Calculation and Verification of Filling Ratios for Liquified Gases

DTRS56-02-X-0049

Final Report Prepared for:

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Introduction

This report describes the work performed and results obtained under Reimbursable Agreement DTRS56-02-X-0049, *Calculation and Verification of Filling Ratios for Liquified Gases*. The major efforts were to establish our best estimates for key properties of select fluids, establish equation of state models to calculate densities at certain conditions, estimate filling ratios for these fluids according to standard protocols, and compare these calculated filling ratios with certain tabulated filling ratios. The fluids studied were those listed in Table 2 of amended Instruction P200 of the UN Model Regulations on the Transport of Dangerous Goods (Committee on the Transport of Dangerous Goods, Report of the Committee of Experts on its Twenty First Session dated 26 January 2001). Filling ratio protocols were developed from the descriptions given in instruction P200 and in DOT 49 CFR, Section 173.304. Comparisons were made with filling ratios (or maximum permitted filling density—percent) tabulated in P200 and in 49 CFR Section 173.304.

The key properties of the fluids are given in Table 1, *Fluid Properties*. The substances are sorted into "high pressure" fluids and "low pressure" fluids, and entries within these two sections are ordered by increasing critical temperature. High pressure fluids are those with critical temperatures between –50 ^{o}C and 65 ^{o}C, and low pressure fluids have critical temperatures greater than 65 ^{o}C, as defined in the P200 document. In Table 1, note that the subscript "c" represents the critical property, so T_c is critical temperature in degrees Celsius, P_c is the critical pressure in megapascals, ρ_c is the critical density in grams per liter (equivalent to grams per cubic decimeter), V_c is the critical volume in liters per kilogram (defined as $1/\rho_c$), and Z_c is the critical compressibility factor (defined by $Z_c = P_c/(\rho_c R T_c)$). Note that the current accepted value of the gas constant[1] is 8.314 472 $J \cdot mol^{-1} \cdot K$; this 1998 CODATA recommended value replaces earlier approximations such as that used in the draft P200 instruction. The sub-heading "ISO" in Table 1 indicates a value taken from the ISO/CD 11622 (Tc-rev1, 2000-09-05) document made available to us by DOT. The values for critical temperature, pressure, and density with the sub-heading "Rec." are our current recommendations; these are consistent with the equation of state reference (EOS ref.) indicated in the final column of the table. The critical volumes and critical compressibility factors were determined from the other table entries as indicated above.

The preferred equation of state sources were the dedicated equations of state that have been thoroughly evaluated and available in NIST standard reference databases[2] 12 or 23; in most of these cases, references to the original literature are given in Table 1. When such an equation of state was not available, calculations were done with the extended corresponding states (EXCST) model used in NIST Standard Reference Database 4; this model has been shown to be generally preferable to cubic equations of state for the calculation of liquid densities. The EXCST model is based on experimental data as available: typically critical properties, vapor pressure curves, and saturated liquid densities are used. For substances not included in Version 3.0 of the NIST Standard

[1] Peter J. Mohr and Barry N. Taylor, *J. Phys. Chem. Reference Data,* Vol. 28, No. 6, pp. 1713-1852, 1999.
[2] Information on NIST Standard Reference Databases are available at http://www.nist.gov/srd/fluids.htm

Reference Database 4, the properties used in the EXCST model were obtained from the American Institute of Chemical Engineers (AIChE) Design Institute for Physical Properties (DIPPR) Project 801 database (Sponsor Version 2.0, DIPPR Diadem, Brigham Young University, 2000). Generally the source data is experimental, but in some cases they are based on evaluated estimation methods. In some cases, experimental data available in the NIST Thermodynamics Research Center Source data system were considered. Note that the molar masses given in Table 1 were chosen to be consistent with the equation of state sources; generally these are based on the 1997 adjustment of the atomic weights of the elements, but for fluids not included in earlier NIST or DIPPR studies, we have used the 1999 IUPAC adjustment[3] for the current project. The differences in the molar masses are generally negligible, and not important for the current study.

The protocols for calculated filling ratios (or maximum permitted filling density—percent) were extracted from the P200 document and 49 CFR Section 173.304. These protocols were established in the first phase of the current project, and the document describing the procedure is included below. Some specific choices, for constants, etc., used in the final calculations are also indicated in this report. Tables 2 and 3 below provide summary comparisons for the "high pressure" fluids and "low pressure" fluids, respectively. Comparisons are provided between the P200 table and current calculations for each test pressure tabulated in P200; comparisons are provided between the CFR 173.304 values and current calculations for fluids and test pressures provided in CFR 173.304. A detailed description of the entries of each column in Table 2 and Table 3 is included below the tables.

More detailed information about each of the calculations can be found in the Excel spreadsheet that accompanies this report. Most of the information in the spreadsheet is self explanatory. Notes attached to some of the cells give information about the source of specific data or estimations, and our estimates of the overall uncertainty in density calculations for each fluid are indicated by the color coding described within the spreadsheet.

[3] T.B. Coplen, Pure Appl. Chem. **73**, No. 4, 667-683, 2001.

