# The BioWin Advantage

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In this edition of **The BioWin Advantage** we will illustrate how to use the Rates Window in BioWin to help interpret model results and gain a deeper understanding of what's going on at various points in your process flowsheet.

## The Rates Window in BioWin


**The Rates Window**

**Extending the Utility of the Rates Window**

**An Example of Using the Rates Window and the Rates Spreadsheet Tool**

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## The Rates Window

BioWin allows you to view the rates of reactions in bioreactor-type elements. To open the **Rates Window** for a bioreactor, you right-click on the bioreactor element in your flowsheet and select **Rates...** from the resulting pop-up menu. An example of a rates window for the secondary anoxic reactor of the **5-stage BNR (N and P removal).bwc** file from the BioWin Filing Cabinet is shown in the figure below. In the left pane of this window, the calculated process rates are shown with units of mg/L/d. In the right pane of this window, the net conversion rates (i.e. reaction term) for each of the State Variables are shown with units of mg/L/d*$m^3$ (or g/d). These conversion rates are a function of the process rates, the model stoichiometry, and the reactor volume and are equivalent to the difference between the mass rate into and out of the reactor.

### Featured Article

**The Rates Window in BioWin**

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Rates for - Sec Anoxic

| # | Process name | Process rate | Units |
|---|---|---|---|
| 0 | Aer. growth of ZBH on SBSC | 0.00 | mgCOD/L/d |
| 1 | Anox. growth of ZBH on SBSC with NO3 | 86.63 | mgCOD/L/d |
| 2 | Anox. growth of ZBH on SBSC with NO2 | 166.54 | mgCOD/L/d |
| 3 | Aer. Growth of ZBH on SBSP | 0 | mgCOD/L/d |
| 4 | Anox. growth of ZBH on SBSP with NO3 | 0.01 | mgCOD/L/d |
| 5 | Anox. growth of ZBH on SBSP with NO2 | 0.02 | mgCOD/L/d |
| 6 | Aer. Growth of ZBH on SBSA | 0.00 | mgCOD/L/d |
| 7 | Anox. growth of ZBH on SBSA with NO3 | 0.08 | mgCOD/L/d |
| 8 | Anox. growth of ZBH on SBSA with NO2 | 0.16 | mgCOD/L/d |
| 9 | Aer. growth of ZBH on SBMETH | 0 | mgCOD/L/d |
| 10 | Decay of ZBH | 365.39 | mgCOD/L/d |
| 11 | Growth of anoxic methanol utilizers with NO3 | 0 | mgCOD/L/d |
| 12 | Growth of anoxic methanol utilizers with NO2 | 0 | mgCOD/L/d |
| 13 | Decay of anoxic methanol utilizers | 0.02 | mgCOD/L/d |
| 14 | Aer. growth of ZBP | 0.00 | mgCOD/L/d |
| 15 | Aer. growth of ZBP (PO4 limited) | 0.00 | mgCOD/L/d |
| 16 | Anox. growth of ZBP with NO3 | 8.78 | mgCOD/L/d |
| 17 | Anox. growth of ZBP with NO2 | 16.87 | mgCOD/L/d |
| 18 | Sequestration of acetate by ZBP | 0.31 | mgCOD/L/d |
| 19 | Sequestration of propionate by ZBP | 0.13 | mgCOD/L/d |
| 20 | Aer. decay of ZBP | 0.00 | mgCOD/L/d |
| 21 | PHA release on aer. decay of ZBP | 0.00 | mgCOD/L/d |
| 22 | PP-LO release on aer. Decay of ZBP | 0.00 | mgP/L/d |
| 23 | PP-HI release on aer. decay of ZBP | 0.00 | mgP/L/d |
| 24 | Ana. decay of ZBP | 16.42 | mgCOD/L/d |
| 25 | PHA release on ana. decay of ZBP | 0.63 | mgCOD/L/d |
| 26 | PP-LO release on ana. decay of ZBP | 1.95 | mgP/L/d |
| 27 | PP-HI release on ana. decay of ZBP | 1.16 | mgP/L/d |
| 28 | Cleavage of PP for ana. maintenance | 15.14 | mgP/L/d |
| 29 | Hydrolysis of stored COD on decay | 429.25 | mgCOD/L/d |

