

PRODUCTION CALCULATOR, VERSION 1.5 OPERATIONS MANUAL

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PRODUCTION CALCULATOR, VERSION 1.5

OPERATIONS MANUAL

Introduction

The following manual has been prepared to assist people in the use of Production Calculator software program. This software was written to be used as a macro program within Excel since it was thought that more potential users would have access to and knowledge of this Microsoft® product. This version is based on the result of two earlier versions that we continuously updated and improved on as our use and needs of this program became more sophisticated and demanding. The impetus for the development of this program came from our initial work quantifying dissolved oxygen (DO) in small, low-gradient streams in the Central Plains region. Using a dissolved oxygen and temperature logger made by the former BioDevices Corporation of Ames Iowa (now Eco Instruments™, <http://www.aquasonde.com/>) we generated thousands of dissolved oxygen and temperature measurements over days, weeks and months. Graphical plots of the diel, weekly, and monthly flux of these variables provided visual records of DO flux and facilitated graphical interpretations of the temporal patterns of these data. However, more sophisticated analyses of these data required that the raw logger data be readily converted to discrete numerical variables (e.g. means, quartiles, medians) suitable for statistical analysis. A relatively simple program was developed in Microsoft® Excel that generated a number of numeric variables. The logical extension of this research was to estimate primary production and community respiration from the temporally robust dissolved oxygen and temperature data and other stream data collected in conjunction

with our dissolved oxygen flux investigations. It became apparent that stream and watershed factors that might be affecting DO flux might also be controlling or mediating instream primary production. Therefore, the original procedures of Odum (Odum 1956, 1957) for estimating primary production from dissolved oxygen measures were examined and a method was developed to use the temporally intense data sets generated by the loggers to calculate net and gross production estimates as well as 24-hour respiration values. Because the amount of data was extremely large when examining daily, weekly, and monthly conditions a computer model was developed in Microsoft Excel[®] to perform the required calculations using these large datasets. The Production Calculator has first developed in the spring of 2003 and since then a number of newer versions has been created - each newer version enhancing modeling capabilities and offering more options to the user. The current version allows the user to select the most appropriate reaeration coefficients for the type of stream and stream conditions being monitored, the instrument recording interval, and account for effects of temperature, barometric pressure and salinity on the calculated saturation values for dissolved oxygen.

This manual consists of two parts. The first is a basic user's guide for the Production Calculator (version 1.5) with step-by-step instructions on stream and data parameterization, data import and export, graphical and numerical displays of intermediate output variables and productivity output variables. The Production Calculator is intuitive to use and only a few general rules need to be followed to successfully operate the program. The program is displayed as five separate work sheets within the Excel shell. The use of the program and the parameterization of the model with data follow from sheet one through the last sheet where the daily and average values

for the deployment period are recorded for net production, gross production and 24-hour community respiration.

The second portion of this manual describes the theoretical and technical basis for the calculation of primary production based on Odum's original work (Odum 1956) and others that have used *in situ* dissolved oxygen change techniques (e.g. Hoskin 1959, Edwards and Owens 1962, Gunnerson and Baily 1963, Flemer 1970, Hall 1972, Hornberger et al. 1977). The procedures for using diel oxygen cycle information to estimate primary production in flowing water can be found in a number of contemporary scientific publications including "Standard Methods" (e.g. APHA, et al. 1995, 1998), Hauer and Lamberti (1996) and Wetzel and Likens (1991), while several computer models (Stephens and Jennings 1976, McBride 1995, <http://home.arcor.de/Limnologie/MB.htm>) have been developed to calculate primary productivity parameters from these data. None of the existing computer programs we have examined are as complete and user friendly as this Excel program. However, each program has certain characteristics or calculations that investigators might find useful and we encourage others to explore the potential use of these and other programs that calculate primary production in streams. Similarly, the authors continue to seek comments and suggestions on how this program maybe made more useful to researchers. Corresponds can be directed to the authors listed on the title page of this manual or posted on the Central Plains Center for BioAssessment website (www.cpcb.ku.edu)

USER'S GUIDE

User Information – Sheet 1

The *User Information* sheet contains basic descriptive information about the Production Calculator including the version and release date. A brief introduction to the operation of each worksheet is explained, along with contact information for the authors and general references for the reaeration equations available for use in the program.

Stream Variables – Sheet 2

Several stream variables that must be collected by the investigator are input into the Production Calculator in this worksheet (Figure 1).

The *Stream Variables* header allows the user to enter the stream name, stream identification number or code, and sampling date for the stream site being analyzed. In addition, the user also has the options to enter the date the Production Calculator was run and any notes the user wants to include. All of the header information entered in this worksheet will also be displayed in the *Productivity Results* sheet (sheet 5).

