Supplement of

Global Annual Mean Atmospheric Histories, Growth Rates and Seawater Solubility Estimations of the Halogenated Compounds HCFC-22, HCFC-141b, HCFC-142b, HFC-134a, HFC-125, HFC-23, PFC-14 and PFC-116

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Section S1: Smoothing spline method

We collected data from in situ, flask, archived air, firn air measurements. Database containing replicate times have been converted into a value without such replicates by using the mean of values at each replicate time. The error of the means will be the root-mean-square (RMS) of standard deviation values of replicate values. Then the data is sorted as $x_1 < x_2 <\ldots< x_i <\ldots< x_n$.

Set $x_i, y_i, \delta y_i$ $(i = 1, 2, \ldots, n)$ to be the decimal time, the corresponding atmospheric mole fractions and the standard deviation.

Normalize the *x* vector

$$t_i = (x_i - min(x_i))/(max(x_i) - min(x_i)) \qquad (1)$$

The smoothing function $f(t)$ to be constructed shall

$$\text{Minimize } p\sum_{i=0}^{n}[\frac{g(t_i)-y_i}{\delta y_i}]^2 + \int g''(t)^2 dt \qquad (2)$$

The solution of the minimum principle is a cubic spline. By introducing the auxiliary variable *z* together with the Lagrangian parameter *p*, we have to look for the minimum of the functional

$$\int_{t_1}^{t_n} g''(t)^2 dt + p[\sum_{i=0}^{n}\left(\frac{g(t_i)-y_i}{\delta y_i}\right)^2 + z^2] \qquad (3)$$

From the corresponding Euler-Lagrange equations, we determine the optimal function $f(t)$.

$$f(t) = a_i + b_i(t-t_i) + c_i(t-t_i)^2 + d_i(t-t_i)^3, \quad t_i \le t < t_{i+1} \qquad (4)$$

We obtain the spline coefficients (Reinsch, 1967).

$$c_i = \frac{pQ^T y}{B}, c = [0;\ c_i;\ 0]^T \qquad (5)$$

$$a = y - W^2 Qc/p \qquad (6)$$

$$d_i = (c_{i+1} - c_i)/(3h_i) \tag{7}$$

$$b_i = (a_{i+1} - a_i)/h_i - c_i h_i - d_i h_i^2 \tag{8}$$

$$coeffs = [d, c, b, a] \tag{9}$$

Here, the following notation is used:

$$h_i = t_{i+1} - t_i, \tag{10}$$

$$W = diag(\delta y_1, \dots, \delta y_n), \tag{11}$$

T is the $(n-1) \times (n-1)$ dimensional positive tridiagonal matrix with entries t_{ij} $(i, j = 1, 2, \dots, \mathrm{n} - 1)$ given by

$$t_{ii} = 2(h_{i-1} + h_i)/3, \quad t_{i,i+1} = t_{i+1,i} = h_i/3 \tag{12}$$

Q is the $(n) \times (n-2)$ dimensional tridiagonal matrix with with entries q_{ij} $(i = 1, 2, \dots, n;\ j = 1, 2, \dots, n-2)$ given by

$$q_{i-1,i} = 1/h_{i-1}, \qquad q_{i,i} = -1/h_{i-1} - 1/h_i, \qquad q_{i+1,i} = 1/h_i \tag{13}$$

The elements in the ith column of Q given by the coefficients of the 2th order divided differences based on $t_i, \dots, t_{i+2}$. Let the coefficient matrix be denoted by

$$B_p = Q^T W^2 Q + pT \tag{14}$$

The *influence matrix* associated with the smoothing spline is the unique $n \times n$ symmetric matrix A_p satisfying

$$a = A_p y \tag{15}$$

The error

$$error = y - a = W^2 Q B_p^{-1} Q^T y \tag{16}$$

So that

$$I - A_p = W^2 Q B_p^{-1} Q^T \tag{17}$$

The weighted residual sum of squares

$$RSS = \left\| (I - A_p) y / W \right\|^2 = \left\| W^2 Q B_p^{-1} Q^T y \right\|^2 \tag{18}$$

The estimate value of the generalized cross-validation (*GCV*) minimization function *V* of *p* used in the experiments below is the minimizer of the GCV function V_p defined

$$V_p = \frac{n \left\| (I - A_p) y / W \right\|^2}{[Tr(I - A_p)]^2} \tag{19}$$

The estimated degrees of freedom (Hutchinson and De Hoog, 1985)

$$Tr(I - A_p) = n - 2 - pTr(T/B) \tag{20}$$

The estimated variance

$$VAR = RSS/Tr(I - A_p) \tag{21}$$

The estimated 95 % Bayesian confidence intervals (*CI*) for the Cross-validated Smoothing Spline (Wahba, 1983) are given by

$$CI = 1.96 \sqrt{VAR * diag(A_p)} \tag{22}$$

Table S2. Comparison among the calculated Ostwald solubility coefficients (L_0, L L^{-1}) by the poly-parameter linear free energy relationships (pp-LFERs), observed ones and calculated ones by the Clark-Glew-Weiss (CGW) fit of target compounds and CFC-12 in water at 298.15 K and 310.15 K