Protocol for DOT Project

(Revised 4/5/02 after discussions with M. Toughiry)

1. Choose 30 fluids from P200 (Table 2).
2. Enter critical temperature from ISO/CD 11622
    a. Verify with IUPAC temperature
    b. Use NIST temperature for work
3. Sort into "high pressure" (-50 ^{o}C < T_c < 65 ^{o}C) and "low pressure" (T_c > 65 ^{o}C)
4. Calculate filling ratios according to UN Reg.
    a. High Pressure, for each "test pressure," P_{test}, in Table 2: Note P_{test} is guage—use 1 bar to convert to absolute.
        i. Check service pressure as 2/3 test pressure—no need to check (as per Mark Toughiry 4/5/02)
        ii. Calculate filling density, ρ_F, as $\rho_F = \rho(65\ ^{o}C, P_{test})$ from NIST database
        iii. Calculate filling ratio as $f = \rho_F / \rho_o$; For ρ_o, use density of water at 15 ^{o}C and 0.101 325 MPa (as per MT); may change later
        iv. Compare calculated filling ratio with Table 2
    b. Low Pressure, for each "test pressure," P_{test}, (guage pressure) in Table 2
        i. Check that test pressure is greater than or equal to $P_\sigma(65\ ^{o}C) - 0.1$ MPa using NIST database: use absolute P for each and then don't subtract 0.1 MPa.
        ii. Calculate test density as $\rho_{test} = \rho(50\ ^{o}C, P_{test})$ from NIST database;
        iii. Calculate filling density as $\rho_F = 0.95\ \rho_{test}$
        iv. Compare ρ_F with $\rho_\sigma(60\ ^{o}C)$ from NIST database; ensure that $\rho_F < \rho_\sigma(60\ ^{o}C)$
        v. Calculate filling ratio as $f = \rho_F / \rho_o$ (Use ρ_o from above.)
        vi. Compare calculated filling ratio with Table 2
    c. Check for any notes in P200 relevant to fluids selected.
5. Calculate filling ratios according to 49 CFR 173.304 (a) (2)
    a. For each test pressure in P200, determine a nominal service pressure by multiplying by 3/5 (must use absolute test pressure).
    b. Convert nominal service pressure to psig.
    c. Choose service pressure from 49 CFR 173.304 (a) (2) list—final digits in container code is psig; choose closest to result from 5b.
    d. Determine test pressure using $P_{test} = 5/3\ P_s$ (use absolute)
    e. Calculate filling density, ρ_F, as $\rho_F = \rho(130\ ^{o}F, P_{test})$ from NIST database
    f. Compare ρ_F with $\rho_\sigma(130\ ^{o}F)$ from NIST database; ensure that $\rho_F < \rho_\sigma(130\ ^{o}F)$

g. Calculate filling ratio as $f = \rho_F / \rho_o$; Use density of water at 60 ^oF equal to 27.737 in^3/lb (as per MT; may change later)

h. Compare calculated filling ratio with 49 CFR 173.304 (a) (2).

i. Use test pressure of 3000 psig; calculate filling density, ρ_F, as $\rho_F = \rho(130\ ^oF, 3000\ psig)$ from NIST database

j. Calculate filling ratio as $f = \rho_F / \rho_o$; use ρ_o from above.

k. Compare calculated filling ratio with 49 CFR 173.304 (a) (2).

l. Check for any notes in 49 CFR 173.301 to 304 relevant to fluids selected.

6. Compile critical temperatures, pressures, compressibility factors, and references for each fluid.

7. Prepare written report summarizing findings. Primary result will be table comparing 5 filling ratios: UN, 49 CFR 173.304 (a) (2), our calculation using UN method, our calculation using 49 CFR 173.304 (a) (2) method, and our calculation using 3000 psig. (MT will send copies of ANSI 239.18 and SF 298 for possible final format; but this is not important.)