| State variable | Reaction term | Units |
|---|---|---|
| Non-polyP heterotrophs | -671457.82 | mgCOD/L/d * m |
| Anoxic methanol utilizers | -106.50 | mgCOD/L/d * m |
| Ammonia oxidizing biomass | -14250.39 | mgCOD/L/d * m |
| Nitrite oxidizing biomass | -6926.47 | mgCOD/L/d * m |
| Anaerobic ammonia oxidizers | -72.00 | mgCOD/L/d * m |
| PolyP heterotrophs | 55400.07 | mgCOD/L/d * m |
| Propionic acetogens | -63.22 | mgCOD/L/d * m |
| Acetoclastic methanogens | -139.88 | mgCOD/L/d * m |
| Hydrogenotrophic methanogens | -178.14 | mgCOD/L/d * m |
| Endogenous products | 201753.54 | mgCOD/L/d * m |
| Slowly bio. COD (part.) | -538416.62 | mgCOD/L/d * m |
| Slowly bio. COD (colloid.) | -106.70 | mgCOD/L/d * m |
| Part. inert. COD | | mgCOD/L/d * m |
| Part. bio. org. N | 22413.30 | mgN/L/d * m3 |
| Part. bio. org. P | 1423.87 | mgP/L/d * m3 |
| Part. inert N | | mgN/L/d * m3 |
| Part. inert P | | mgP/L/d * m3 |
| Stored PHA | -297698.83 | mgCOD/L/d * m |
| Releasable stored polyP | -6259.92 | mgP/L/d * m3 |
| Fixed stored polyP | -728.07 | mgP/L/d * m3 |
| PolyP bound cations | -4743.56 | mg/L/d * m3 |
| Readily bio. COD (complex) | -181257.72 | mgCOD/L/d * m |
| Acetate | -147.44 | mgCOD/L/d * m |
| Propionate | -402.84 | mgCOD/L/d * m |
| Methanol | 0.00 | mgCOD/L/d * m |
| Dissolved H2 | -9295.94 | mgCOD/L/d * m |
| Dissolved methane | -7.18 | mg/L/d * m3 |
| Ammonia N | 95352.50 | mgN/L/d * m3 |
| Sol. bio. org. N | -88330.55 | mgN/L/d * m3 |
| Nitrite N | -122153.15 | mgN/L/d * m3 |
| Nitrate N | -430714.40 | mgN/L/d * m3 |

It should be noted that the units of the reaction term are always in g/d regardless of your current project unit selection - so if you're working in US units, you'll need to convert these to lbs/d. This is due to the fact that even when you are working in US units, BioWin still does all of its underlying calculations in SI.

