**Using Excel Solver to Fit an Equation**

1. Convert BOD\_mg/L (raw data) to CO2\_mg/L by dividing 32 (molecular weight of oxygen) and multiplying 44 (molecular weight of CO2), assuming 1:1 molar ratio of oxygen consumption to CO2 generation.

Convert CO2 unit from mg/L to mg/g by multiplying 0.97 L (volume of incubation jar headspace) and dividing 50 g (soil dry weight).

Column A and D are the kinetics data to fit.

|  |  |  |  |
| --- | --- | --- | --- |
| A | B | C | D |
| Time\_hr | BOD\_mg/L | CO2\_mg/L | CO2\_mg/g |
| 0 | 0.0 | 0 | 0.000 |
| 2 | 22.0 | 30.25 | 0.618 |
| 4 | 22.0 | 30.25 | 0.618 |
| 6 | 24.0 | 33 | 0.674 |
| 8 | 24.0 | 33 | 0.674 |
| 10 | 32.0 | 44 | 0.899 |
| 12 | 32.0 | 44 | 0.899 |

1. Fit the kinetics data with 1st order respiration model:

CO2 = B + A\*(1-exp(-k\*t))

CO2 is the CO2 concentration, B is the initial CO2 concentration at time 0, A is the maximum CO2 generation in the sample, k is the rate constant (hr-1), t is the time (hr).

Column E is the predicted CO2 values from the equation above with the guess values of B in cell E1, A in cell E2 and k in cell E3.

An example of cell E7 is ‘=$E$1+$E$2\*(1-EXP(-$E$3\*A7))’

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | A | B | C | D | E | F |
| 1 |  |  |  | B | 1 |  |
| 2 |  |  |  | A | 2 |  |
| 3 |  |  |  | k | 0.1 |  |
| 4 |  |  |  | Sum of sq er |  |  |
| 5 |  |  |  |  |  |  |
| 6 | Time\_hr | BOD\_mg/L | CO2\_mg/L | CO2\_mg/g | Predicted CO2 |  |
| 7 | 0 | 0.0 | 0 | 0.000 | 0.000 |  |
| 8 | 2 | 22.0 | 30.25 | 0.618 | 0.246 |  |
| 9 | 4 | 22.0 | 30.25 | 0.618 | 0.458 |  |
| 10 | 6 | 24.0 | 33 | 0.674 | 0.642 |  |
| 11 | 8 | 24.0 | 33 | 0.674 | 0.801 |  |
| 12 | 10 | 32.0 | 44 | 0.899 | 0.938 |  |
| 13 | 12 | 32.0 | 44 | 0.899 | 1.057 |  |

1. Column F is the square of the difference between the measured data (column D) and the predicated data (column E), called chi squared (χ2).

The following formula should be entered into cell F7: =(D7-E7)^2 and copied into all of column F.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | A | B | C | D | E | F |
| 1 |  |  |  | B | 0.108 |  |
| 2 |  |  |  | A | 1.714 |  |
| 3 |  |  |  | k | 0.068 |  |
| 4 |  |  |  | Sum of chi sq | 0.527 |  |
| 5 |  |  |  |  |  |  |
| 6 | Time\_hr | BOD\_mg/L | CO2\_mg/L | CO2\_mg/g | Predicted CO2 | Chi sq |
| 7 | 0 | 0.0 | 0 | 0.000 | 0.108 | 0.012 |
| 8 | 2 | 22.0 | 30.25 | 0.618 | 0.326 | 0.085 |
| 9 | 4 | 22.0 | 30.25 | 0.618 | 0.516 | 0.010 |
| 10 | 6 | 24.0 | 33 | 0.674 | 0.682 | 0.000 |
| 11 | 8 | 24.0 | 33 | 0.674 | 0.827 | 0.023 |
| 12 | 10 | 32.0 | 44 | 0.899 | 0.954 | 0.003 |
| 13 | 12 | 32.0 | 44 | 0.899 | 1.064 | 0.027 |

1. Cell E3 is the sum of all the chi square values in column F. The best curve fit is expected to have the minimum value of the sum of chi squares.
2. Load the “Solver” Add-in in Excel

Windows:

* 1. go to **File > Options**
  2. Click **Add-Ins**, and then in the **Manage** box, select **Excel Add-ins**.
  3. Click **Go**.
  4. In the **Add-Ins available** box, select the **Solver Add-in** check box, and then click **OK**.
     1. If the **Solver Add-in** is not listed in the **Add-Ins available** box, click **Browse** to locate the add-in.
     2. If you get prompted that the Solver Add-in is not currently installed on your computer, click **Yes** to install it.
  5. After you load the Solver Add-in, the **Solver** command is available in the **Analysis** group on the **Data** tab.

MacOS:

* 1. On the **Tools** menu, select **Excel Add-Ins**.
  2. In the **Add-Ins available** box, select the **Solver Add-In** check box, and then click **OK**.
     1. If **Solver Add-in** is not listed in the **Add-Ins available** box, click **Browse** to locate the add-in.
     2. If you get a prompt that the Solver add-in is not currently installed on your computer, click **Yes** in the dialog box to install it.
  3. After you load the Solver add-in, the **Solver** button is available on the **Data** tab.

1. Procedure to fit the data with Solver:
   1. Click “Solver” in the “Data” tab in Excel.
   2. In the pop-up window, select cell E3 as Set Objective.
   3. Choose To: “Min”.
   4. Select cell E2 and E3 as By Changing Variable Cells
   5. In the “Select a Solving Method”, choose “GRG Nonlinear”.
   6. Click “Solve”
   7. A new pop-up window will appear asking if you want to keep the new values or restore original values. Select “Keep Solver Solution” and click the “OK” button.
2. The Predicted CO2 (column E) should be updated with new values of B, A and k from Solver. Plot Predicted CO2 with time as curve together with a scatter plot of measured CO2 and time.