The first stream variables to be entered are the calculated means for stream depth (m) and velocity (m/sec) for that stream segment above the point of measure for DO and stream temperature (i.e. the logger deployment site). We are not aware of any published guidance regarding the length of the upstream area that should be considered when attempting to calculate average depth and velocity values for a particular stream segment or reach. Our own experiences suggest that both flow conditions and geomorphic complexity of the stream channel must be considered when selecting a length of stream

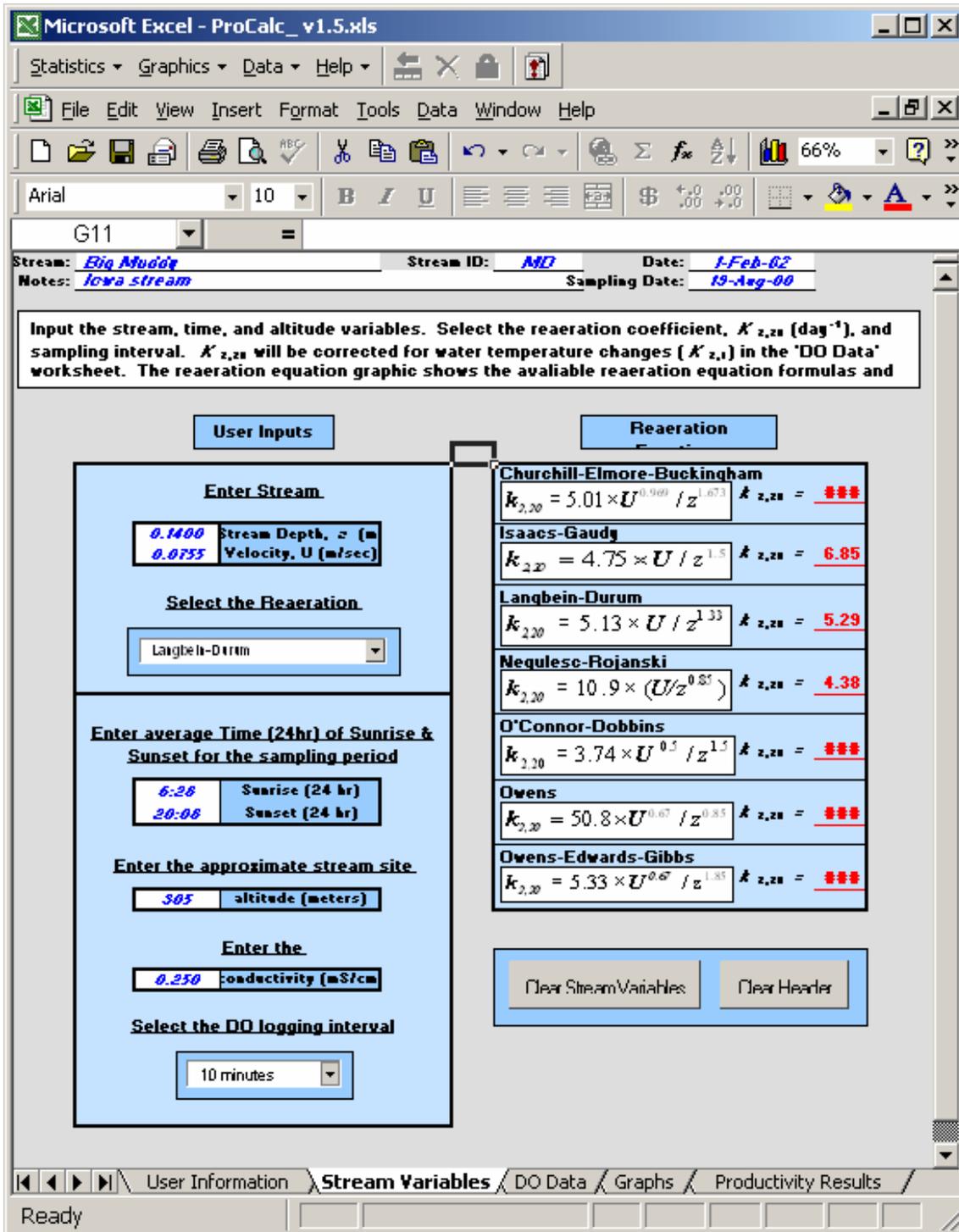


Figure 1. Stream Variables sheet (Sheet 2) showing stream, sunrise/sunset and altitude data settings for Big Muddy Creek in Iowa (USA). A data collection time interval of 10 minutes and the Langbein-Durum reaeration coefficient have also been selected for use.

