Calculating Molecular SO_2

Molecular SO_2 is calculated using the free SO_2 of a wine and a molecular SO_2 factor related to the pH of the wine. The effectiveness of the SO_2 to protect the wine from oxidation and microbial spoilage is dependant upon the pH of the wine. Therefore, the higher the pH a wine has, the less effective the SO_2. A molecular SO_2 of 0.8 ppm, while an acceptable maximum for some wines, is not recommended for all wines. Wineries adjusting to a standard free SO_2 level instead of monitoring molecular SO_2 will have varying SO_2 impact on their wines; adjusting to molecular SO_2 provides consistency in SO_2 management.

In general, we suggest a lower molecular SO_2 for reds than for whites, perhaps around 0.4-0.6 ppm at bottling. Wines with higher pH levels, red or white, may require too high a total SO_2 level to achieve desired free SO_2 levels. Rather than have excessive bound SO_2 (which may give a "chemical" taste), it is best to rely on a combination of factors, including susceptibility to spoilage. Some pH problems can be relieved by adjusting the pH downward with tartaric acid.

Distribution of free SO_2 at various pH's — *Free SO_2 needed to achieve molecular SO_2 of:*

pH	$\%SO_2$	$\%HSO_3$-	$\%SO_3$	0.8 ppm	0.5 ppm
2.90	7.5	92.5	0.009	1 ppm free	7 ppm free
2.95	6.6			12	7
3.00	6.1	93.9	0.012	13	8
3.05	5.3			15	9
3.10	4.9	95.1	0.015	16	10
3.15	4.3			19	12
3.20	3.9	96.1	0.019	21	13
3.25	3.4			23	15
3.30	3.1	96.8	0.024	26	16
3.35	2.7			29	18
3.40	2.5	97.5	0.030	32	20
3.45	2.2			37	23
3.50	2.0	98.0	0.038	40	25
3.55	1.8			46	29
3.60	1.6	98.4	0.048	50	31
3.65	1.4			57	36
3.70	1.3	98.7	0.061	63	39
3.75	1.1			72	45
3.80	1.0	98.9	.077	79	49
3.85	0.9			91	57
3.90	0.8	99.1	0.097	99	62
3.95	0.7			114	71
4.00	0.7	99.2	0.122	125	78

**Adapted from: Enology Briefs I (#1), Feb/Mar 1982. University of California Cooperative Extension*

Free SO_2 consists of 3 species: molecular SO_2 (directly active in preventing oxidation and spoilage), and two ions, HSO_3- (bisulfite) and SO_3= (sulfite), which comprise the majority of the free SO_2 but are MUCH less reactive than molecular SO_2. The percentage of free SO_2 existing as molecular SO_2 drops as pH rises (2nd column). Thus, at the SAME free SO_2 level, wines with higher pH have less molecular SO_2, and therefore less SO_2 protection.

The last 2 columns show free SO_2 level needed at different pHs to achieve two levels of molecular SO_2: 0.5 ppm and 0.8 ppm, a normal range in wine.

The molecular SO_2 level can be extrapolated from the chart or calculated by using this formula:

Molecular SO_2 = free SO_2 divided by $(1 + 10^{pH - 1.8})$

English to Metric to English Calculations

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English	=	Metric
1 oz (fluid)	=	30 ml (29.6 ml)
1 quart (2 pints)	=	0.95 L
1 Gallon (128 oz)	=	3,785 ml
1 oz (weight)	=	28.35 g
1 lb (16 oz)	=	453.6 g
1 ton (2,000 lbs)	=	907 kg

Metric	=	English
1 ml (1 cc)	=	0.035 fluid oz
1 L (1,000 ml)	=	1.06 quart (0.26 G)
1 hl (100 L)	=	26.4 G
1 gram (1,000 mg)	=	0.035 oz
1 kg (1,000 g)	=	2.204 lbs
1 ton (1,000 kg)	=	2,204 lbs

Abbreviations:

oz = ounce	g = gram
lb = pound	kg = kilogram
G = gallon	ml = milliliter
L = liter	hl = hectoliter

Common units of measure

1 lb / 1,000 G = 0.45 g / G = 0.012 g / 100 ml = 0.12 g / L = 12 g / hl

0.1 g / 100 ml = 1 g / L = 100 g / hl = 0.75 g / 750 ml = 3.78 g / G = 8.3 lbs / 1,000 G

Addition Formulas

Compound	Lab Addition Rate	Cellar Addition Rate
Acids (increase TA)	+ 0.1 g / 100 ml	= 3.8 g tartaric / G wine = 8.3 lb tartaric / 1,000 G wine = 7.4 lb malic / 1,000 G wine = 7.1 lb citric / 1,000 G wine
Ascorbic acid (treat disulfides, add copper and carbon afterwards)	+ 10 ppm	= 0.1 ml of 1% solution in 100 ml wine = 3.78 ml / G = 37.85 g ascorbic acid crystals in 1,000 G wine
Potassium carbonate	reduce TA by 0.1 g/100 ml	= 2.5 g / G calcium carbonate = 5.5 lbs / 1,000 G wine = 3.8 g / G potassium carbonate = 8.3 lbs / 1,000 G wine
Copper (treat sulfides) DO TRIALS FIRST	+ 0.1 ppm as Cu	= 0.15 ml of 1% $CuSO_4$ solution / G wine = 0.1 ml of 0.05% $CuSO_4$ in 120 ml (4 oz) wine = 1.5 grams $CuSO_4$-$5H_2O$ per 1,000 G wine
Hydrogen peroxide (reduce SO_2) (Not legal for commercial wine)	~10 ppm SO_2	approx 1 ml H_2O_2 3% / G wine DO TRIALS FIRST!
Potassium metabisulfite (add SO_2)	+ 100 ppm SO_2	= 0.76 g / G = 760 g / 1,000 G = 20 g / hl = 0.2 g / L = 7.6 ml / G = 2 ml / L of 10% KMBS solution (~5% SO_2)
Any soluble compound	1% + 1 lb / 1,000 G	1 g / 100 ml = 7.50 g / 750 ml = 37.85 g / G = 0.45 g / G = 0.012 g / 100 ml = 0.09 g / 750 ml

Other Useful Calculations

Normality:

Normality (1) x Volume (1) = Normality (2) x Volume (2)

OR amount to add = $\dfrac{\text{normality desired x volume desired}}{\text{Normality of concentrated solution}}$

Percentage (% additions):

% (1) x Volume (1) = % (2) x Volume (2)

OR volume to add = $\dfrac{\text{\% desired x total volume desired}}{\text{\% solution to be added}}$

Parts per million (ppm) = mg / L

Amount to add in grams = $\dfrac{\text{(gallons wine) x 3.785 x desired ppm}}{1{,}000}$