Table 1. Fluid Properties

UN #	Fluid	T_c(°C) ISO	T_c (°C) Rec.	P_c(MPa) Rec.	ρ_c(g/l) Rec.	V_c(l/kg) Rec.	Molar mass	Z_c	EOS ref.
1982	Tetrafluoromethane (R14)	-45.7	-45.64	3.75	625.66	1.598	88.005	0.279	[1]
2451	Nitrogen Trifluoride	-39.3	-39.15	4.46	562.47	1.778	71.019	0.289	[2]
1859	Silicon tetrafluoride	-14.2	-14.15	3.72	515.46	1.940	104.079	0.349	[3]
1008	boron trifluoride, BF3	-12.2	-12.25	4.99	549.44	1.820	67.806	0.284	[4]
2203	Silane	-3.5	-3.45	4.84	242.13	4.130	32.117	0.286	[5]
1962	Ethylene	9.2	9.2	5.04	214.25	4.667	28.054	0.281	[6]
2417	carbonyl fluoride	14.7	23.85	5.76	467.29	2.140	66.007	0.329	[7]
1911	Diborane	16	16.65	4.05	159.74	6.260	27.67	0.291	[8]
2036	Xenon	16.6	16.584	5.84	1099	0.910	131.3	0.290	[9]
2599	R503	na	18.595	4.30	552.93	1.809	87.247	0.280	[10]
2198	phosphorous pentafluoride	19	18.95	3.39	623.59	1.604	125.966	0.282	[11]
2193	Hexafluoroethane (R116)	19.7	19.88	3.04	622	1.608	138.01	0.277	[12]
1984	Trifluoromethane (R23)	26	26.143	4.83	526.5	1.899	70.014	0.258	[13]
1022	Chlorotrifluoromethane (R13)	28.8	28.85	3.88	582.88	1.716	104.46	0.277	[14]
1959	1,1-difluoroethylene	29.7	29.65	4.46	416.67	2.400	64.035	0.273	[15]
1013	Carbon Dioxide	30.1	30.978	7.38	467.6	2.139	44.01	0.275	[16]
1035	Ethane	32.3	32.18	4.87	206.58	4.841	30.07	0.279	[17]
1081	Tetrafluoroethylene	33.3	33.3	3.94	581.4	1.720	100.016	0.266	[18]
2192	Germane	34.8	34.85	5.55	546.45	1.830	76.642	0.303	[19]
1001	Acetylene	na	35.15	6.14	232.5	4.301	26.038	0.268	[20]
1070	Nitrous oxide	36.4	36.42	7.25	452.49	2.210	44.013	0.274	[21]
1080	Sulphur Hexafluoride	45.6	45.583	3.75	743.81	1.344	146.06	0.278	[22]
2454	Methyl Fluoride (R41)	na	44.13	5.90	316.51	3.159	34.033	0.240	[23]
1050	Hydrogen chloride	51.5	51.5	8.31	450.45	2.220	36.461	0.249	[24]
2199	Phosphine	51.9	51.6	6.54	301.2	3.320	33.998	0.274	[25]
1860	vinyl fluoride	54.7	54.65	5.24	319.49	3.130	46.044	0.277	[26]
3220	Pentafluoroethane (R125)	66.3	66.015	3.63	568	1.761	120.02	0.272	[27]
1009	Bromotrifluoromethane (R13B1)	66.8	67	3.97	746.27	1.340	148.91	0.281	[28]
2424	Octafluoropropane (R218)	71.9	71.95	2.67	627.98	1.592	188.02	0.279	[29]
3337	R404A	na	71.977	3.72	487.85	2.050	97.604	0.260	[30]
2035	1,1,1-trifluoroethane (R143a)	73.1	72.707	3.76	431	2.320	84.041	0.255	[31]

UN #	Fluid	T_c(°C) ISO	T_c (°C) Rec.	P_c(MPa) Rec.	ρ_c(g/l) Rec.	V_c(l/kg) Rec.	Molar mass	Z_c	EOS ref.
3339	R407B	na	74.284	4.07	563.43	1.775	102.94	0.257	[32]
3252	Difluoromethane (R32)	78	78.105	5.78	424	2.358	52.024	0.243	[33]
1020	Chloropentafluoroethane (R115)	80	79.95	3.12	613.1	1.631	154.47	0.268	[34]
1973	R502	na	80.727	3.97	568.92	1.758	111.63	0.264	[35]
3338	R407A	na	81.864	4.48	531.97	1.880	90.111	0.257	[36]
2195	telurium hexafluoride	83.2	107.03	3.45	961.6	1.040	241.59	0.274	[37]
2420	Hexafluoroacetone	84.1	83.99	2.84	505.05	1.980	166.023	0.314	[38]
3340	R407C	na	86.021	4.63	513.21	1.949	86.204	0.261	[39]
1858	Hexafluoropropylene	86.2	94.85	2.90	558.66	1.790	150.023	0.254	[40]
3153	perfluoromethylvinylether	87	89.85	3.11	574.71	1.740	166.023	0.298	[41]
1048	Hydrogen bromide	89.9	90.0	8.55	806.45	1.240	80.912	0.283	[42]
2191	sulphuryl fluoride	91	67.85	7.50	515.45	1.940	102.06	0.524	[43]
2418	sulphur tetrafluoride	91	90.95	4.60	600.33	1.666	108.0596	0.274	[44]
1077	Propylene	92.4	92.42	4.66	223.39	4.476	42.08	0.289	[45]
3083	Perchloryl fluoride	95.2	95.25	5.37	636.94	1.570	102.449	0.282	[46]
2194	selenium hexafluoride	na	95.65	4.48	1027.8	0.973	192.95	0.274	[47]
1018	Chlorodifluoromethane (R22)	96.2	96.145	4.99	523.84	1.909	86.468	0.268	[48]
1978	Propane	96.8	96.675	4.25	218.5	4.577	44.096	0.279	[49]
2422	octafluorobut-2-ene	98.3	118.85	2.33	578.03	1.730	200.031	0.248	[50]
2188	Arsine	99.9	99.85	6.55	800	1.250	77.945	0.207	[51]
1053	Hydrogen sulphide	100	100.45	9.01	347.06	2.881	34.082	0.285	[52]
3296	heptafluoropropane (R227ea)	100	101.65	2.93	573	1.745	170.03	0.279	[53]
3159	1,1,1,2-tetrafluoroethane (R134a)	101.1	101.06	4.06	511.9	1.954	102.03	0.260	[54]
2204	carbonyl sulphide	102	105.65	6.35	444.44	2.250	60.076	0.272	[55]
2602	R500	na	102.15	4.17	491.98	2.033	99.303	0.270	[56]
2453	Ethyl fluoride (R161)	102.2	102.16	5.03	293.26	3.410	48.06	0.264	[57]
1082	Trifluorochloroethylene	105.8	106.0	4.05	549.45	1.820	116.47	0.273	[58]
3057	Trifluoroacetylchloride	109	112.85	4.40	538.49	1.857	132.4696	0.337	[59]
1028	Dichlorodifluoromethane (R12)	112	111.97	4.14	565	1.770	120.91	0.276	[60]
1030	1,1-difluoroethane (R152a)	113.5	113.26	4.52	368	2.717	66.051	0.252	[61]
1976	Octafluorocyclobutane (RC318)	115.3	115.23	2.78	619.97	1.613	200.03	0.278	[62]
2200	Propadiene	120.7	120.85	5.25	242.72	4.120	40.065	0.264	[63]
1021	1-chloro-1,2,2,2-tetrafluoroethane (R124)	na	122.28	3.62	560	1.786	136.48	0.269	[64]
1027	Cyclopropane	125.2	125.15	5.58	258.5	3.868	42.081	0.274	[65]

