

Calculation of O₂ Saturation and of the Oxyhemoglobin Dissociation Curve for Different Species, Using a New Programmable Pocket Calculator*

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Summary. The degree of O₂ saturation and different data of acid-base status are determined from pO_2 , pH, and pCO_2 values by a programmable pocket calculator. Since the operating program should be usable for different species and also in the range of very low O₂ saturations, obviously the usual Hill equation for calculating the oxygen dissociation curve of hemoglobin is not applicable; the same is true in some cases for the Adair equation. Thus a 3-fold subdivision of the dissociation curve was undertaken and programmed. Suitable programs for several species could be established despite the limited number of program steps in the new calculator, giving systematic deviations in calculated O₂ saturations of $\leq \pm 0.9$ saturation percent over the full range of dissociation curves. A reverse procedure for calculation of pO_2 from saturation is added. In situations where pCO_2 or base excess are not known or only estimated, limits of the arising error are stated. In the acid-base program 7 parameters are evaluated partially using empirical formulae derived from nomograms. The programmable pocket calculator offers advantages of small size, economy, and independence of line voltage compared to much more spacious units and a precision equal or superior to nomograms.

Key words: Computer Programs — Bohr Effect — Acid-Base Status — Base Excess — pO_2 — Oxyhemoglobin Dissociation Curve.

With the development of programmable pocket calculators difficult calculations can be carried out at relatively low cost and immediately at the site where measurements are taken. In addition, the further evaluation and elaboration of experimental results can be done at almost any place. It was our purpose to calculate the oxygen saturation from measured pO_2 , pH, and partially pCO_2 values for different species, considering largely the present knowledge of mutual influence of various factors. In spite of the limited number of programmable steps in the described calculators one can achieve an accuracy which could not be guaranteed by the use of even very exact and consequently very extensive nomograms. The following study elaborates on the programming and the degree of accuracy that can be obtained from evaluation of dissociation curves of different species as described by several authors.

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Methods

Using a special experimental arrangement (Lutz *et al.*, 1974), the following values were determined from blood flowing with constant velocity through a temperature-regulated electrode assembly: pO_2 (Pt-electrode of Clark type, according to Lübbers and Windisch, 1963; produced by Eschweiler, Kiel), pH (microelectrodes Ingold KG Frankfurt), and in extension of the experimental procedure pCO_2 (electrode according to Gleichmann and Lübbers, 1960; produced by Eschweiler, Kiel). For the determination of the O_2 consumption and its variations in organ circulations the oxygen saturation (SO_2) should be detected down to very low values. For this a new programmable pocket calculator HP-65 (Hewlett-Packard) was used. This may be easily moved to every measuring location as it has dimensions of only $15 \times 8 \times 3.5$ cm and 312 g weight. For the programming 100 single steps are available. Calculating the oxygen saturation from the values of blood was done in the following manner. First the oxygen tension was converted to standard conditions (pH = 7.4, $pCO_2 = 40$ mm Hg, BE = 0 mval/l, respectively). Then the resulting standardized pO_2 value was inserted in equations describing the S-shaped dissociation curve and the appropriate oxygen saturation was determined. A correction for different temperature values is given in three of the programs; however, in order to obtain a good reproduction and calibration a constant temperature of $37^\circ C$ in the electrode units is usual in most species. Various arithmetical methods were applied and specially checked in regard to their applicability for different animal species. The exclusive use of Hill's equation was abandoned already in preliminary tests, since it causes greater deviations; the same was true for the Adair equation in some species other than man. Furthermore the reverse procedure, calculation of pO_2 from saturation, would require a multistep iteration by this equation.

1. Equation of Adair

Although the value of the equation of Adair (1925) today is to be seen more as a formal than as a causal description (Hutten, 1968; Yoder *et al.*, 1973), it permits a sufficiently exact description of the human oxyhemoglobin dissociation curve. The most appropriate form for the computing process is found by the following equations (SO_2 in % saturation):

$$SO_2 = 25 \frac{A_1 pO_2 + 2A_2 pO_2^2 + 3A_3 pO_2^3 + 4A_4 pO_2^4}{1 + A_1 pO_2 + A_2 pO_2^2 + A_3 pO_2^3 + A_4 pO_2^4} \quad \text{after Adair} \quad (1)$$

further by differential calculus:

$$SO_2 = 25 pO_2 \frac{d}{dpO_2} \left\{ \ln (1 + A_1 pO_2 + A_2 pO_2^2 + A_3 pO_2^3 + A_4 pO_2^4) \right\} \quad (2)$$

continued:

$$SO_2 = 125 pO_2 \cdot$$

$$\ln \left\{ \frac{1 + A_1(pO_2 + 0.1) + A_2(pO_2 + 0.1)^2 + A_3(pO_2 + 0.1)^3 + A_4(pO_2 + 0.1)^4}{1 + A_1(pO_2 - 0.1) + A_2(pO_2 - 0.1)^2 + A_3(pO_2 - 0.1)^3 + A_4(pO_2 - 0.1)^4} \right\} \quad (3)$$