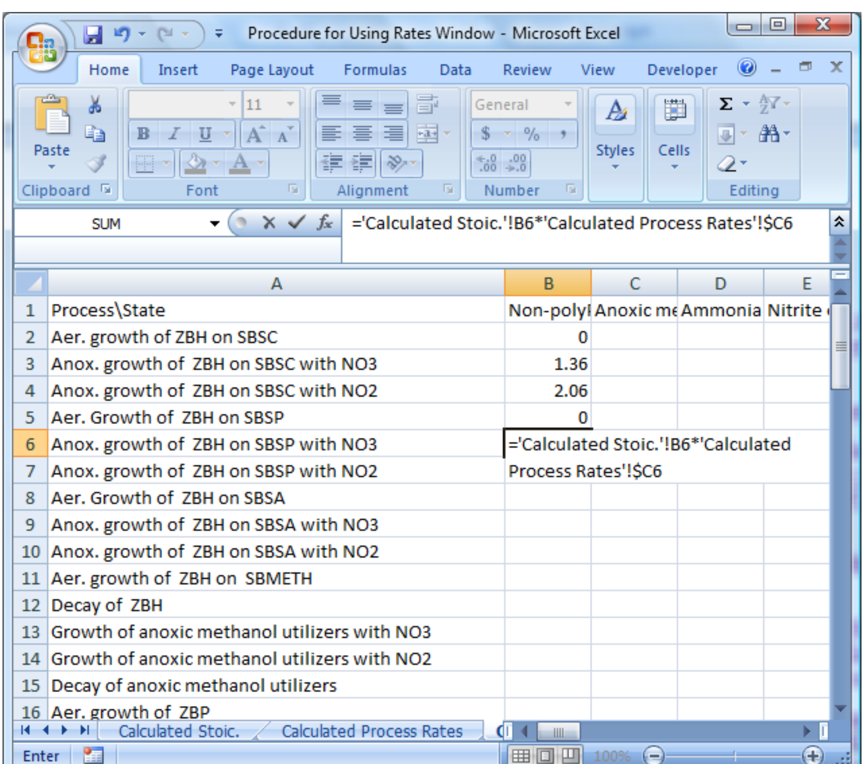
Just by looking at the **Rates Window**, you can find out good information about what's going on at that point in your process. For example, by looking at the calculated process rates in the left-hand portion of the window, you can see if certain processes are active or not. For example, for the secondary anoxic reactor in our process we can see that the aerobic processes are zero (as we'd expect), the anoxic process are non-zero (again, we'd expect that we have denitrification occurring here), and if we look at Processes 11 and 12, we see that there are no anoxic methanol-utilizers growing in our secondary anoxic reactor (which is expected in this case, because there is no methanol being added!). These examples are all obvious, but in other cases just having a quick look down the list of processes in a reactor and seeing what's "on" and what's "off" can be a very useful trouble-shooting and/or results interpretation tool.

Looking at the net conversion rates in the right-hand side of the **Rates Window** is useful for seeing what's happening to the various state variables that BioWin tracks in that zone of your process. Recall that the net conversion rate is equivalent to the difference between the mass rate into and out of the reactor in g/d. For example, the net conversion rate of ammonia is 95,352.50 g/d, or about 95.4 kg/d. That is, about 95.4 kg/d more ammonia is leaving than entering the secondary anoxic reactor - there is a ***net generation*** of ammonia in the secondary anoxic reactor. Likely this is mainly due to nitrogen release upon organism decay - we often see this slight increase in ammonia across secondary anoxic zones because the nitrifiers can't remove it in these unaerated zones! To take another example, we can see that the net conversion rates for nitrite and nitrate are -122,153.15 and -430,714.40 g/d, respectively (about -122.2 and -430.7 kg/d). The negative values tell us that there is a net consumption of nitrite and nitrate in the secondary anoxic reactor - as we'd expect since we're looking for denitrification to occur in that zone! In the next section, we'll see how we can extend the utility of the **Rates Window** even further by looking at the individual contributions to a state variable's net conversion rate.

## Extending the Utility of the Rates Window

It is possible to get more detail about the processes contributing to the net conversion rates of the individual State Variables using information from the **Rates Window** and the **Calculated Stoichiometry** for the model. The following steps walk you through the creation of a spreadsheet that will do this (this is mainly for explanation - EnviroSim has created one for you and it is included with this newsletter!):