UN #	Fluid	T_c(°C) ISO	T_c (°C) Rec.	P_c(MPa) Rec.	ρ_c(g/l) Rec.	V_c(l/kg) Rec.	Molar mass	Z_c	EOS ref.
1033	dimethyl ether	126.9	126.95	5.37	271	3.690	46.069	0.274	[66]
1026	Cyanogen	126.6	127.0	5.98	266.67	3.750	52.036	0.351	[67]
1005	Ammonia, Anhydrous	132.4	132.25	11.33	225	4.444	17.03	0.254	[68]
3154	perfluoroethylvinylether	132.8	127.85	2.80	602.41	1.660	216.031	0.301	[69]
1969	Isobutane	134.9	134.67	3.64	224.35	4.457	58.122	0.278	[70]
2517	1-chloro-1,1-difluoroethane (R142b)	137.1	137.11	4.07	446	2.242	100.5	0.269	[71]
2202	Hydrogen selenide	138	138.0	8.92	675.68	1.480	80.976	0.313	[72]
2548	chlorine pentafluoride	142.6	142.85	5.26	564.92	1.770	130.44	0.351	[73]
1063	Methyl chloride	143	143.1	6.68	353.36	2.830	50.488	0.276	[74]
1017	Chlorine	144	144.0	7.71	571.43	1.750	70.905	0.276	[75]
1055	Isobutylene (2-methylpropene)	144.7	144.75	4.00	234.74	4.260	56.108	0.275	[76]
1958	1,2-dichloro-1,1,2,2-tetrafluoroethane (R114)	145.7	145.68	3.26	579.97	1.724	170.92	0.276	[77]
1012	1-butylene	146.4	146.35	4.02	232.56	4.300	56.108	0.241	[78]
1983	1-chloro-2,2,2-trifluoroethane (R133a)	150	156.85	3.84	497.51	2.010	118.486	0.256	[79]
2197	Hydrogen iodide	150.8	150.7	8.31	1052.63	0.950	127.912	0.287	[80]
1011	Butane	152	151.98	3.80	227.84	4.389	58.122	0.274	[81]
1010	1,3-butadiene	152	151.85	4.32	244.5	4.090	54.092	0.270	[82]
1749	chlorine trifluoride	153.7	182.85	5.00	674.81	1.482	92.4484	0.181	[83]
1974	Chlorodifluorobromomethane (R12B1)	153.7	153.0	4.25	671.14	1.490	165.365	0.295	[84]
1012	Trans-2-butylene	155.5	155.45	4.10	235.85	4.240	56.108	0.274	[85]
1086	Vinyl chloride	156.5	158.85	5.67	349.65	2.860	62.499	0.283	[86]
1061	Methylamine	156.9	156.9	7.46	201.61	4.960	31.057	0.321	[87]
1079	Sulphur Dioxide	157.5	157.49	7.88	525.01	1.905	64.065	0.269	[88]
1067	nitrogen dioxide	158	158.0	10.13	558.66	1.790	46.006	0.233	[89]
1083	Trimethylamine	160.2	160.1	4.07	232.72	4.297	59.111	0.287	[90]
2044	2,2-dimethylpropane (neopentane)	160.6	160.65	3.20	234.74	4.260	72.15	0.272	[91]
1012	cis-2-butylene	162.4	162.35	4.21	239.81	4.170	56.108	0.272	[92]
1032	Dimethylamine	164.6	164.05	5.34	250.63	3.990	45.084	0.264	[93]
1039	Ethyl methyl ether	164.7	164.65	4.40	271.74	3.680	60.096	0.267	[94]
1069	nitrosyl chloride	167.5	167.5	9.12	471.7	2.120	65.459	0.346	[95]
2196	tungsten hexafluoride	170	179.55	4.57	2978.4	0.336	297.84	0.121	[96]
1087	Vinyl methyl ether	171.6	163.85	4.67	276.24	3.620	58.08	0.270	[97]
2676	Stibine	173	167.2	7.31	793.7	1.260	124.77	0.314	[98]
1010	1,2-butadiene	176.1	178.85	4.36	245.7	4.070	54.092	0.255	[99]