Program 1 (Adair)

LBL	R/S	7	R/S	STO3	EEX	CHS	□	+	÷
A	.	-	x	.	CHS	□	+	RCL2	f
7	0	.	STO1	2	□	+	RCL2	x	ln
.	0	0	.	CHS	RCL2	RCL2	x	1	1
4	1	3	3	STO	x	x	²⁾ □	+	2
-	3	1	+	+	⁴⁾ □	³⁾ □	□	RCL3	5
.	x	x	STO2	2	□	□	□	gx=y	×
¹⁾ □	+	-	CLX	⁵⁾ □	□	□	EEX	gx>y	RCL1
□	R/S	f ⁻¹	LBL	□	□	EEX	CHS	GTO	x
x	3	log	8	□	EEX	CHS	□	8	RTN

The sign □ is used for digits and exponents of constants to be set in:

Man^a: 1) B = 0.48; 2) A₁ = 257 EEX CHS4; 3) A₂ = 780 EEX CHS6; 4) A₃ = 4440 EEX CHS9; 5) A₄ = 255 EEX CHS8.

(Maximal deviation from listed values: ΔS = ± 1.2 S%, compare with Fig. 1).

Man (own calculation^b): 1) B = 0.48; 2) A₁ = 972 EEX CHS5; 3) A₂ = 177 EEX CHS5; 4) A₃ = 210 CHS EEX CHS7; 5) A₄ = 259 EEX CHS8.

(Maximal deviation from listed values: ΔS = ± 0.7 S%).

Rat^c: 1) B = 0.47; 2) A₁ = 310 EEX CHS4; 3) A₂ = 190 EEX CHS6; 4) A₃ = 5200 EEX CHS9; 5) A₄ = 077 EEX CHS8.

(No listed values available, deviation therefore not to be calculated).

Running program:

Input	Units	Key	Output	Units
pH		A		
BE (or zero)	mval/l	R/S		
T	°C	R/S		
pO ₂	mm Hg	R/S	SO ₂	S%

The first 33 steps are used for standardizing the pO₂ according to Eq. (2), steps 34—100 to Eq. (1).

^a A₁—A₄ after Roughton and Severinghaus (1973).

^b Executed after the method of smallest squared deviations on a Telefunken TR 440 computer (Rechenzentrum der Universität Würzburg).

^c B after Turek *et al.* (1972); A₁—A₄ after Turek *et al.* (1973).

The 4 determined coefficients A₁₋₄ were ascertained from a recent article (Roughton and Severinghaus, 1973) and are given in Program 1. In this Program 1 the conversion of pO₂ to SO₂ requires 67 program steps (including the insertion of the constants); there remain 33 steps for determining the standardized pO₂ in the beginning of the program, so that it was calculated with a constant Bohr factor B and an inserted base excess (BE), which can be obtained from the values of the acid-base status according to Program 4¹. In the relationship between SO₂ and

¹ Equations for the standardization of the pO₂, in which pCO₂ enters directly instead of BE, were not used, because there are no data available concerning the resulting much lower Bohr factor in other species (man: B = -0.40).

pO_2 , a variable Bohr factor for different species can be used. The appropriate standardization corresponds to the equation specified by Severinghaus (1966):

$$\Delta (\log pO_2) = B \cdot (pH - 7.4) + 0.0013 \text{ BE} - 0.031 (T - 37); \quad (4)$$

[BE in mval, T in °C].

The maximal systematic deviations of oxygen saturation appearing from the use of Program 1 are for man ± 1.2 % saturation (S^0_0) compared with the original values. If the BE is determined only by sample taking at random or is unknown entirely, the following deviations of the calculated saturations arise additionally:

A deviation of the real BE from the keyed BE (or from a BE = 0) called Δ BE leads to the following differences in per cent saturation ΔSO_2 :

Δ BE \leq 5 mval/l	leads to $\Delta SO_2 \leq \pm 1.5 S^0_0$
5.1 to 10 mval/l	leads to $\Delta SO_2 \leq \pm 2.0 S^0_0$
10.1 to 15 mval/l	leads to $\Delta SO_2 \leq \pm 3.0 S^0_0$
15.1 to 20 mval/l	leads to $\Delta SO_2 \leq \pm 4.0 S^0_0$

[The deviations were calculated according to Mengden *et al.* (1969) and Thews (1971)]. Therefore it is necessary to decide in each individual case, how much of an expected deviation of BE may be tolerated.