Species	Chemical Formula	T (K)	Calculated log L_0 by pp-LFERs [a]	Calculated L_0 by pp-LFERs [a]	Calculated log L_0_cV by pp-LFERs [b]	Calculated L_0_cV by pp-LFERs [b]	Observed log L_0 [c]	Observed L_0 [c]	Calculated L_0 by the CGW fit [d]	RSD [e] (%)	RSD_cV [f] (%)
HCFC-22	$CHClF_2$	298.15	-0.017	0.961	-0.052	0.888	-0.091	0.811	0.844	9.18	3.53
HCFC-141b	$C_2H_3Cl_2F$	298.15	-0.136	0.731	-0.154	0.702	-0.148	0.711	0.711	1.97	0.92
HCFC-142b	$C_2H_3ClF_2$	298.15	-0.405	0.394	-0.440	0.363	-0.449	0.356	0.352	7.97	2.33
HFC-134a	CH_2FCF_3	298.15	-0.326	0.472	-0.407	0.392	-0.408	0.391	0.381	15.10	2.02
HFC-125	C_2HF_5	298.15	-1.003	0.099	-1.130	0.074	-1.059	0.087	0.086	9.79	10.78
HFC-23	CHF_3	298.15	-0.453	0.352	-0.505	0.313	-0.510	0.309	0.313	8.31	0.14
PFC-14	CF_4	298.15	-2.241	0.00574	-2.296	0.00505	-2.306	0.00494	0.00513	7.98	1.04
PFC-116	C_2F_6	298.15	-2.658	0.00220	-2.763	0.00173	-	-	0.00143	29.80	13.24
CFC-12	CCl_2F_2	298.15	-1.120	0.076	-1.155	0.070	-1.129	0.074	0.069	6.61	0.94
HCFC-22	$CHClF_2$	310.15	-0.161	0.691	-0.203	0.626	-	-	0.598	10.23	3.27
HCFC-141b	$C_2H_3Cl_2F$	310.15	-0.306	0.494	-0.327	0.471	-0.336	0.461	0.484	1.43	2.06
HCFC-142b	$C_2H_3ClF_2$	310.15	-0.571	0.269	-0.614	0.243	-0.605	0.248	0.246	6.14	0.80
HFC-134a	CH_2FCF_3	310.15	-0.563	0.274	-0.621	0.239	-0.547	0.284	0.269	1.10	8.30
HFC-125	C_2HF_5	310.15	-1.208	0.062	-1.339	0.046	-1.203	0.063	0.062	0.10	21.10
HFC-23	CHF_3	310.15	-0.618	0.241	-0.683	0.208	-0.622	0.239	0.225	4.87	5.62
PFC-14	CF_4	310.15	-2.310	0.00490	-2.382	0.00415	-2.386	0.00411	0.00437	8.12	3.60
PFC-116	C_2F_6	310.15	-2.755	0.00176	-2.883	0.00131	-	-	0.00110	32.53	12.15
CFC-12	CCl_2F_2	310.15	-1.213	0.061	-1.256	0.055	-1.275	0.053	0.048	17.00	10.00

[a] Calculated log L_0 and L_0 are calculated by the pp-LFERs, which are obtained from Table 6,7,9,12-15 in Abraham et al. (2001) and Table 2 in Abraham et al. (2012)

[b] Calculated log L_{0_cV} and L_0_cV are calculated by the pp-LFERs based on the corrected V

[c] Observed log L_0 and L_0 are measured by experiments, which are also obtained from Table 6,7,9,12-15 in Abraham et al. (2001) and Table 2 in Abraham et al. (2012)

[d] Calculated L_0 by the CGW fit are calculated based on the Combined Method for water solubility

[e] Relative standard deviation (RSD) of calculated L_0 by the pp-LFERs and calculated L_0 by the CGW fit

[f] Relative standard deviation (RSD) of calculated L_0_cV by the pp-LFERs and calculated L_0 by the CGW fit

Table S3. Ostwald solubility function of PFC-14 in seawater estimated by Method I

Compound	a_1	a_2	a_3	c_1	c_2	c_3	T_{min} (K)	T_{max} (K)	L_0 at 1 atm, 25 °C (L L^{-1})	L at 1 atm, 25 °C, 35.0 ‰ (L L^{-1})
PFC-14	-113.8218	162.6686	49.4215	$6.60 \cdot 10^{-5}$	0.003341	0.21307	273.15	328.15	0.00513	0.004027

$$lnL = \left[a_1 + a_2 \cdot \left(\frac{100}{T}\right) + a_3 \cdot ln\left(\frac{T}{100}\right)\right] \times exp[-(c_1(T-273.15)^2 + c_2(T-273.15) + c_3) \times \frac{0.03600}{1.80655} \times S \times \rho(T,S)]$$

Table S4. Ostwald solubility function of target compounds and CFC-12 in water estimated by Method II at 298.15 K and 310.15 K