from which to estimate average stream depth and velocity. Intuitively, segments comprised of alternating pools and riffles should be long enough to include two or more altering pool/riffle or glide sequences. For small wadeable streams we derive our depth and velocity means from eight or more points along each of five individual cross sectional transects evenly spaced along a 100-meter or longer segment starting immediately above the DO logger. In general, we use a 20 to 40 meter interval between transects with the number of transects dependant on the complexity of the stream reach. Once these values are entered, the user can examine the reaeration equations to determine which $k_{2,20}$ value to select from the *Reaeration Coefficient* drop-down list. The reaeration rate coefficient (k_2) is temperature dependant so the standardized reporting value is the coefficient value at 20 degrees Celsius. It is critical to select the most appropriate reaeration coefficient for the type of stream or river that you are monitoring. If possible actual measurement of the reaeration coefficient should be done, however this is seldom practical. The $k_{2,20}$ values calculated on this sheet allow users to observe similarities and differences between values generated by the reaeration coefficients equations included in this program. These standardized reaeration coefficient values are calculated for a water temperature of 20° Celsius. During later computations, the $k_{2,20}$ values will be adjusted for each recorded temperature to compensate for effects related to stream temperature changes associated with the diel cycles. Wilcock (1982) examined six of the most commonly used reaeration equations and evaluated them based on their acceptance in the literature and their predictability over varying stream velocities and depths. Wilcock found that the estimates from these equations were very similar to the actual values for stream conditions that were used in their derivation, but generated poor predictive values

when equations were used in streams that were dissimilar to the modeled streams (i.e. greater or lesser depth and velocity ranges). A guide to the selection of the most appropriate equations for various stream conditions is presented in Table 1, which is based on Wilcock's original findings.

Table 1. Suggested reaeration equations for differing depths and velocities.

Velocity U (m/s)	Depth - z (m)			
	0.25-0.50	0.50-1.0	1.0-3.0	3.0-6.5
0.1-0.3	E	E	E	E
0.3-0.5	E	E	E	E
0.5-1.0	C	B	A	A
1.0-2.0	C	B	A	A

Churchill-Elmore-Buckingham, A; Issacs-Gaudy, B; Langbien-Durum, C; Negulescu-Rojanski, D; O'Connr-Dobbins, E; Owens-Edwards-Gibbs, F.

The next variables to be entered are the average times of sunrise and sunset reported in 24-hour time format for the deployment period of the data. We use mean sunrise and sunset values because our deployment periods are of short duration (< 30 days) and sunrise/sunset time changes are generally small (minutes) for weekly to monthly time periods. These times are input in Microsoft's twenty-four hour format with a colon separating the hour and minute columns. Night (*i.e.* dark cycle) is defined as the period between sunset and sunrise and is used in calculating 24-hour community respiration values. Several source of sunrise and sunset data are available on the World Wide Web (e.g. www.google.com/sun/; aa.usno.navy.mil/data/; www.mindspring.com/~cavu/sunset.html; www.weatherimages.org/latlonsun.html).

Next the user enters the approximate altitude of the stream sampling site in meters. Altitude is used as a surrogate measure of atmospheric pressure, which directly affects the solubility of oxygen in water. Though short-term changes in atmospheric

pressure occur due to fluctuations in climate and weather, from a stream monitoring perspective the most influential and predictable factor affecting atmospheric pressure is altitude (www.geog.ouc.bc.ca/physgeog/contents/7d.html). The calculator uses the quantifiable relationship between altitude and pressure to estimate the solubility of DO in the stream segment or reach being monitored.

Stream conductivity (mS/cm) measured during the period of study is used to correct for the effects of salinity on dissolved oxygen solubility in water. Conductivity is easily and accurately measured *in situ* or in the laboratory making it a commonly available water quality parameter. We used the tabular data in US Geological Survey's *National Field Manual for the Collection of Water-Quality Data* (USGS 1997) to develop a mathematical model to account for solubility changes as a result of salinity (i.e. conductivity). Conductivity is entered in units of mS/cm.

The final user selected variable in the *Stream Variables* sheet is the selection of the *Dissolved Oxygen logging interval*. This is the recording interval for the DO and temperature measurements. From the drop-down list, the user selects one of thirteen different intervals ranging from four to 30 minutes. These intervals were chosen because they divide evenly into a 24-hour period (day) thus simplifying calculation procedures. Recording intervals smaller than three minutes have little meaning as it takes about this length of time for the instrument to register the next stable measurement. No interval options over thirty minutes were included due to the increased error (i.e. reduced data resolution) associated with using larger sampling intervals with this production estimation method.

Two command buttons, *Clear Stream Variables* and *Clear Header*, allow the user to clear the previous values and to enter new values when necessary. These two buttons are located at the bottom of the reaeration equation list near the bottom, right-hand side of the worksheet.

DO Data – Sheet 3

The dissolved oxygen and temperature data along with the corresponding collection times are input in this worksheet (Figure 2). Once entered, the rates of change in DO concentrations can be calculated using the appropriate command button. General user information about the worksheet is contained in the header along with reminder information about user selected options and input data from the *Stream Variables* worksheet (i.e. reaeration coefficient, coefficient equation, and DO logging interval).