An attempt to express the oxyhemoglobin dissociation curve for various animal species by the Adair equation by means of calculated factors A_1 — A_4 partially resulted in greater systematic deviations. Kelman (1966) used an analogous equation with 7 coefficients which, however, becomes inexact in the range of lower saturations. A later paper of Thomas (1972) avoids this shortcoming, but it is very difficult or impossible to calculate the given coefficients with a comparable accuracy in some species. The same holds for an Fortran subroutine of Aberman *et al.* (1973) with 8 constants. A method of approximation according to Heise and Schmidt (1973) involves considerable requirements to the computer and must be performed each time for a special species with supporting points. Relationships used by Maas *et al.* (1972) in the course of a determination of acid-base parameters trace back to Hill's equation and involve the restrictions mentioned above. However, it appeared that deviations of $\pm 0.9 S^0_0$ may be obtained with a much less extensive method, additionally making possible a reverse procedure to calculate pO_2 from saturation values (Program 3). The method is described in the following section.

II. 3-Segment Equations

The oxyhemoglobin dissociation curve may be described by 3 segments, whereby the curve is approximated by a parabola in the first segment (low saturations; SO₂ in % saturation):

$$SO_2 = K_1 pO_2^2 + K_2 pO_2. \tag{5}$$

This equation is valid in different species up to a SO₂ of 19–51 S% (“a”). In the following segment the curve is reproduced by the equation of a straight line:

$$SO_2 = K_3 pO_2 - K_4. \tag{6}$$

In the last segment, beginning in different species at 41–80 S% (“b”) the dissociation curve is approximated by the equation:

$$SO_2 = \frac{100}{\left(\frac{K_5}{pO_2}\right)^{K_6} + 1}. \tag{7}$$

The equivalent programming (Program 2) requires 62 steps with 2 logical decisions for the limits a and b, so that 38 steps remain for the

Program 2 (3 segments)

LBL	R/S	7	R/S	RCL1	gx ≤ y	□	⁶⁾ □	□	x
A	.	—	x	³⁾ □	GTO	.	□	g	RTN
7	0	.	STO1	□	8	□	.	y ^x	LBL
.	0	0	↑	□	⁴⁾ □	—	□	1	8
4	1	3	x	□	.	^{b)} □	□	+	RTN
—	3	1	²⁾ .	x	□	□	RCL1	g	
¹⁾ .	x	x	□	+	□	gx ⇒ y	÷	1/x	
□	+	—	□	^{a)} □	RCL1	gx ≤ y	⁷⁾ □	1	
□	R/S	f ⁻¹	□	□	x	GTO	.	0	
x	3	log	x	gx ⇒ y	⁵⁾ □	8	□	0	

Input	Units	Keys	Output	Units
pH		A		
BE	mval/l	R/S		
T	°C	R/S		
pO ₂	mm Hg	R/S	SO ₂	S%

Program 2 (continued)

Species	1. Bohr factor	Change segments		2. K_1	3. K_2	4. K_3	5. K_4	6. K_5	7. K_6	ΔS [S%]
		[S%]								
		a	b							
Man ¹	0.48 ¹	40	56	0.062	0.351	2.50	16.9	27.00	2.80	± 0.6
Horse ²	0.48 ²	19	46	0.075	0.244	2.86	22.1	25.18	2.87	± 0.3
Cow ³	0.49 ⁶	28	38	0.052	0.109	2.38	24.9	30.80	3.25	± 0.6
Pig ³	0.42 ⁶	22	41	0.041	0.331	2.56	27.7	30.60	2.79	± 0.5
Sheep ³	0.43 ⁶	19	41	0.040	0.113	2.35	28.8	33.70	2.87	± 0.3
Dog ³	0.50 ⁶	23	46	0.059	0.267	2.35	18.9	29.11	3.13	± 0.5
Rabbit ³	0.45 ⁶	29	58	0.022	0.806	2.53	27.7	30.70	3.28	± 0.6
Cat ³	0.54 ⁶	40	66	0.035	0.192	1.87	18.4	38.80	4.10	± 0.9
Guinea pig ³	0.47 ⁶	40	66	0.047	0.622	2.38	15.4	28.45	3.48	± 0.9
Rat ⁴	0.47 ⁷	22	58	0.020	0.535	1.91	20.8	36.71	2.70	± 0.5
Golden Hamster ⁵	0.41 ⁵	51	64	0.028	1.04	2.77	26.3	26.39	2.78	± 0.9
White mouse ⁵	0.63 ⁵	25	80	0.021	0.975	1.65	05.3	40.69	5.70	± 0.9