UN #	Fluid	T_c(°C) ISO	T_c (°C) Rec.	P_c(MPa) Rec.	ρ_c(g/l) Rec.	V_c(l/kg) Rec.	Molar mass	Z_c	EOS ref.
1029	dichlorofluoromethane (R21)	178.5	178.43	5.18	526.33	1.900	102.923	0.271	[100]
1741	boron trichloride	178.8	178.8	3.87	787.4	1.270	117.169	0.153	[101]
1076	Phosgene	182.3	181.85	5.67	520.83	1.920	98.916	0.285	[102]
1036	Ethylamine	183.4	183.0	5.62	217.86	4.590	45.084	0.307	[103]
1051	Hydrogen cyanide	183.5	183.5	5.39	194.55	5.140	27.026	0.197	[104]
2419	bromotrifluoroethylene	184.8	158.85	4.48	671.14	1.490	160.921	0.298	[105]
2189	Dichlorosilane	176.3	185.85	4.59	425.53	2.350	101.007	0.285	[106]
2601	Cyclobutane	186.8	186.78	4.98	267.38	3.740	56.108	0.273	[107]
1037	Ethyl chloride	187.2	187.2	5.27	322.58	3.100	64.514	0.275	[108]
1052	Hydrogen fluoride	na	188.0	6.48	289.86	3.450	20.006	0.117	[109]
2452	Ethylacetylene	190.5	166.85	4.60	259.74	3.850	54.092	0.262	[110]
1062	Methyl bromide	194	193.85	8.00	609.76	1.640	94.939	0.321	[111]
1040	ethylene oxide	195.8	196.0	7.19	314.47	3.180	44.053	0.259	[112]
1064	Methyl mercaptan	196.8	196.8	7.23	332.23	3.010	48.109	0.268	[113]
1085	Vinyl bromide	198	199.85	7.18	534.76	1.870	106.95	0.365	[114]
1589	Cyanogens chloride	215	175.85	5.99	377.36	2.650	61.47	0.262	[115]
1745	bromine pentafluoride	na	213.85	4.20	780.8	1.281	174.9	0.232	[116]
2495	iodine pentafluoride	na	305.85	3.70	887.6	1.127	221.9	0.192	[117]
1746	bromine trifluoride	na	362.85	5.30	805.29	1.242	136.9	0.1704	[118]
2901	bromine chloride	na	Na	Na	na	na	115.36	na	[119]

Table 2. "High Pressure" fluids (-50˚C <Tc <65˚C)

UN Number	Name	T_c (°C)	P_{test}(bar) UN, gauge	Filling ratio UN	Filling ratio, UN, NIST	NIST: 130 °F, 3000 psig fill ratio	test P (bar) from CFR 173.304	CFR 173.304 filling ratio NIST	CFR 173.304 filling ratio
1982	Tetrafluoromethane (R14)	-45.64	200	0.62	0.71	0.77			
1982	Tetrafluoromethane (R14)	-45.64	300	0.94	0.90	0.77			
2451	Nitrogen Trifluoride	-39.15	200	0.50	0.63	0.69			
2451	Nitrogen Trifluoride	-39.15	300	0.75	0.82	0.69			
1859	silicon tetrafluoride	-14.15	200	0.74	0.96	1.04			
1859	silicon tetrafluoride	-14.15	300	1.10	1.17	1.04			
1008	Boron trifluoride, BF3	-12.25	225	0.72	0.76	0.78			
1008	Boron trifluoride, BF3	-12.25	300	0.86	0.89	0.78			
2203	Silane	-3.45	225	0.32	0.33	0.34			
2203	Silane	-3.45	250	0.36	0.35	0.34			
1962	Ethylene	9.2	225	0.34	0.34	0.35	208.5	0.35	0.31
1962	Ethylene	9.2	300	0.37	0.38	0.35	277.5	0.39	0.36
2417	carbonyl fluoride	23.85	200	0.47	0.72	0.77			
2417	carbonyl fluoride	23.85	300	0.70	0.83	0.77			
1911	Diborane	16.65	250	0.07	0.30	0.29			
2036	Xenon	16.584	130	1.24	1.28	1.86			
2599	R503	18.595	31	0.11	0.12	1.02			
2599	R503	18.595	42	0.20	0.17	1.02			
2599	R503	18.595	100	0.66	0.64	1.02			
2198	phosphorous pentafluoride	18.95	200	0.90	1.12	1.18			
2198	phosphorous pentafluoride	18.95	300	1.34	1.25	1.18			
2193	Hexafluoroethane (R116)	19.88	200	1.10	1.13	1.19			
1984	Trifluoromethane (R23)	26.143	190	0.87	0.88	0.96			
1984	Trifluoromethane (R23)	26.143	250	0.95	0.96	0.96			
1022	Chlorotrifluoromethane(R13)	28.85	100	0.83	0.82	1.10			
1022	Chlorotrifluoromethane(R13)	28.85	120	0.90	0.90	1.10			
1022	Chlorotrifluoromethane(R13)	28.85	190	1.04	1.04	1.10	208.5	1.11	1.00
1022	Chlorotrifluoromethane(R13)	28.85	250	1.10	1.11	1.10			

Table 2. "High Pressure" fluids (-50˚C <Tc <65˚C), continued.