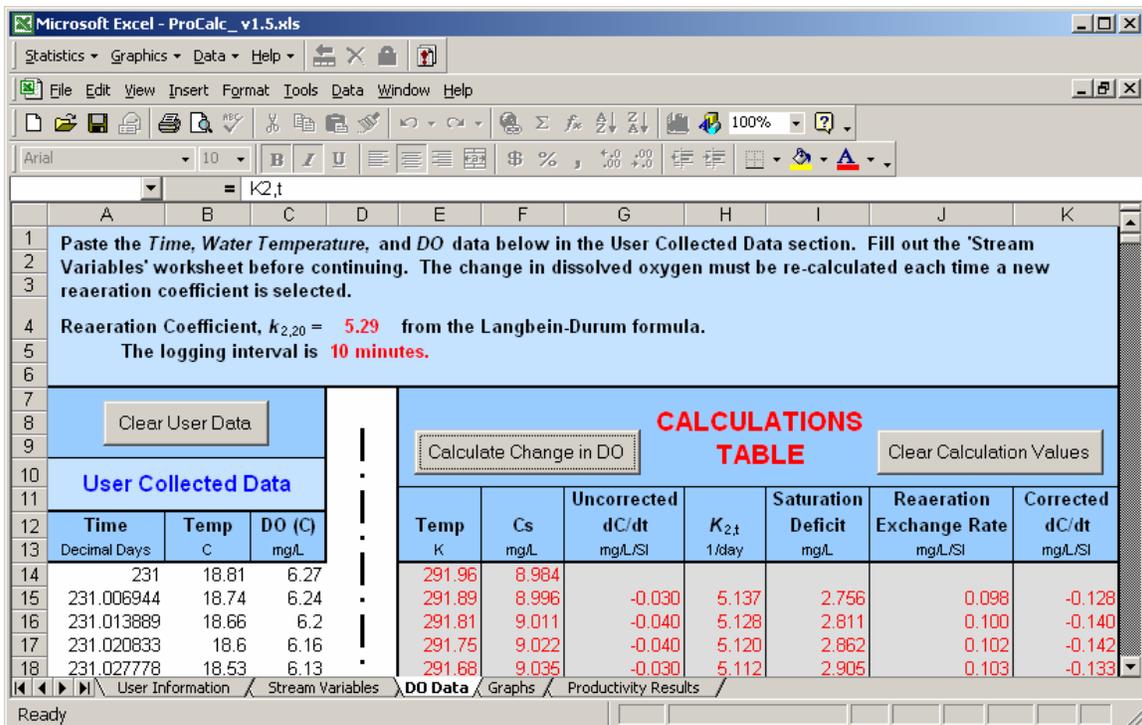


Figure 2. DO Data sheet (Sheet 3) showing both raw data and calculated variable values.

First under the *User Collected Data* heading copy and paste three columns of data from the logger; the time of each measurement (decimal days) and the temperature (C°) and DO (mg/L) values.

Later versions of the DO logger made by Eco Instruments recorded date and time in both decimal days and as mm/dd/yyyy. The Production Calculator can only process data based on decimal time intervals. Then click the *Calculate Change in DO* command button is pressed to calculate the necessary variables in the *Calculations Table*. It is during these calculations that the reaeration coefficients are corrected for each recorded temperature change. After calculating the variables in the *Calculations Table*, should the user choose to alter any of the data entered in the *Stream Variables* worksheet, the *Calculate Change in DO* button must be pressed again to recalculate the values in the *Calculations Table* in order for the changes made to translate to the *Calculations Table*. Two additional command buttons, *Clear User Data* and *Clear Calculation Values*, are included to allow the deletion of old and irrelevant data.

Graphs – Sheet 4

This worksheet displays data calculated in the *DO Data* worksheet. Data values from the *Calculations Table* are shown in graphical format to allow visualization of relevant temperature and dissolved oxygen variables generated as intermediate factors used in the final productivity calculations. The first of these graphs displays the cyclic flux of stream DO and temperature values through one or more night/day periods. Other graphs show the calculated DO concentrations at saturation for non standard pressure, both the uncorrected and corrected changes in DO concentrations over time, and changes

