

## Solubility of ClO<sub>2</sub> (Handbook of Chemistry and Physics, 88 ed.)

$$\ln(X) = A + B/T^* + C \cdot \ln(T^*) \quad T^* = T/100 \text{ K}$$

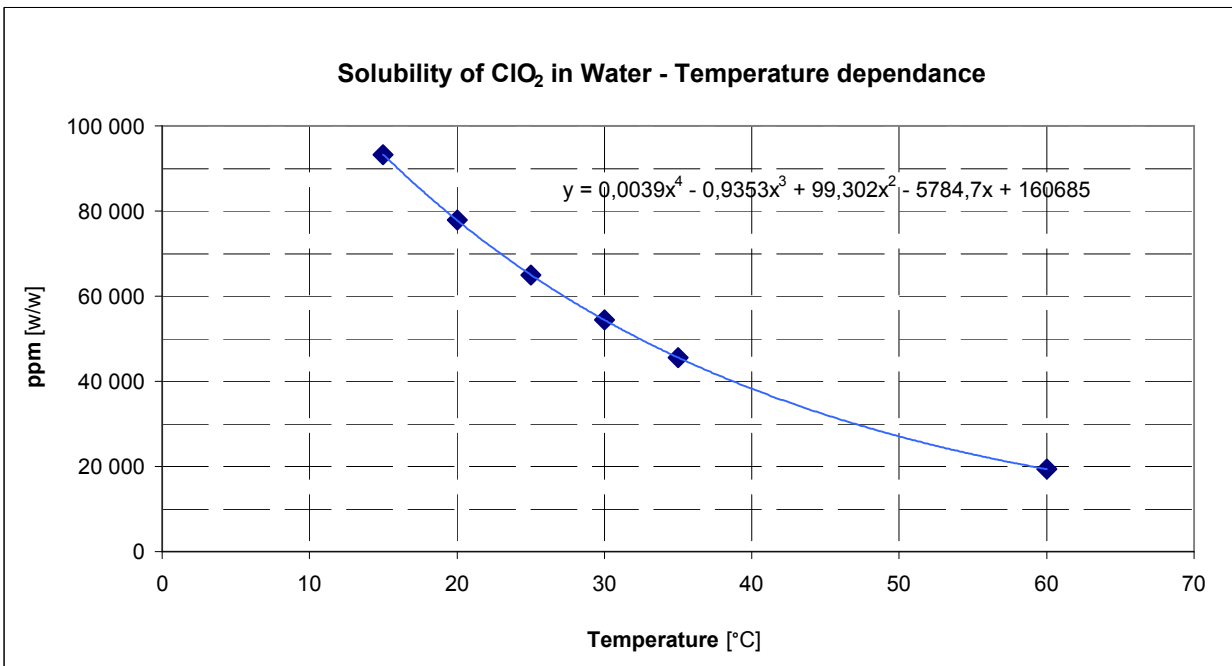
$$\begin{aligned} \text{Mw}(\text{ClO}_2) &= 67,4515 \\ \text{Mw}(\text{H}_2\text{O}) &= 18,01 \end{aligned} \quad X = \frac{m(\text{H}_2\text{O})/\text{Mw}(\text{H}_2\text{O})}{m(\text{ClO}_2)/\text{Mw}(\text{ClO}_2) + m(\text{H}_2\text{O})/\text{Mw}(\text{H}_2\text{O})} \quad \text{Eq. (1)}$$

$$\begin{aligned} A &= 7,9163 \\ B &= 0,4791 \\ C &= -11,0593 \end{aligned} \quad m(\text{H}_2\text{O}) + m(\text{ClO}_2) = 100 \quad \text{Eq. (2)}$$

$$k = \text{Mw}(\text{ClO}_2) / \text{Mw}(\text{H}_2\text{O}) = 3,745$$

$$\text{Solution of Eq (1) and (2):} \quad \text{Solubility (g ClO}_2 \text{ in 100 g of solution)} = \frac{100kX}{1 + X(k - 1)}$$