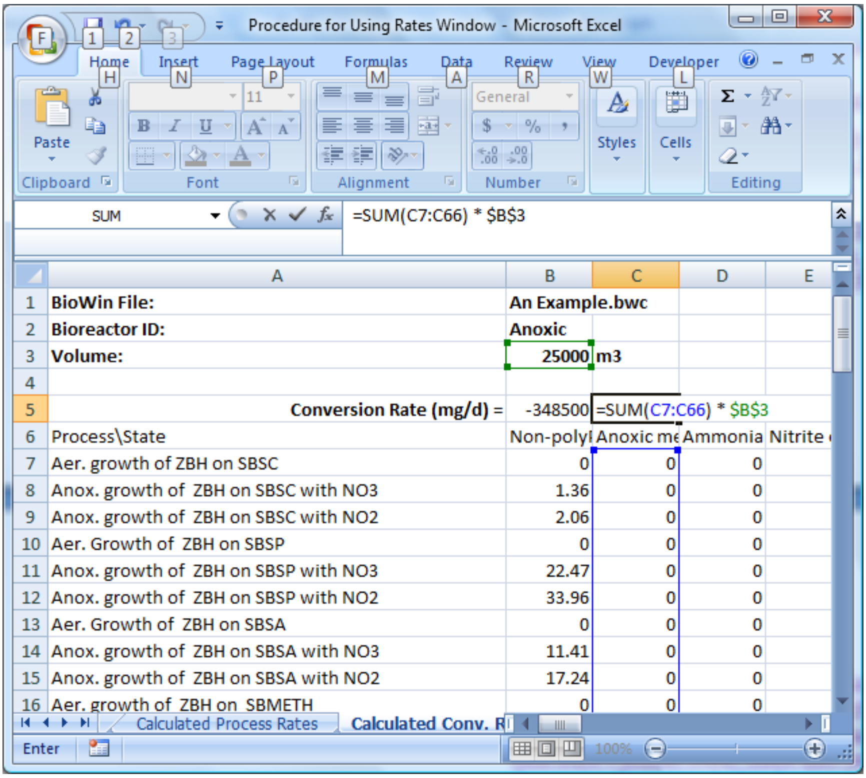
- Open up **Project|Current Project Options|Model|Show calculated stoichiometry...**
- Right-click on a column heading and select **Copy** from the pop-up menu to copy the stoichiometry matrix to the Windows clipboard. Next, open Excel, switch to an empty worksheet, and paste the information in the upper left-hand cell (**A1**). Give the worksheet a descriptive name, e.g. "**Calculated Stoich**.".
- Switch back to BioWin and close the calculated stoichiometry window, and then click **Cancel** or **OK** to close the **Current Project Options** dialog box.
- Right-click on the bioreactor you are interested in and open the **Rates Window**.
- Right-click on the column heading in the left pane of the **Rates Window** and select **Copy** from the pop-up menu to copy the table of the calculated **Process Rates** to the Windows clipboard. Next, paste the copied information into a second worksheet (tab) in your spreadsheet program. Give this worksheet a descriptive name, e.g. "**Calculated Process Rates**".
- Create a third worksheet in the spreadsheet program and name it "**Calculated Conv. Rates**".
- In the first column of the "**Calculated Conv. Rates**" worksheet, copy the names of the process rates from the "**Calculated Stoic**." worksheet. In the first row, also copy the names of the State Variables from the "**Calculated Stoic**." worksheet.
- In the first open cell of the "**Calculated Conv. Rates**" worksheet, enter a formula to determine the product of the first calculated stoichiometry matrix entry and the first calculated process rate. For example, the conversion rate for **Non-polyP heterotrophs due to Aer. Growth of ZBH on SBSC** is equal to the **Calculated Stoichiometry** for that process and state variable multiplied by the rate for that process. If you have been following the placement of information into your worksheets exactly as described in the steps above, the equation entered into the first cell will be **"='Calculated Stoic.'!B2*'Calculated Process Rates'!$C2"**



*Calculating Conversion Rates (mg/L/d) due to individual Processes*

- Copy this equation across the entire matrix.
- At this point it may be useful to add a few extra rows at the top of the worksheet along with the details of the BioWin file, Bioreactor ID and Bioreactor Volume under investigation.
- The net conversion rate for each of the State Variables can next be calculated as the sum of the **Conversion Rates** due to each of the

individual processes multiplied by the volume of the bioreactor.




*Calculating Net Conversion Rates (mg/ d) as a function of volume and sum of individual conversion rates*

- This value is equivalent to the reaction term calculated for each state variable in the right pane of the **Rates Window** for a BioWin flowsheet element, but offers the added benefit of being able to identify which processes are contributing to the net conversion rate for each State Variable. Note that there may be some difference between your calculated conversion rate and those shown in BioWin's **Rates Window**. This is because BioWin carries many significant figures in its calculations.