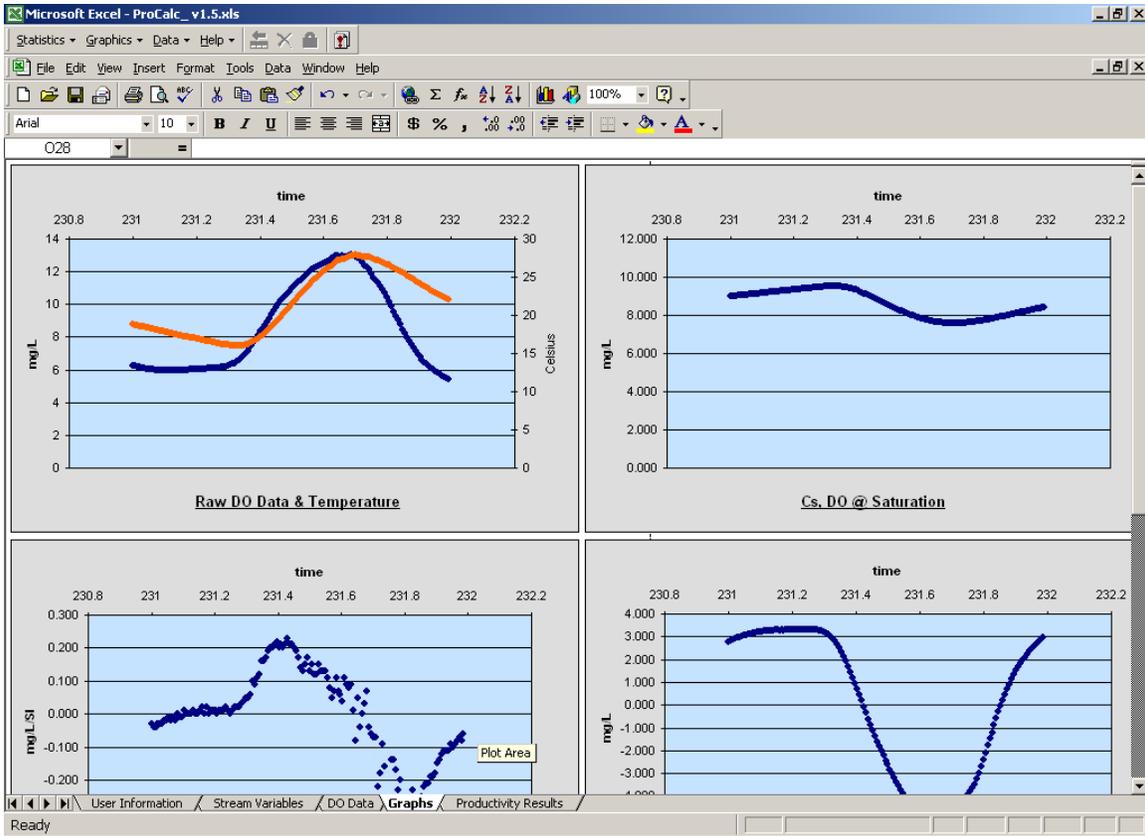


Figure 3. Graphs sheet (Sheet 4) showing some of the data graphs generated by the program to visualize the data and check for potential data quality issues.

in the DO saturation deficit and reaeration exchange rates. For stream data collected during the growing season the user will see a series of cyclic changes as a result of the light/dark cycle that influences both temperature and photosynthetic activities both of which affect productions and respiration (oxygen evolution and consumption). While changes in the size and shape of flux cycles can be expected due to actual stream and climate changes, abrupt and erratic changes in flux patterns or excessive data scatter should be cause for data quality concerns.

Productivity Results – Sheet 5

Computed estimates of production, respiration and the P/R ratio are displayed in the *Productivity Results* worksheet. Also included is the P/R ratio. Once the user presses the *Calculate Production* button, daily estimates and the sampling period averages for net production, gross production, and respiration are computed from the *Calculations Table* values calculated and displayed on DO Data worksheet (Sheet 3) and displayed as standard rates ($O_2/m^2/day$). To aid in printing the results, the previously entered header information along with the production estimates are formatted to be “printer friendly” and fit on letter size paper. The *Clear Values* command button erases the estimates and resets the page.