¹ Roughton and Severinghaus (1973).⁵ Ulrich *et al.* (1963).² Baumann *et al.* (1963).⁶ Hilpert *et al.* (1961).³ Bartels and Harms (1959).⁷ Turek *et al.* (1972).⁴ Turek *et al.* (1973).

initial standardization. Gaps at the transition of the segments lead to errors in the limits mentioned below the program. A fixed value for BE is to be keyed; this (just as for the first program) is evaluated besides other values of the acid-base status with a special program (nr. 4). A comparison of the systematic deviations between values of the human dissociation curve taken from Roughton and Severinghaus (1973) and those calculated after the Adair method and our 3-segment method is given in Fig. 1.

In a third program the reverse conversion of O_2 saturation into standardized pO_2 is made possible using the same 7 constants as in Program 2. Either an additional temperature correction or a correction for the actual pH value using the special Bohr factor can be made.

Programs for the calculation of the acid-base status by computers have been described to a different extent by Jalowaysky *et al.* (1968), Hardt (1972), Maas *et al.*, (1972). It could be shown, however, that already 7 important values may be determined with a limited number of steps to a great degree of accuracy by a selection of relationships—partly taken from nomograms empirically. The equations underlying these calculations are presented below Program 4.

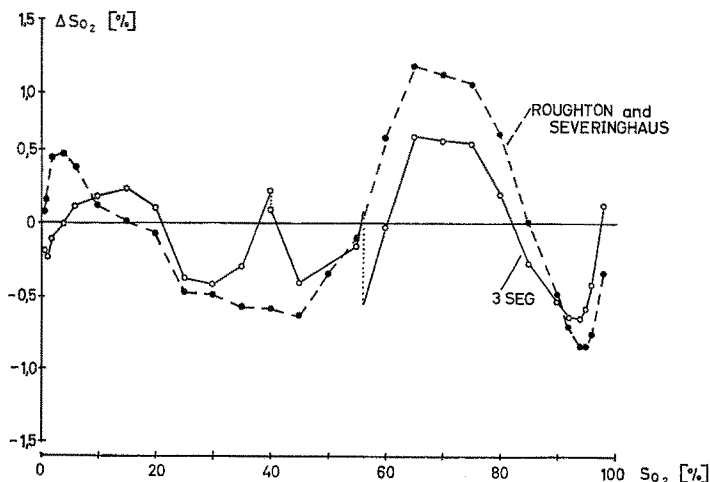


Fig. 1. Systematic deviations between 27 values of the oxyhemoglobin dissociation curve for humans according to Roughton and Severinghaus (1973) and their Adair approximation (dashed line) and the 3-segment approximation (solid line). In the latter in no case the deviation exceeds $\pm 0.7 S^0/0$. The dotted line stands for the gaps

Discussion

The handiness of a pocket calculator opens ranges of application which hitherto were covered either exclusively by nomograms or by a system in which compiled data were fed into a much larger computer, frequently loaded with numerous other functions. As has been described, substantial information is available already from 100 program steps; for more extensive calculations additional programs may be attached. The lack of a printout of numerical values has to rank as a disadvantage; but it should be taken into consideration that the normal one-column printing of most desk calculators requires further tabulation; a multi-column printing to tabulations is possible only with much larger computers.