## An Example of Using the Rates Window and the Rates Spreadsheet Tool

To make your life easier, EnviroSim has set up a template spreadsheet with most of the above steps completed for you. Using this template (which is attached to this newsletter and called **BW Conversion Rates Calculator - BioWin Advantage.xls**) cuts the steps outlined above to a few copy/paste operations. Let's apply the template to investigate the formation of ammonia in the secondary anoxic zone of the **5-stage BNR (N and P removal).bwc** file from the BioWin Filing Cabinet.

Recall that earlier, we had used the **Rates Window** to tell us that there was about 95.4 kg/d more ammonia leaving the secondary anoxic zone of the 5 Stage BNR system than entering it. Our initial thought was that this likely was from decay. Let's check on that.

First, open the **Rates Window** for the secondary anoxic zone and copy the contents of the left-hand pane by right-clicking. Now go to the **Step 1** tab of the spreadsheet template we've provided, click on cell **A3** (which will contain a '#' sign), and paste what you just copied. Also, while you're on this tab, enter the secondary anoxic zone volume of 6,000 $m^3$.

Next, access the calculated stoichiometry matrix for your file as outlined above, and copy that over to the **Step 2** tab of the spreadsheet template. Because we've already entered the formulas for calculating the net conversions on the **Step 3** tab, you're all done. Now it's a matter of using the information that we can see on the Step 3 tab.

If you click on cell **AC13**, you will see the net conversion of ammonia that we saw in BioWin; in the BioWin **Rates Window** it was 95.4 kg/d, but here it is calculated as 95.2 kg/d due to the significant figures issue flagged earlier. Looking down column **AC** tells us what's contributing to that net generation of ammonia. For example, the first large numbers we see are negative values; if we look across to column **A** we can see that these are associated with ammonia assimilation for synthesis purposes during growth of ordinary heterotrophs that are denitrifying. Scrolling further down, we see a positive number associated with decay of phosphorus accumulating organisms. And going down a bit further, we see a large positive number (208.5 kg/d) associated with ammonification, which is the conversion of soluble biodegradable organic nitrogen to ammonia. It looks like this is the main contributor to the net generation of ammonia in this secondary anoxic zone, and to verify that it came from decay processes, we can "follow the nitrogen" (i.e. look in further detail at the ammonification process).

For the ammonification process (Row 39), we can see exactly one column to the right of ammonia (**column AD**) a conversion rate of -208.5 kg/d for soluble biodegradable organic nitrogen - so as stated above, the ammonia is indeed coming from ammonification of soluble biodegradable organic nitrogen. In this same column, if we look up a few rows, we can see that over half (120.2 kg/d) of this soluble biodegradable organic nitrogen is being generated within the Secondary Anoxic zone by the process **Hydrolysis of Stored N on Decay** (see column **A**). That is to say that decay, followed by ammonification of decay products, is indeed the reason there is a net generation of ammonia across the secondary anoxic zone.

Once you get the hang of using the **Rates Window** and the spreadsheet template we've provided, you will find that this is a very powerful tool for interpreting your BioWin results, trouble-shooting, etc. For example, you can use it to answer questions like:

- In an aerobic zone, how much ammonia is being used for synthesis by ordinary heterotrophs and how much is being converted to nitrite by ammonia oxidizing bacteria?
- In an anoxic zone of a biological phosphorus removal process, how much denitrification is being carried out by phosphorus accumulating organisms?
- How much "new growth" am I getting in a given zone?
- In a secondary anoxic zone with methanol addition, how much NOX-N is removed by the methanol utilizers relative to the ordinary heterotrophic denitrification?

## In Conclusion

In this edition of **The BioWin Advantage**, we've introduced you to a feature of BioWin that when combined with the spreadsheet template we've provided is a powerful diagnostic tool.

We trust that you found this technical topic both interesting and informative.

Please feel free to contact us at **info@envirosim.com** (Subject: The BioWin Advantage) with your comments on this article or suggestions for future article.

Thank you and good modeling

**The EnviroSim Team**

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