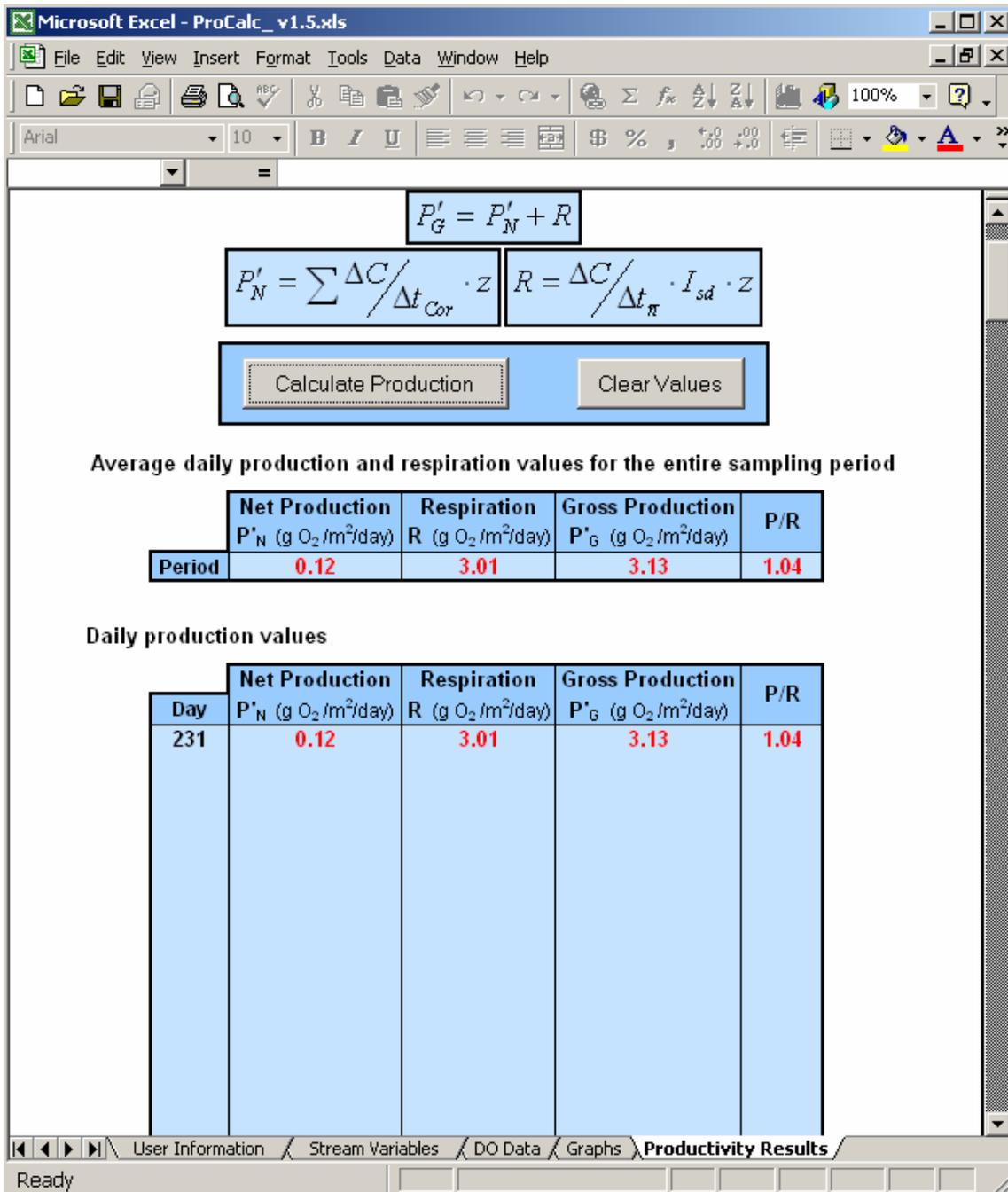


Figure 4. Productivity Results sheet (Sheet 5) showing production, respiration and P/R ratio values for a single day (24-hour period) of DO and temperature measurements of Big Muddy Creek, Iowa.

TECHNICAL GUIDE

The estimates of gross primary production and community respiration computed by the Production Calculator are calculated from diel oxygen and temperature data curves following the widely used and generally accepted method first proposed by Odum (1956). According to Odum the rate of change of dissolved oxygen (Q) is affected by four main factors that include the rate of gross primary production (P), the rate of community respiration (R), the rate of oxygen diffusion (D), and the rate of drainage accrual (A). The majority of studies conducted on estimates of production derived from diel oxygen data follow the method set forth by Odum (1956).

The rate of change of dissolved oxygen can be determined by subtracting both the rate of community respiration (R) and the rate of oxygen diffusion (D) from the rate of gross primary production (P) plus the rate of drainage accrual (A).

$$Q = P - R - D + A \quad (1)$$

The fluctuation of dissolved oxygen levels in the stream due to drainage accrual is assumed negligible relative to the other factors, but as a precaution, monitoring days in which dissolved oxygen readings could have been impacted by runoff should be removed from the deployment period dataset. While we assume that groundwater accrual is zero this may not be true for all streams and potential groundwater contributions may have to be examined. Elimination of drainage accrual reduces Equation 1 to Equation 2, the basic equation used to compute gross production.

$$Q = P - R - D \quad (2)$$

There are several climate and stream factors that also affect the concentration of dissolved oxygen in streams and must be examined in order to provide accurate estimates of production. These factors are temperature, reaeration, pressure and salinity.

The single most important factor regulating the concentration of dissolved oxygen in water is temperature (Horne and Goldman 1994). The concentration of oxygen in water is inversely proportionally to water temperature. Cold waters contain higher oxygen concentrations than the same volume of warm water at a given pressure.

Reaeration of streams is primarily the result of two phenomena: entrainment of oxygen due to turbulent flow and the replacement of oxygen due to a deficit from saturation caused by the combustion of organic matter. Reaeration was originally defined in the Streeter-Phelps (1925) equation as the reoxygenation (k_2) of streams. Today it is largely understood that the effects of the hydraulic properties of water (i.e. turbulent flow) are expressed as the coefficient of reaeration, k_2 (Langbein and Durum 1967).