Species	Chemical Formula	*T* (K)	*c*	*e*	*s*	*a*	*b*	*v*	K_s	L_0 at 1 atm, 25 °C (L L^{-1})	*L* at 1 atm, 25 °C, 35.0 ‰ (L L^{-1})
HCFC-22	$CHClF_2$	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.169 ± 0.037	0.888	0.703
HCFC-141b	$C_2H_3Cl_2F$	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.204 ± 0.043	0.702	0.530
HCFC-142b	$C_2H_3ClF_2$	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.198 ± 0.037	0.363	0.277
HFC-134a	CH_2FCF_3	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.193 ± 0.034	0.392	0.300
HFC-125	C_2HF_5	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.224 ± 0.028	0.091	0.067
HFC-23	CHF_3	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.168 ± 0.028	0.313	0.248
PFC-14	CF_4	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.202 ± 0.016	0.00505	0.00382
PFC-116	C_2F_6	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.244 ± 0.017	0.00173	0.00123
CFC-12	CCl_2F_2	298.15	-0.994	0.577	2.549	3.813	4.841	-0.869	0.204 ± 0.034	0.070	0.053
HCFC-22	$CHClF_2$	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.169 ± 0.037	0.626	0.530
HCFC-141b	$C_2H_3Cl_2F$	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.204 ± 0.043	0.471	0.385
HCFC-142b	$C_2H_3ClF_2$	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.198 ± 0.037	0.243	0.200
HFC-134a	CH_2FCF_3	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.193 ± 0.034	0.239	0.198
HFC-125	C_2HF_5	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.224 ± 0.028	0.059	0.047
HFC-23	CHF_3	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.168 ± 0.028	0.208	0.176
PFC-14	CF_4	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.202 ± 0.016	0.00415	0.00340
PFC-116	C_2F_6	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.244 ± 0.017	0.00131	0.00103
CFC-12	CCl_2F_2	310.15	-0.966	0.698	2.412	3.393	4.577	-1.072	0.204 ± 0.034	0.055	0.045

$$L = 10^\wedge\left[-K_S \cdot \frac{S}{M_{NaCl}} + c + eE + sS + aA + bB + vV\right]$$, (*V* for HFC-125, corrected *V* for other compounds)

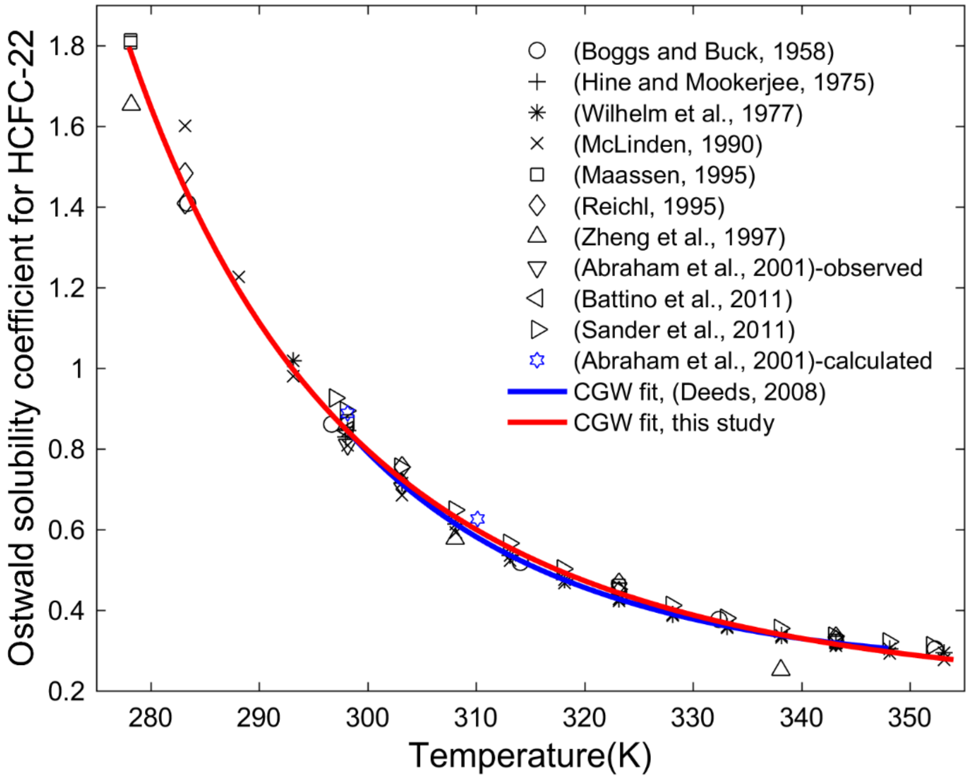

Figure S1. The freshwater solubility (Ostwald solubility coefficients) for HCFC-22 as a function of temperature by collecting data from previous studies (Boggs and Buck Jr, 1958; Hine and Mookerjee, 1975; Wilhelm et al., 1977; Mclinden, 1990; Maaßen, 1995; Reichl, 1995; Zheng et al., 1997; Abraham et al., 2001; Battino et al., 2011; Sander et al., 2011). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from Deeds (2008) and from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 4.0 % with two-thirds of the data.