UN Number	Name	T_c (°C)	P_{test}(bar) UN, gauge	Filling ratio UN	Filling ratio, UN, NIST	NIST: 130 °F, 3000 psig fill ratio	test P (bar) from CFR 173.304	CFR 173.304 filling ratio NIST	CFR 173.304 filling ratio
1959	1,1-difluoroethylene	29.65	250	0.77	0.77	0.77	254.5	0.80	0.73
1013	Carbon Dioxide	30.978	190	0.66	0.68	0.77	208.5	0.77	0.68
1013	Carbon Dioxide	30.978	250	0.75	0.76	0.77	231.5	0.80	0.68
1035	Ethane	32.18	95	0.25	0.25	0.38			
1035	Ethane	32.18	120	0.29	0.30	0.38	208.5	0.38	0.36
1035	Ethane	32.18	300	0.39	0.40	0.38	231.5	0.39	0.37
1081	Tetrafluoroethylene	33.3	200	Na	1.04	1.10	208.5	1.10	0.90
2192	Germane	34.85	250	1.02	1.00	1.00			
1001	Acetylene	35.15	60	na	0.08	0.41			
1001	Acetylene	35.15	52	na	0.07	0.41			
3374	Acetylene	35.15	52	na	0.07	0.41			
3374	Acetylene	35.15	60	na	0.08	0.41			
1070	nitrous oxide	36.42	180	0.68	0.66	0.76			
1070	nitrous oxide	36.42	225	0.74	0.73	0.76	208.5	0.77	0.68
1070	nitrous oxide	36.42	250	0.75	0.76	0.76			
1080	SulphurHexafluoride	45.583	70	1.04	1.06	1.49			
1080	SulphurHexafluoride	45.583	140	1.33	1.34	1.49	116.6	1.36	1.20
1080	SulphurHexafluoride	45.583	160	1.37	1.38	1.49			
2454	MethylFluoride(R41)	44.13	300	0.36	0.63	0.61			
1050	Hydrogen chloride	51.5	100	0.30	0.38	0.78			
1050	Hydrogen chloride	51.5	120	0.56	0.59	0.78			
1050	Hydrogen chloride	51.5	150	0.67	0.66	0.78			
1050	Hydrogen chloride	51.5	200	0.74	0.72	0.78	208.5	0.78	0.65
2199	Phosphine	51.6	225	0.30	0.50	0.52			
2199	Phosphine	51.6	250	0.45	0.51	0.52			
1860	vinyl fluoride	54.65	250	0.64	0.65	0.65	208.5	0.65	0.62

Table 3. "Low Pressure" Fluids (Tc > 65˚C)

UN Number	Name	T_c (°C)	P_{test}(bar) UN, gauge	Filling ratio UN	Filling ratio, UN, NIST	NIST: 130 °F, 3000 psig fill ratio	test P (bar) from CFR 173.304	CFR 173.304 filling ratio NIST	CFR 173.304 filling ratio
3220	Pentafluoroethane (R125)	66.015	49	0.95	0.87	1.25			
3220	Pentafluoroethane (R125)	66.015	36	0.72	0.87	1.25			
1009	Bromotrifluoromethane (R13B1)	67	42	1.13	1.15	1.62	47.7	1.24	1.24
1009	Bromotrifluoromethane	67	120	1.44	1.15	1.62			
1009	Bromotrifluoromethane	67	250	1.60	1.15	1.62			
2424	Octafluoropropane (R218)	71.95	25	1.09	1.04	1.41			
3337	R404A	71.977	36	0.82	0.81	1.09			
2035	1,1,1-trifluoroethane (R143a)	72.707	35	0.75	0.73	0.97			
3339	R407B	74.284	38	0.93	0.93	1.20			
3252	Difluoromethane (R32)	78.105	48	0.78	0.77	0.96			
1020	Chloropentafluoroethane (R115)	79.95	25	1.08	1.05	1.35	27.5	1.10	1.10
1973	R502	80.727	31	1.05	1.01	1.25			
3338	R407A	81.864	36	0.94	0.94	1.16			
2195	telurium hexafluoride	107.03	20	1.00	2.37	2.71			
2420	hexafluoroacetone	83.99	22	1.08	1.11	1.38			
3340	R407C	86.021	35	0.95	0.95	1.15			
1858	hexafluoropropylene	94.85	22	1.11	1.11	1.33			
3153	perfluoromethylvinylether	89.85	20	0.75	1.02	1.29			
1048	Hydrogen bromide	90	60	1.54	1.48	1.71			
2191	Sulphuryl fluoride	67.85	50	1.10	1.09	1.40	56.8	1.14	1.06
2418	sulphur tetrafluoride	90.95	30	0.91	1.37	1.55			
1077	Propylene	92.42	30	0.43	0.43	0.52			
3083	Perchloryl fluoride	95.25	33	1.21	1.21	1.41			
2194	selenium hexafluoride	95.65	36	1.46	1.74	2.09			
1018	Chlorodifluoromethane (R22)	96.145	29	1.03	1.03	1.19	29.3	1.06	1.05
1978	Propane	96.675	25	0.42	0.43	0.50			
2422	octafluorobut-2-ene	118.85	12	1.34	1.31	1.51			

Table 3. "Low Pressure" Fluids (Tc > 65˚C), continued.