The constants used for the programs can also be replaced by additional instructions later on. Thus studies have been presented for the influence of 2,3-diphosphoglycerate (Benesch and Benesch, 1967; Chanutin and Curnish, 1967; Sigaard-Andersen and Salling, 1961), for the variation of the Bohr factor in the range of extreme oxygen saturations (Glauser and Forster, 1967; Kernohan and Forster, 1967; Kernohan and Roughton, 1972), for large variations of pH (Karmann *et al.*, 1971; Roughton and Severinghaus, 1973), and for the different influence of fixed acids against $p\text{CO}_2$ variations (Naeraa *et al.*, 1963; Kirschbaum,

Program 3 (reverse program)

LBL	\square	\div	⁶⁾ \square	RCL1	\div	2	\uparrow	STO5
A	gx>y	⁷⁾ \square	\square	⁵⁾ \square	STO5	\div	RCL1	RTN
STO1	GTO	.	.	\square	RTN	\uparrow	x	
^{a)} \square	1	\square	\square	.	LBL	\uparrow	+	
\square	1	\square	\square	\square	2	x	f	
gx>y	0	CHS	x	+	³⁾ \square	²⁾ .	$\sqrt{\quad}$	
GTO	0	g	STO5	⁴⁾ \square	\square	\square	gx \Leftrightarrow y	
2	RCL1	1/x	RTN	.	\square	\square	-	
RCL1	-	g	LBL	\square	\square	\square	RCL2	
^{b)} \square	RCL1	y ^x	1	\square	\uparrow	STO2	\div	

Factors to be set in see below program 2.

Continued by

	1
	x
LBL	f ⁻¹
B	log
3	RCL5
7	x
-	RTN
.	
0	
3	

	\square
	CHS
LBL	x
B	f ⁻¹
7	log
.	RCL5
4	x
-	RTN
¹⁾ .	
\square	

temp. correction

pH correction

	Input	Units	Key	Output	Units
(O ₂ saturation)	SO ₂	S%	A	pO ₂ st	mm Hg
(temp. correction)	T	°C	B	pO ₂ T-cor	mm Hg
(pH correction)	pH		B	pO ₂ pH-cor	mm Hg

1963; Garby *et al.*, 1972), whereby decisive evaluations of the degree of their mutual influence are not yet possible. These studies mainly refer to the problem of the pO₂ conversion to standard conditions, from which the oxygen saturation is determined as described with a fixed program. Even when several supplementary programs are needed the instant availability of a pocket calculator provides important advantages.

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Program 4 (acid-base status)

LBL	.	STO2	6	9	4	÷	STO5	4	.
A	1	R/S	.	—	1	1	R/S	+	2
.	—	RCL1	8	STO3	.	—	.	STO6	x
0	f ⁻¹	.	8	R/S	7	RCL8	0	6	STO7
3	log	7	x	STO8	+	.	1	.	RTN
x	RCL7	7	+	.	STO4	2	4	1	
STO7	x	5	2	4	R/S	x	5	—	
R/S	STO1	x	1	2	1	x	x	f ⁻¹	
STO6	RCL7	RCL6	7	x	0	RCL3	7	log	
6	+	2	.	+	0	+	.	1	

Input	Units	Key	Output	Units	Content of register	Register number
pCO ₂	mm Hg	A	0.03 pCO ₂	mm Hg	HCO ₃ ⁻	1
pH		R/S	tot. CO ₂	mmol/l	tot. CO ₂	2
		R/S	BE _{ac}	mval/l	BE _{ac}	3
Hb	g/100 ml	R/S	BB	mval/l	BB	4
	bl.					
SO ₂	S%	R/S	BE _{ox}	mval/l	BE _{ox}	5
		R/S	HCO ₃ ⁻ _s	mval/l	pH _s	6
					HCO ₃ ⁻ _s	7

$\text{HCO}_3^- = 0.3 \text{ pCO}_2 \cdot 10^{(\text{pH}-6.1)}$ (Henderson-Hasselbalch equation).

$\text{tot. CO}_2 = \text{HCO}_3^- + 0.03 \text{ pCO}_2$

$\text{BE}_{ac} = 0.775 \text{ HCO}_3^- + 26.88 \text{ pH} - 217.9$ (empirical after Thews nomogram, 1971)

$\text{BE}_{ox} = \text{BE}_{ac} + 0.2 \text{ Hb} \left(\frac{\text{SO}_2}{100} - 1 \right)$ (after Siggaard-Andersen and Salling, 1971)

$\text{BB} = \text{BE}_{ac} + 41.7 + 0.42 \text{ Hb}$ (after Siggaard-Andersen, 1963).

$\text{pH}_s = 0.0145 \text{ BE}_{ox} + 7.4$ (empirical after Thews nomogram, 1971).

$\text{HCO}_3^-_s = 1.2 \cdot 10^{(\text{pH}_s-6.1)}$ (Henderson-Hasselbalch equation).

Hb = hemoglobin; BE_{ac} = actual BE; BB = buffer base; BE_{ox} = BE for oxygenated blood; pH_s = standard pH; HCO₃⁻_s = standard bicarbonate.

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