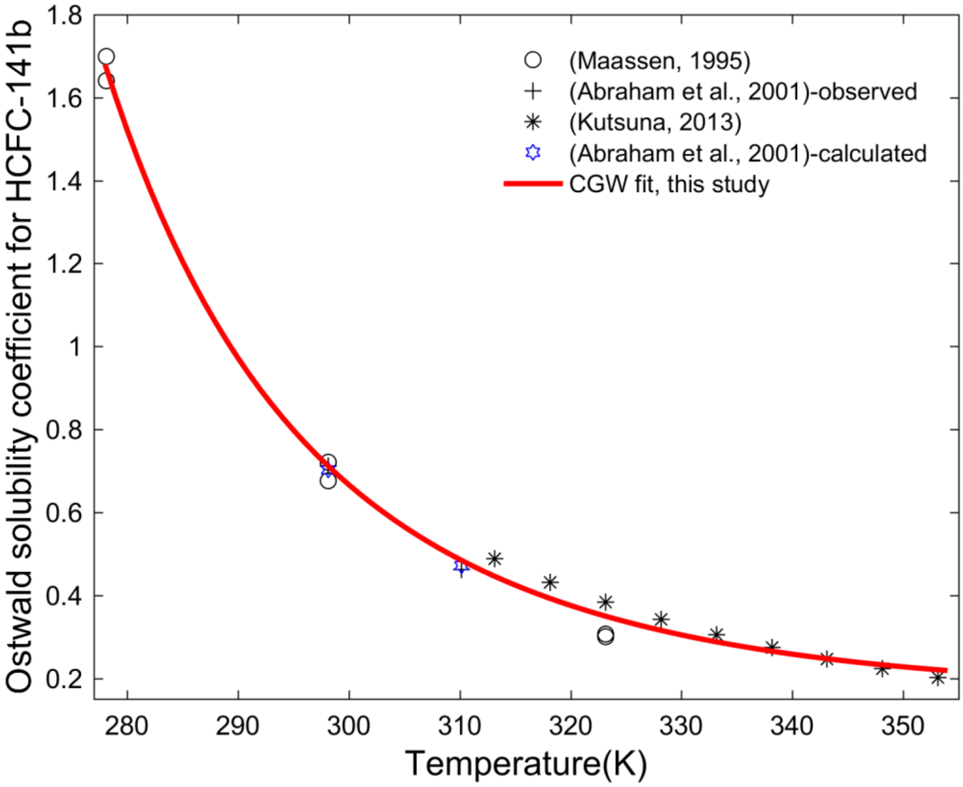

Figure S2. The freshwater solubility (Ostwald solubility coefficients) for HCFC-141b as a function of temperature by collecting data from previous studies (Maaßen, 1995; Abraham et al., 2001; Kutsuna, 2013). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 7.8 % with two-thirds of the data.

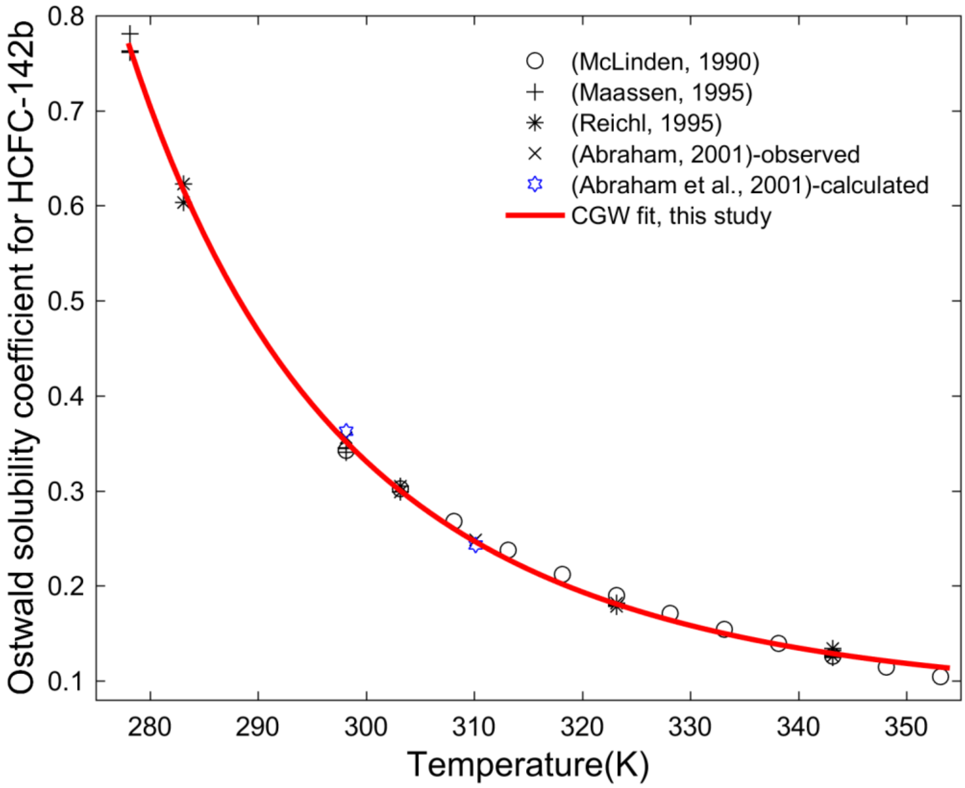

Figure S3. The freshwater solubility (Ostwald solubility coefficients) for HCFC-142b as a function of temperature by collecting data from previous studies (Mclinden, 1990; Maaßen, 1995; Reichl, 1995; Abraham et al., 2001). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 2.5 % with two-thirds of the data.