UN Number	Name	T_c (°C)	P_{test}(bar) UN, gauge	Filling ratio UN	Filling ratio, UN, NIST	NIST: 130 °F, 3000 psig fill ratio	test P (bar) from CFR 173.304	CFR 173.304 filling ratio NIST	CFR 173.304 filling ratio
2188	Arsine	99.85	42	1.10	1.16	1.32			
1053	hydrogen sulphide	100.45	55	0.67	0.67	0.76	56.8	0.69	0.63
3296	heptafluoropropane (R227ea)	101.65	15	1.20	1.22	1.42			
3159	1,1,11,2-tetrafluoroethane (R134a)	101.06	22	1.04	1.05	1.21			
2204	carbonyl sulphide	105.65	26	0.84	0.89	1.00			
2602	R500	102.15	22	1.01	1.00	1.16			
2453	ethyl fluoride	102.16	30	0.57	0.63	0.71			
1082	Trifluorochloroethylene	106	19	1.13	1.12	1.28	36.2	1.15	1.15
3057	Trifluoroacetylchloride	112.85	17	1.17	1.21	1.38			
1028	Dichlorodifluoromethane (R12)	111.97	18	1.15	1.16	1.33	27.5	1.20	1.19
1030	1,1-difluoroethane (R152a)	113.26	18	0.79	0.79	0.90	18.9	0.82	0.79
1976	Octafluorocyclobutane (RC318)	115.23	11	1.34	1.33	1.52			
2200	Propadiene	120.85	22	0.50	0.51	0.57			
1021	1-chloro-1,2,2,2-tetrafluoroethane (R124)	122.28	12	1.20	1.21	1.36			
1027	Cyclopropane	125.15	20	0.53	0.55	0.62	27.5	0.57	0.55
1033	dimethyl ether	126.95	18	0.58	0.58	0.65			
1026	Cyanogens	127	100	0.70	0.79	0.85			
1005	Ammonia, Anhydrous	132.25	33	0.53	0.55	0.58	56.8	0.56	0.54
3154	Perfluoroethylvinylether	127.85	10	0.98	1.22	1.42			
1969	Isobutane	134.67	10	0.49	0.49	0.56			
2517	1-chloro-1,1-difluoroethane (R142b)	137.11	10	0.99	0.99	1.11	18.9	1.03	1.00
2202	hydrogen selenide	138	31	1.60	1.57	1.71			
2548	chlorine pentafluoride	142.85	13	1.49	1.61	1.77			
1063	methyl chloride	143.1	17	0.81	0.82	0.89	27.5	0.85	0.84
1017	Chlorine	144	22	1.25	1.25	1.37	56.8	1.30	1.25
1055	Isobutylene	144.75	10	0.52	0.53	0.59			
1958	1,2-dichloro-1,1,2,2-tetrafluoroethane (R114)	145.68	10	1.30	1.31	1.46			

Table 3. "Low Pressure" Fluids (Tc > 65˚C), continued.

UN Number	Name	T_c (^oC)	P_{test}(bar) UN, gauge	Filling ratio UN	Filling ratio, UN, NIST	NIST: 130 ^oF, 3000 psig fill ratio	test P (bar) from CFR 173.304	CFR 173.304 filling ratio NIST	CFR 173.304 filling ratio
1012	1-butylene	146.35	10	0.53	0.53	0.59			
1983	1-chloro-2,2,2-trifluoroethane	156.85	10	1.18	1.19	1.31			
2197	hydrogen iodide	150.7	23	2.25	2.28	2.49			
1011	Butane	151.98	10	0.51	0.52	0.58			
1010	1,3-butadiene	151.85	10	0.55	0.55	0.61			
1749	chlorine trifluoride	182.85	30	1.40	1.51	1.71			
1974	Chlorodifluorobromomethane	153	10	1.61	1.63	1.81			
1012	trans-2-butylene	155.45	10	0.54	0.54	0.60			
1086	vinyl chloride	158.85	12	0.81	0.82	0.90	18.9	0.85	0.84
1061	methylamine	156.9	13	0.58	0.59	0.63	18.9	0.61	0.60
1079	Sulphur Dioxide	157.49	14	1.23	1.23	1.33	18.9	1.28	1.25
1067	nitrogen dioxide	158	10	1.30	1.31	1.38			
1083	trimethylamine	160.1	10	0.56	0.57	0.63	18.9	0.59	0.57
2044	2,2-dimethylpropane	160.65	10	0.53	0.53	0.59			
1012	cis-2-butylene	162.35	10	0.55	0.56	0.62			
1032	dimethylamine	164.05	10	0.59	0.59	0.64	18.9	0.62	0.59
1039	ethyl methyl ether	164.65	10	0.64	0.63	0.69			
1069	nitrosyl chloride	167.5	13	1.10	1.15	1.24	47.7	1.17	1.10
2196	tungsten hexafluoride	179.55	10	2.70	3.13	3.41			
1087	vinyl methyl ether	163.85	10	0.67	0.67	0.74	18.9	0.70	0.68
2676	Stibine	167.2	20	1.20	1.94	2.10			
1010	1,2-butadiene	178.85	10	0.59	0.58	0.64			
1029	dichlorofluoromethane (R21)	178.43	10	1.23	1.24	1.35			
1741	Boron trichloride	178.8	10	1.19	1.20	1.31			
1076	Phosgene	181.85	20	1.23	1.24	1.35			
1036	Ethylamine	183	10	0.61	0.61	0.66			
1051	hydrogen cyanide	183.5	100	0.55	0.61	0.64			
2419	bromotrifluoroethylene	158.85	10	1.19	1.64	1.81			
2189	dichlorosilane	185.85	10	0.90	1.10	1.21			

Table 3. "Low Pressure" Fluids (Tc > 65˚C), continued.