Changes in barometric pressure alter the concentration of dissolved oxygen, since all gases are more soluble at higher pressures. This same principle is directly applicable to increases in altitude as reductions in atmospheric pressure are related to elevation increases. In these instances where pressures are less due to increased altitude, concentrations of dissolved oxygen are reduced. Additionally, barometric pressure changes associated with some weather changes can potentially alter DO levels in streams but these changes are episodic and often short lived.

Salinity has a minor effect on dissolved oxygen concentrations in fresh waters when compared to the other constituents. Increases in dissolved salts can affectively reduce the amount of intermolecular space within water molecules that would be

available to oxygen thus limiting oxygen saturation. However, salinities must be very high for increases in salt concentrations to effect dissolved oxygen concentrations. Because of its known relationship to salinity and greater commonality of measure, conductivity was used in the calculator as a surrogate measure of salinity

An understanding of these influencing factors allows us to parameterize and solve Equation 2 to calculate gross production. The first component of Equation 2 to solve is D , the rate of oxygen diffusion. There are several aspects that affect the rate of oxygen diffusion (D). The reaeration coefficient $k_{2,20}$, in units of 1/day, is one of the first variables to define. Several authors, Owens et al. (1964) and O'Connor and Dobbins (1958) among others, have developed simple predictive equations for the estimation of $k_{2,20}$. Wilcock (1982) has provided an overview of some of the most widely used reaeration equations and the stream conditions for which the equations are most viable. The vast majority of these equations are of the form:

$$k_{2,20} = aU^b \cdot z^c \quad (3)$$

Where U is the mean stream velocity (m/s), z is the mean stream depth (m), and a , b , and c are constants. Once $k_{2,20}$ is computed, it must be corrected for temperature. This conversion is accomplished using the Elmore and West (1961) equation.

$$k_{2,T} = k_{2,20} \cdot 1.024^{T_c-20} \quad (4)$$

A new temperature corrected reaeration coefficient, $k_{2,T}$, can be calculated for each recorded measurement of temperature and dissolved oxygen since both fluctuate throughout each day and the sample period. These changes in reaeration must be taken into account to provide an accuracy estimate of DO concentrations related solely to productivity and respiration processes.

After calculating $k_{2,T}$, the concentration of dissolved oxygen at saturation for each recorded temperature must be calculated. During these computations, corrections for salinity and pressure will be addressed. In order to calculate the dissolved oxygen concentration in mg/L at the standard pressure of one atmosphere, C_p , all temperature values are converted from Celsius to Kelvin, Equation 5.

$$T_K = T_C + 273.15 \quad (5)$$

The temperature in Kelvin, T_K , is used to calculate the dissolved oxygen concentration in mg/L at the standard pressure of one atmosphere, C_p .

$$C_p = e^{(-139.34411 + (157.570.1/T_K) - (66.423.080/T_K^2) + (1.2438 \times 10^{10}/T_K^3) - (8.621949 \times 10^{11}/T_K^4))} \quad (6)$$

In order to utilize the user's conductivity value as the correction of salinity, several steps must first take place. The conductivity units must be converted from the user entered units mS/cm to μ S/cm, Equation 7.

$$cond_2 = cond_1 \times 1000 \quad (7)$$

Then the conductivity correction factor for salinity is computed, Equation 8.

$$f_{cond} = -0.000003 \times cond_2 + 1.0002 \quad (8)$$

Once calculated, the correction factor is multiplied by C_p to correct the dissolved oxygen concentration at saturation and standard pressure for salinity, Equation 9.

$$C_{p,sal} = f_{cond} \times C_p \quad (9)$$

Having solved for, $C_{p,sal}$, we will calculate the nonstandard air pressure at the sampling site. This is accomplished using a measure of the site altitude as a surrogate for

air pressure. The altitude is entered into the calculator in meters (A_m) and then converted to feet, Equation 10.

$$A_{ft} = A_m \times 3.280839895 \quad (10)$$

The equation that converts altitude to nonstandard pressure, P , in atmospheres was derived from a table relating pressure and altitude created by Cole-Palmer Instrument Co. (www.coleparmer.com/techinfo/techinfo.asp?htmlfile=PEquationsTables.htm). This conversion is calculated using Equation 11.

$$P = -3 \times 10^{-5} A_{ft} + 0.996 \quad (11)$$

Now the partial pressure of water vapor, P_{wv} , in atmospheres, can be computed. Equation 12 uses the measured water temperature, in Kelvin.

$$P_{wv} = e^{(11.8571 - (3,840.7/T_k) - (216,961/T_k^2))} \quad (12)$$

The final variable required for the calculation of the dissolved oxygen concentration at saturation for nonstandard pressure corrected for salinity and pressure is theta, θ . Theta is a temperature adjustment needed to calculate the final corrected concentration at saturation, Equation 13.