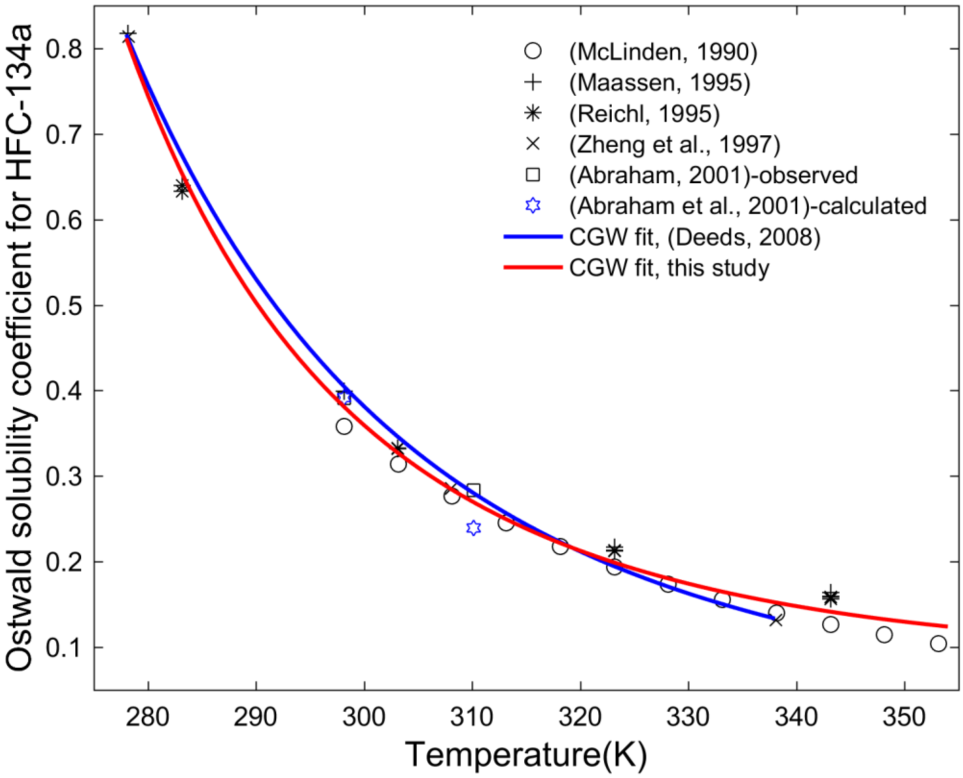

Figure S4. The freshwater solubility (Ostwald solubility coefficients) for HFC-134a as a function of temperature by collecting data from previous studies (Mclinden, 1990; Maaßen, 1995; Reichl, 1995; Zheng et al., 1997; Abraham et al., 2001). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from Deeds (2008) and from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 6.8 % with two-thirds of the data.

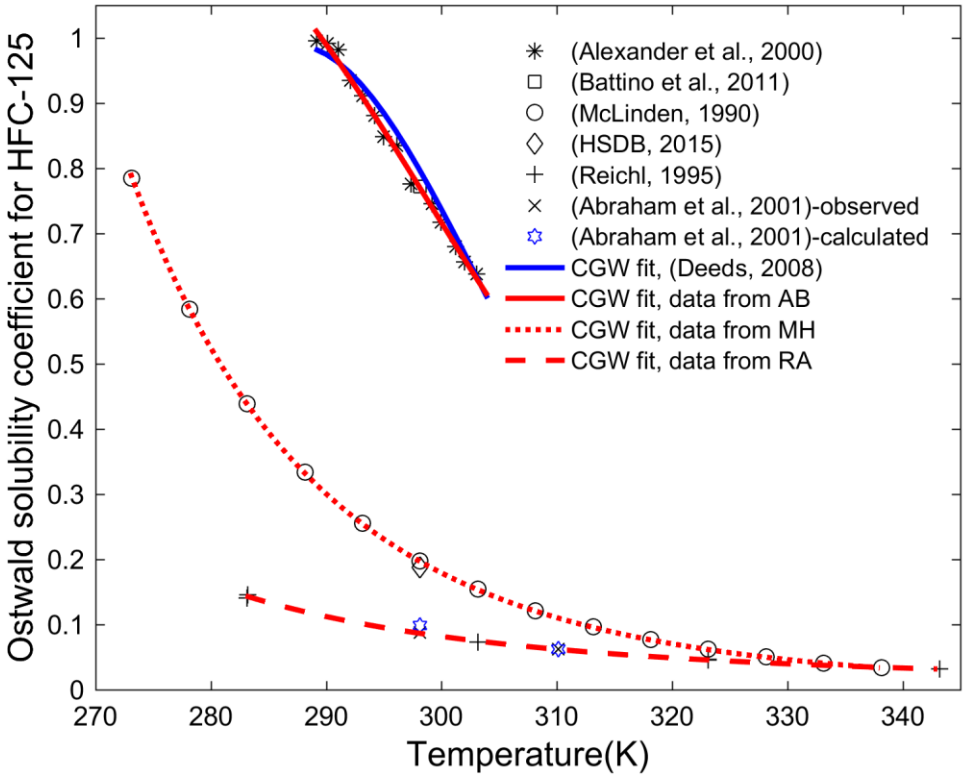

Figure S5. The freshwater solubility (Ostwald solubility coefficients) for HFC-125 as a function of temperature by collecting data from previous studies (Alexandre et al., 2000; Battino et al., 2011; Mclinden, 1990; HSDB, 2015; Reichl, 1995; Abraham et al., 2001). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from Deeds (2008) and from (Abraham et al., 2001)-calculated (Hexagram, calculated by Method II). The CGW fit in this study agrees to within 2.1 % with all data. There are three CGW fit curves from these literatures. Curve 1 is the upper and red solid line fitted the data (Alexandre et al., 2000; Battino et al., 2011) in the temperature range of 289.15 K ~ 303.15 K. This fit agrees to within 1.0 % with 2/3 data. Curve 2 is the middle and red dotted line fitted the data (Mclinden, 1990; HSDB, 2015) from 273.15 K to 338.15 K. This fit agrees to within 0.75 % with 2/3 data. Curve 3 is the bottom and red dashed line fitted the data (Reichl, 1995; Abraham et al., 2001) in the temperature range of 283.15 K ~ 343.15 K. This fit agrees to within 3.3 % with two-thirds of the data.

