCs in drum
c y(i,n) - i-th VOC concentration in n-th layer of confinement, (mol/cm3)
c n=1, small bag headspace (for 3 identical bags)
c n=2, small bag headspace (for 4th small bag)
c** allows user to specify unique conditions of one of four small bags
c n=3, large bag headspace
c n=4, drum liner headspace
c n=5, drum headspace
c ap(n) - permeation surface area around n-th layer of confinement (cm2)
c ad(n) - cross-sectional area for diffusion out of n-th layer
c of confinement (cm2)
c xp(n) - thickness of permeable surface (cm)
c xd(n) - length of diffusional path between layers of confinement (cm)
c v(n) - void volume in n-th layer of confinement (cm3)
c *****
c ivoc - VOC identification number
c 1 - CC14 2 - cyclohexane 3 - methanol 4 - CH2Cl2
c 5 - toluene 6 - TCA 7 - TCE 8 - Freon-113 9 - p-xylene
c *****
vocid(1)='carbon tetrachloride'
vocid(2)='cyclohexane'
vocid(3)='methanol'
vocid(4)='methylene chloride'
vocid(5)='toluene'
vocid(6)='1,1,1-trichloroethane'
vocid(7)='trichloroethylene'
vocid(8)='Freon-113'
vocid(9)='p-xylene'

```

```

c yvoc(i) - concentration of VOC i in drum headspace, ppmv
c nft - if = 1, temperature = constant
c       if = 2, temperature = f(t)
c thr1 - approximate number of hours after t=0 when heating cycle begins
c thr2 - approximate number of hours after t=0 when small bags first sampled
c temp - drum temperature, C
c pHg - atmospheric pressure, cm Hg
c dfh - carbon composite filter H2-diffusion constant, mol/s/mol fraction
c -----
c initial conditions
  read(3,*)test.ofname
  open(unit=2,file=ofname,status='unknown')
  read(3,*)nvoc
c neq - number of layers of confinement inside waste drum
  neq=5
  do 8 i=1,nvoc
    read(3,*)ivoc(i),(yy(i,j),j=1,neq)
  8 continue
  read(3,*)(ap(j),ad(j),v(j),xp(j),xd(j),j=1,neq)
  read(3,*)nft,thr1,thr2,temp,pHg,dfh
c -----
c r0 - gas constant (cm3 atm/mol K)
c patm - atmospheric pressure (atm)
  r0=82.06
  pi=3.141592654
c convert pHg (cm Hg) to patm (atm)
  patm=pHg/76.0
c temp0 - initial drum temperature, K
  temp0=temp+273.2
c c0 - initial gas concentration in each layer of confinement (mol/cm3)
  c0=patm/(r0*temp0)
cccccc*****
cccccc  calculate concentration throughout waste drum for each VOC
cccccc*****
  nv=nvoc
  do 43 i=1,nv
c -----
c convert VOC gas concentration from ppmv to mol/cm3
  do 37 j=1,neq
    yz(j)=yy(i,j)*c0*1.e-6
  37 continue
c VOC conc. in polymer walls (6(3); 9(1) -small bag, 7 -large bag, 8 - liner)
c (cm3 VOC/cm3 polymer)
  yz(6)=0.
  yz(7)=0.
  yz(8)=0.
  yz(9)=0.
  nq=9
c y0 - initial VOC concentration in gas feed, mol/cm3
  y0=yz(1)
c -----
c set param to default values
  mxparm=50
  CALL SSET(mxparm,0.0,param,1)
  param(4)=150000
  param(10)=2
c param(12): 1=Adams' method; 2=Gear's backward difference method
  param(12)=2
c -----
c initialization of other variables
c t - time (sec)
  t=0.

```