UN Number	Name	T_c (°C)	P_{test}(bar) UN, gauge	Filling ratio UN	Filling ratio, UN, NIST	NIST: 130 °F, 3000 psig fill ratio	test P (bar) from CFR 173.304	CFR 173.304 filling ratio NIST	CFR 173.304 filling ratio
2601	Cyclobutane	186.78	10	0.63	0.63	0.69			
1037	ethyl chloride	187.2	10	0.80	0.81	0.88			
1052	hydrogen fluoride	188	10	0.84	0.83	0.87			
2452	ethylacetylene	166.85	10	0.57	0.59	0.64			
1062	methyl bromide	193.85	10	1.51	1.51	1.63			
1040	ethylene oxide	196	15	0.78	0.79	0.85			
1064	methyl mercaptan	196.8	10	0.78	0.79	0.85	29.3	0.82	0.80
1085	vinyl bromide	199.85	10	1.37	1.38	1.49			
1589	cyanogen chloride	175.85	20	1.03	1.06	1.14			
1745	bromine pentafluoride	213.85	10	Na	2.26	2.42			
2495	iodine pentafluoride	305.85	10	Na	2.95	3.14			
1746	bromine trifluoride	362.85	10	Na	2.49	2.63			
2901	bromine chloride		10	1.50					

Explanation of columns in Tables 2 and 3

1. UN number.	The 4 digit UN identification number of the fluid.
2. Name.	Chemical name of the fluid.
3. T_c(^{o}C).	The critical temperature, in ^{o}C, recommended by NIST, as given in Table 1.
4. P_{test}(bar).	The gauge test pressure, in bar, as given in the packing instruction P200, Table2 of UN Model regulation, Twelfth Edition.
5. Filling Ratio, UN	The Filling Ratio as given in the packing instruction P200, Table 2 of UN Model regulation, Twelfth Edition.
6. Filling Ratio UN, NIST	The Filling Ratio, f, computed by NIST. a.) For high-pressure fluids, $f = \rho_F/\rho_{water}$. The fluid density ρ_F is calculated from NIST databases at T=65 ˚C and $Ptest_{abs}$ (bar) where $Ptest_{gauge}=Ptest_{abs}-1$ and ρ_{water}=999.10262 g/L (the density of water at 15 ˚C, 0.101 325 MPa as given in Wagner, W. and Pruss, A., "The IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use," J. Phys. Chem. Ref. Data, 31(2): 387-535, 2002.) b.) For low-pressure fluids, $f = \rho_F/\rho_{water}$. The fluid density is calculated from NIST databases according to $\rho_F = 0.95\rho_{test}$, where ρ_{test} is evaluated at T=50 ˚C and P=min($Ptest_{abs}$,P_{sat}(T= 65˚C)) where $Ptest_{abs}$ is found as described in a.) and P_{sat}(T=65 ˚C) is the saturation pressure of the fluid calculated from a NIST database at T=65 ˚C expressed in bar (absolute). Check that ρ_F is less than or equal to the saturation density of the fluid, calculated at T=60 ˚C using a NIST database.
7. NIST, 130 ^{o}F, 3000 psig	The filling ratio, computed by NIST, according to the 130 ^{o}F, 3000 psig definition , $f = \rho_F/\rho_{water}$. In this case, ρ_F is found using NIST databases at the conditions *T*=130 ˚F, *P*=3000 psig and ρ_{water} = (1.0/27.737) lb/in^3 (water density supplied by sponsor). The same method is used for both high-pressure and low-pressure fluids.
8. Test P (bar) from CFR 173.304	Test pressure (in bar) from 49 CFR 173.304 computed in the following manner: For each $Ptest_{abs}$ in bar for fluids listed in P200, computed as described in column 4 above, determine a nominal service pressure P_s = (3/5) $Ptest_{abs}$ and then convert this number to gauge units. Compare with service pressures in 49 CFR 173.304 and select closest one to nominal service pressure P_s. P_{test} is then found with $P_{test}=(5/3)\ P_s$, using absolute pressure units. Test P is then reported in bar.

9. CFR 173.304 Filling ratio NIST	The filling ratio, computed by NIST, according to the definition, $f = \rho_F/\rho_{water}$. In this case, ρ_F is found using NIST databases at T=130˚F, $P = P_{test}$ (bar) where the pressure is found as described in column 8 above. Check that ρ_F is less than or equal to the saturation density of the fluid, calculated at *T*=130 ˚F using a NIST database. ρ_{water} = (1.0/27.737) lb/in^3 (water density supplied by sponsor).
10. CFR 173.304 Filling ratio	The filling ratio is computed by taking the maximum permitted filling density (percent) given in 49 CFR 173.304 divided by 100.

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