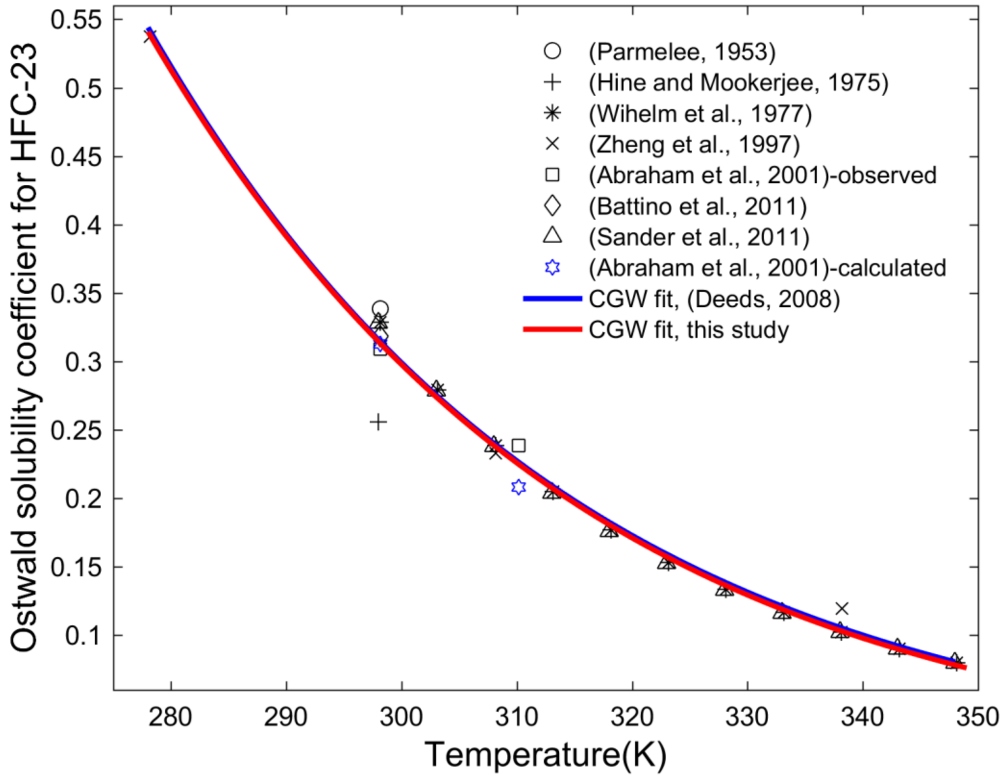

Figure S6. The freshwater solubility (Ostwald solubility coefficients) for HFC-23 as a function of temperature by collecting data from previous studies (Parmelee, 1953; Hine and Mookerjee, 1975; Wilhelm et al., 1977; Zheng et al., 1997; Abraham et al., 2001; Battino et al., 2011; Sander et al., 2011). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from Deeds (2008) and from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 2.3 % with two-thirds of the data.