$$\theta = 9.75 \times 10^{-4} - (1.426 \times 10^{-5} T_C) + (6.436 \times 10^{-8} T_C^2) \quad (13)$$

Having calculated all the necessary variables, the dissolved oxygen concentration at saturation for nonstandard pressure corrected for salinity and pressure in mg/L, C_s , can be computed, Equation 14.

$$C_s = C_{p,sal} P \left[\frac{(1 - P_{wv}/P)(1 - \theta P)}{(1 - P_{wv})(1 - \theta)} \right] \quad (14)$$

These calculations result in a corrected value of dissolved oxygen at saturation for every measure of temperature logged.

The next portion of the procedure involves calculating the reaeration exchange rate, r . The reaeration exchange rate incorporates all the corrections previously calculated, salinity, pressure, reaeration, and temperature, into the determination of gross production. This begins with the calculation of the dissolved oxygen deficit in mg/L, C_d , Equation 15.

$$C_d = C_s - C_t \quad (15)$$

The dissolved oxygen deficit, C_d , is the difference between the corrected dissolved oxygen concentration, C_s , and the recorded dissolved oxygen concentration at some time, t . The dissolved oxygen deficit is then multiplied by the temperature corrected reaeration coefficient, $k_{2,T}$, and divided by the number of recording intervals per day, I_{sd} , resulting in the reaeration exchange rate, Equation 16.

$$r = k_{2,T} \cdot C_d / I_{sd} \quad (16)$$

The number of recording intervals per day, I_{sd} , is calculated from the logging interval, l_i , selected by the user in the *Stream Variables* worksheet.

From here the uncorrected change in dissolved oxygen concentration over time, $\Delta C / \Delta t_{Uncor}$, is computed. This is found by subtracting the current measure of dissolved oxygen, C_t , from the next measure, C_{t+1} , Equation 17.

$$\Delta C / \Delta t_{Uncor} = C_{t+1} - C_t \quad (17)$$

Since the program is calculating a rate, a change in concentration over unit time, the units for $\Delta C / \Delta t_{Uncor}$ are in mg/L/ l_i , where l_i , the selected logging interval,

With the reaeration exchange rate and the uncorrected change in dissolved oxygen concentration over time calculations completed, we can correct the change in dissolved oxygen concentration over time for salinity, pressure, reaeration, and temperature by subtracting the reaeration exchange rate, Equation 18.

$$\frac{\Delta C}{\Delta t_{Cor}} = \frac{\Delta C}{\Delta t_{Uncor}} - r \quad (18)$$

With all the preliminary calculations completed, it is now possible to begin calculating estimates of production and respiration. The first step is the estimation of respiration, R . Because these respiration rates encompass all stream respiration including insects and microorganisms, Since no photosynthesis occurs at night the only biologic activity should be respiration. Using this concept, the program will determine the average change in dissolved oxygen concentrations at night and then extrapolate the value over the entire day to generate a daily rate of respiration. The average nighttime $\Delta C / \Delta t_{Cor}$ is calculated by summing all $\Delta C / \Delta t_{Cor}$ values that occur before sunrise and after sunset. The values for sunrise and sunset are input by the user. All individual nighttime values are summed then divided by the number of nighttime recording intervals to obtain the average nighttime corrected change in dissolved oxygen concentration over time, $\Delta C / \Delta t_{\bar{n}}$. To extrapolate this nighttime value over the entire day $\Delta C / \Delta t_{\bar{n}}$ is multiplied by the number of recording intervals per day, I_{sd} . And finally, everything is multiplied by

depth, z , to convert the units from volumetric to areal. The resulting Equation 19 has units of $\text{g O}_2/\text{m}^2/\text{day}$.

$$R = \Delta C / \Delta t_{\bar{n}} \cdot I_{sd} \cdot z \quad (19)$$

By reporting oxygen rates as respiration it is understood that an oxygen deficit exists therefore respiration values should be reported as positive numbers. For this purpose, the absolute value of R is reported.

The next estimated component is net primary productivity. Net primary productivity, P'_N , is the sum of the corrected change in dissolved oxygen concentration over time multiplied by depth to produce an areal measure, Equation 20 with units $\text{g O}_2/\text{m}^2/\text{day}$.

$$P'_N = \sum \Delta C / \Delta t_{Cor} \cdot z \quad (20)$$

The final production estimate is gross primary production, P'_G . Gross primary production, units of $\text{g O}_2/\text{m}^2/\text{day}$, is computed from the addition of respiration and net primary productivity, Equation 21. As with R and P'_N gross primary production is has the units of $\text{g O}_2/\text{m}^2/\text{day}$.

$$P'_G = P'_N + R \quad (21)$$

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