T/°K	T/100	T/°C	T/°F	ln(X)	Molar ratio X	Solubility g/100 g	ppm w/w	k <sub>H</sub> mol/kg.bar
278,15	2,7815	5	41	-3,2250	0,03976	13,42	<b>134 242</b>	<b>0,502</b>
283,15	2,8315	10	50	-3,4251	0,03255	11,19	<b>111 896</b>	0,603
288,15	2,882	15	59	-3,6216	0,02674	9,33	<b>93 297</b>	0,723
293,15	2,932	20	68	-3,8147	0,02204	7,78	<b>77 850</b>	0,866
298,15	2,982	25	77	-4,0045	0,01823	6,5034	<b>65 034</b>	<b>1,037</b>
303,15	3,032	30	86	-4,1911	0,01513	5,44	<b>54 406</b>	1,240
308,15	3,082	35	95	-4,3745	0,01259	4,56	<b>45 591</b>	1,479
333,15	3,332	60	140	-5,2489	0,00525	1,94	<b>19 395</b>	3,478



# Content of ClO<sub>2</sub> [ volume %] in air space in a bottle

Concentration and temperature dependance - safety consideration

Henry's law

$$p = k_H c$$

$k_H$  calculated from solubility data HoCP for 25 °C at atmospheric pressure = **1,037** mol/kg.bar is

in accordance with NIST - <http://webbook.nist.gov/cgi/cbook.cgi?ID=C10049044&Units=SI&Mask=10> :

$k_H$  = Henry's law constant for solubility in water at 298.15 K (mol/kg\*bar) = 1; 0,84; 1; three sources

25 °C			
c		p(ClO <sub>2</sub> )	V(ClO <sub>2</sub> )
[ppm]	[mol/kg]	[bar]	[% v/v]
2 000	0,030	0,03	3,1
3 000	0,044	0,05	4,6
4 000	0,059	0,06	6,2
5 000	0,074	0,08	7,7
6 000	0,089	0,09	9,2
<b>7 000</b>	<b>0,104</b>	<b>0,11</b>	<b>10,8</b>
8 000	0,119	0,12	12,3
9 000	0,133	0,14	13,8
10 000	0,148	0,15	15,4
11 000	0,163	0,17	16,9
12 000	0,178	0,18	18,5
13 000	0,193	0,20	20,0
14 000	0,208	0,22	21,5
15 000	0,222	0,23	23,1
20 000	0,297	0,31	30,8
30 000	0,445	0,46	46,1
40 000	0,593	0,62	61,5
50 000	0,741	0,77	76,9
60 000	0,890	0,92	92,3
65 000	0,964	1,00	99,9

5 °C		
c	p(ClO <sub>2</sub> )	V(ClO <sub>2</sub> )
[ppm]	[bar]	[% v/v]
2 000	0,015	1,5
3 000	0,022	2,2
4 000	0,030	3,0
5 000	0,037	3,7
6 000	0,045	4,5
7 000	0,052	5,2
8 000	0,060	6,0
9 000	0,067	6,7
10 000	0,074	7,4
11 000	0,082	8,2
12 000	0,089	8,9
13 000	0,097	9,7
14 000	0,104	10,4
15 000	0,112	11,2
20 000	0,149	14,9
30 000	0,223	22,3
40 000	0,298	29,8
50 000	0,372	37,2
60 000	0,447	44,7
65 000	0,484	48,4

Chlorine dioxide (ClO<sub>2</sub>, Chemical Abstracts Service [CAS] No. 10049-04-4), a free radical, exists as a greenish yellow to orange gas at room temperature with a characteristic pungent chlorine-like odour. Chlorine dioxide gas is strongly oxidizing, **it is explosive in concentrations in excess of 10% v/v** at atmospheric pressure and will easily be detonated by sunlight or heat (Budavari et al., 1996). Its melting point is -59 °C, its boiling point is 11 °C (at 101.3 kPa), and its vapour density is 2.34 (air = 1).

<http://www.inchem.org/documents/cicads/cicads/cicad37.htm#2>.

If the information in bold above and my calculations are correct, then CDS with concentration greater than 6 000 ppm is dangerous (at temperatures above 25 °C).

As the vapor density of chlorine dioxide is rather high, it can concentrate at the bottom (similar to carbon dioxide accumulation in lowest parts of caves).

According to many literature sources **CDS concentration up to 3 000 - 4 000 ppm only is considered safe** at adequate manipulation.

If the solution is kept at 5 °C (at fridge), the partial pressure and volume content of ClO<sub>2</sub> in air in the bottle are lower (about one half of these at 25 °C). That means that the critical amount 10 % (v/v) in the air is not overstepped up to CDS concentration cca 13000 ppm.

Due to lower partial pressure at 5 °C the speed of gas off is slower, too - another beneficial of cold CDS solution.