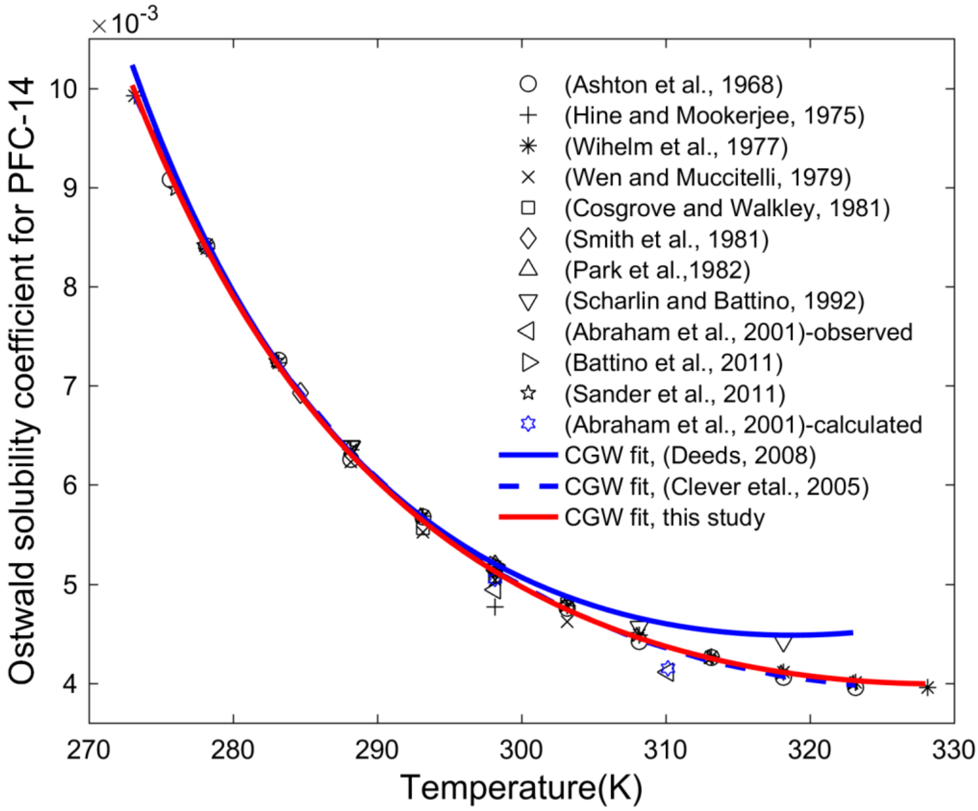

Figure S7. The freshwater solubility (Ostwald solubility coefficients) for PFC-14 as a function of temperature by collecting data from previous studies (Smith et al., 1981; Park et al., 1982; Scharlin and Battino, 1992; Abraham et al., 2001; Battino et al., 2011; Sander et al., 2011). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the results from Deeds (2008), from Clever et al. (2005) and from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 0.95 % with two-thirds of the data.

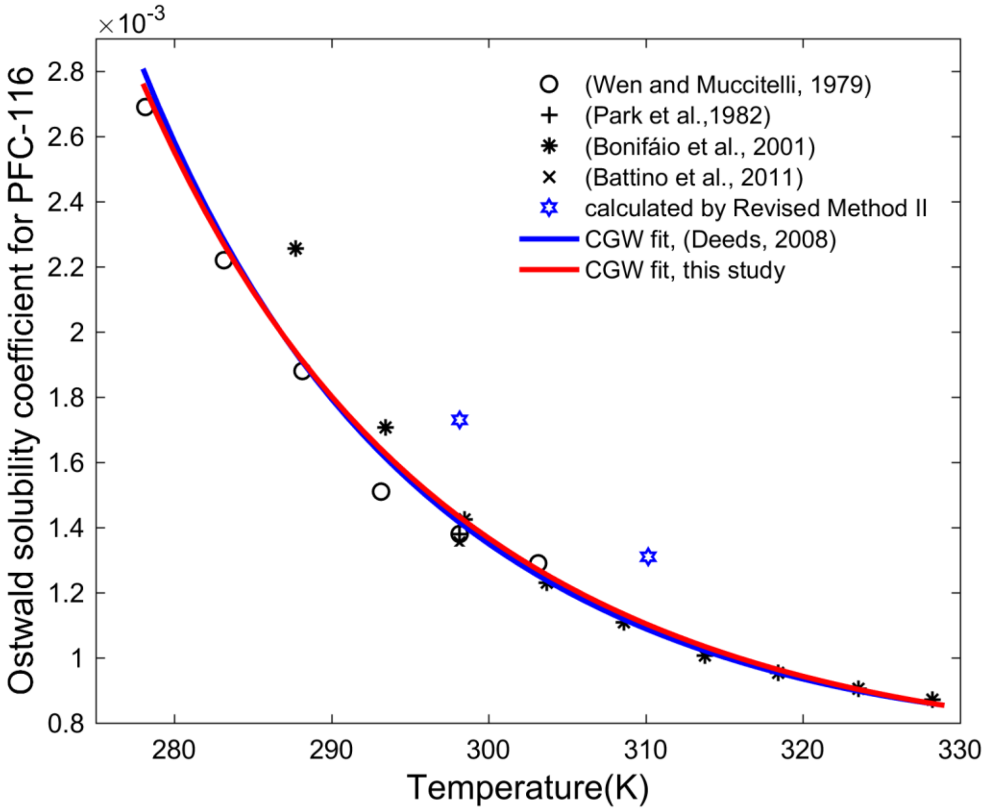

Figure S8. The freshwater solubility (Ostwald solubility coefficients) for PFC-116 as a function of temperature by collecting data from previous studies (Wen and Muccitelli, 1979; Park et al., 1982; Bonifácio et al., 2001; Battino et al., 2011). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the fit results from Deeds (2008) and from the data calculated by Revised Method II (Hexagram). The CGW fit in this study agrees to within 3.5 % with two-thirds of the data.

