**Using Excel Solver to Fit an Equation**

1. Create a spreadsheet similar to the one below. 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 = A\*(1-exp(-k\*t))

CO2 is the CO2 concentration, 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 A in cell E1 and k in cell E2.

An example of cell E6 is ‘=$E$1\*(1-EXP(-$E$2\*A6))’

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | A | B | C | D | E | F |
| 1 |  |  |  | A | 1.816915075 |  |
| 2 |  |  |  | k | 0.072625018 |  |
| 3 |  |  |  | Sum of sq er |  |  |
| 4 |  |  |  |  |  |  |
| 5 | Time\_hr | BOD\_mg/L | CO2\_mg/L | CO2\_mg/g | Predicted CO2 |  |
| 6 | 0 | 0.0 | 0 | 0.000 | 0.000 |  |
| 7 | 2 | 22.0 | 30.25 | 0.618 | 0.246 |  |
| 8 | 4 | 22.0 | 30.25 | 0.618 | 0.458 |  |
| 9 | 6 | 24.0 | 33 | 0.674 | 0.642 |  |
| 10 | 8 | 24.0 | 33 | 0.674 | 0.801 |  |
| 11 | 10 | 32.0 | 44 | 0.899 | 0.938 |  |
| 12 | 12 | 32.0 | 44 | 0.899 | 1.057 |  |

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

The following formula should be entered into cell F6: =(D6-E6)^2 and copied into all of column F.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | A | B | C | D | E | F |
| 1 |  |  |  | A | 1.816915075 |  |
| 2 |  |  |  | k | 0.072625018 |  |
| 3 |  |  |  | Sum of chi sq | 0.555 |  |
| 4 |  |  |  |  |  |  |
| 5 | Time\_hr | BOD\_mg/L | CO2\_mg/L | CO2\_mg/g | Predicted CO2 | Chi sq |
| 6 | 0 | 0.0 | 0 | 0.000 | 0.000 | 0.000 |
| 7 | 2 | 22.0 | 30.25 | 0.618 | 0.246 | 0.139 |
| 8 | 4 | 22.0 | 30.25 | 0.618 | 0.458 | 0.026 |
| 9 | 6 | 24.0 | 33 | 0.674 | 0.642 | 0.001 |
| 10 | 8 | 24.0 | 33 | 0.674 | 0.801 | 0.016 |
| 11 | 10 | 32.0 | 44 | 0.899 | 0.938 | 0.002 |
| 12 | 12 | 32.0 | 44 | 0.899 | 1.057 | 0.025 |

1. Cell E3 is the sum of all the chi square values in column F. The best fit curve 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 A and k from Solver. Plot Predicted CO2 with time as curve together with a scatter plot of real measured CO2 and time.