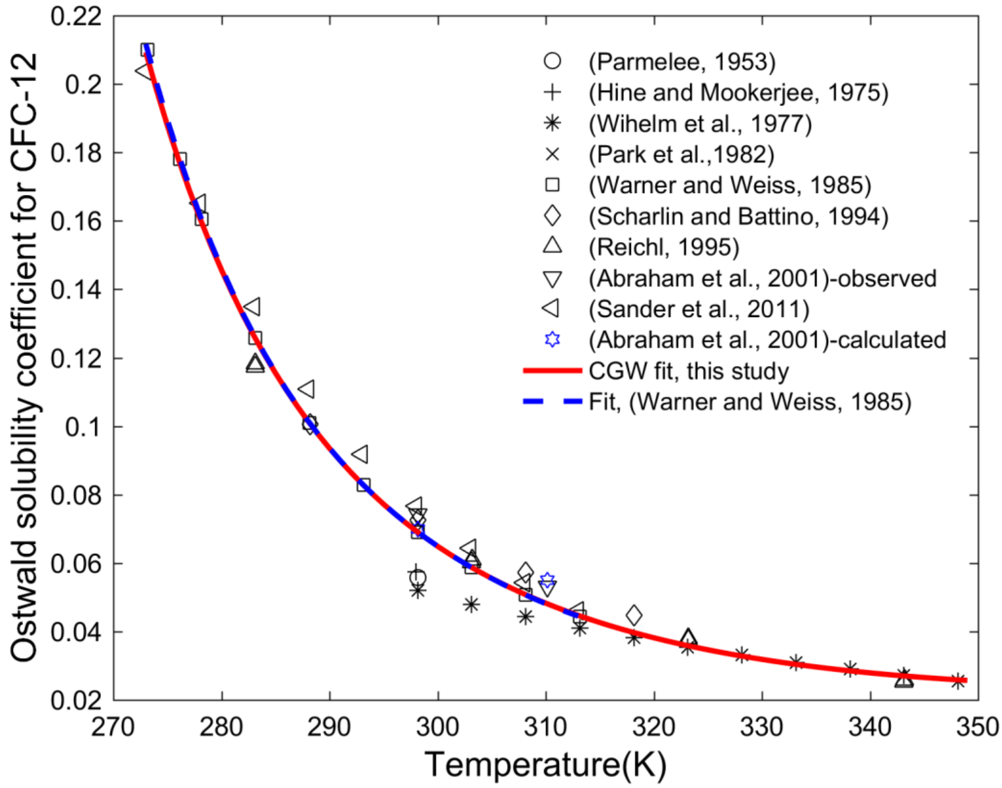

Figure S9. The freshwater solubility (Ostwald solubility coefficients) for CFC-12 as a function of temperature by collecting data from previous studies (Parmelee, 1953; Hine and Mookerjee, 1975; Wilhelm et al., 1977; Park et al., 1982; Warner and Weiss, 1985; Scharlin and Battino, 1994; Reichl, 1995; Abraham et al., 2001; Sander et al., 2011). The Clarke-Glew-Weiss (CGW) is used to fit the data (black markers) and compared with the fit results from Warner and Weiss (1985) and the data from (Abraham et al., 2001)-calculated (Hexagram, calculated by Revised Method II). The CGW fit in this study agrees to within 6.6 % with two-thirds of the data.

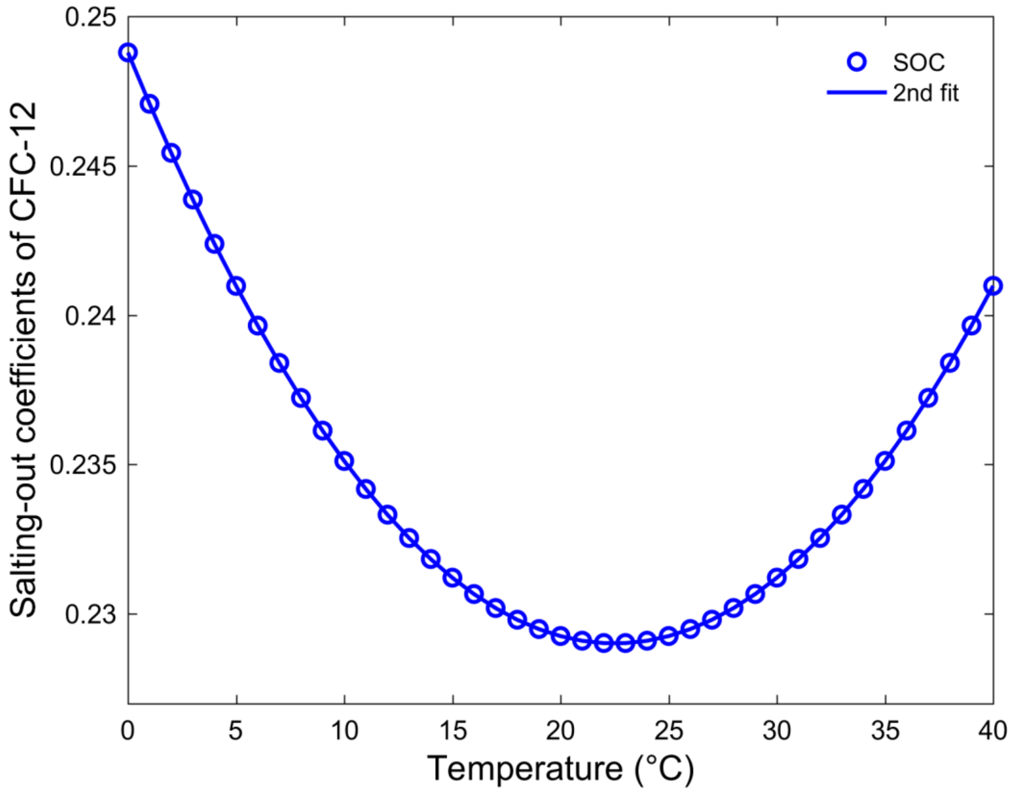

Figure S10. The relationship between salting-out coefficients (SOC) and temperature for CFC-12 calculated by the Combined Method based on the data from Warner and Weiss (1985).

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