

# Athena Visual Studio Algebraic Model Tutorial

- ❖ Start **Athena Visual Studio**
- ❖ From the **File** menu select **New**.
- ❖ You are in the **Process Modeling** tab.
- ❖ Click **Modeling with Pure Algebraic Equations**.
- ❖ Select **A Blank Document** and click **OK**.
- ❖ Enter your data, initial conditions, model equations, and the Athena DAE solver data and options as described in this tutorial.

### When you are done:

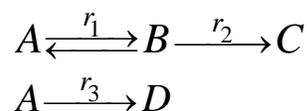
- ❖ From the **File** menu click **Save**.
- ❖ Navigate to the folder where you wish to save and enter a proper filename for your model.
- ❖ From the **Build** menu click **Compile**.
- ❖ From the **Build** menu click **Build EXE**.
- ❖ From the **Build** menu click **Execute**.

Nonlinear Algebraic Models that can be solved with Athena Visual Studio take the form  $\mathbf{F}(\mathbf{u};\boldsymbol{\theta}) = \mathbf{0}$  where  $\mathbf{u}$  is a vector of unknowns, such as the temperature, pressure and composition, and  $\boldsymbol{\theta}$  is a vector of parameters pertinent to the process we are modeling. Algebraic models are ordinarily used to describe steady-state processes such as CSTRs (Continuous Stirred Tank Reactors); they are also used to describe steady-state phase equilibrium, such as single-stage and multi-stage flash calculations, chemical equilibrium and the discretized forms of distributed parameter systems such as steady-state

plug flow and fixed bed reactors. The algebraic equations can be solved using the Athena Visual Studio powerful damped Newton algorithm which is encoded in the **DDAPLUS** solver. The example problem below has been created to illustrate the functionality of Athena Visual Studio in dealing with the solution of nonlinear algebraic equations. Additional features such as sensitivity analysis, parametric continuation and the use of auxiliary variables will also be demonstrated.

## Tutorial: Continuous Stirred Tank Reactor (CSTR) Modeling

The following chemical reactions take place in a Continuous Stirred Tank Reactor (CSTR) under isothermal and isobaric conditions:



The mathematical model that describes the reactor material balance is given by the following system of nonlinear algebraic equations. The last column in Table 1. shows the unknown variables (component molar concentrations) in Athena Visual Studio notation:

**Table 1. CSTR Material Balance Equations**

$C_{A0} + \tau(-r_1 - r_3) - C_A = 0$	$r_1 = \frac{k_1 K_A}{1 + K_A C_A + K_B C_B} \left( C_A - \frac{C_B}{K_{eq}} \right)$	$U(1) := C_A$
$C_{B0} + \tau(r_1 - r_2) - C_B = 0$	$r_2 = \frac{k_2 K_B}{1 + K_A C_A + K_B C_B} C_B$	$U(2) := C_B$
$C_{C0} + \tau r_2 - C_C = 0$	$r_3 = \frac{k_3 K_A}{1 + K_A C_A + K_B C_B} C_A$	$U(3) := C_C$
$C_{D0} + \tau r_3 - C_D = 0$		$U(4) := C_D$

We wish to perform the following tasks:

- ❖ Estimate the concentration of the reaction components in the effluent stream
- ❖ Estimate the sensitivity of the concentrations to changes in rate constants  $k_1, k_2$
- ❖ Estimate the conversion of component A by introducing an auxiliary variable,  $X_A$
- ❖ Create a plot of Residence Time vs. Conversion using Continuation Analysis

The values and description of the parameters for this process model are given in the table below:

<b>MODEL PARAMETERS</b>	<b>Description and Units</b>
$\tau = 90.0$	Residence Time (s)
$C_{A0} = 0.35$	Feed Molar Concentration (mol/m <sup>3</sup> )
$k_1 = 0.01$	Reaction Rate Constant (mol/m <sup>3</sup> s)
$k_2 = 0.01$	Reaction Rate Constant (mol/m <sup>3</sup> s)
$k_3 = 0.001$	Reaction Rate Constant (mol/m <sup>3</sup> s)
$K_A = \exp\left(\frac{35,000}{R_g T} - \frac{91}{R_g}\right)$	Adsorption Constant (m <sup>3</sup> /mol)
$K_B = \exp\left(\frac{20,000}{R_g T} - \frac{53}{R_g}\right)$	Adsorption Constant (m <sup>3</sup> /mol)
$K_{eq} = 4.29 \times 10^{-4} \frac{K_A}{K_B} \exp\left(\frac{30,000}{R_g T}\right)$	Equilibrium Constant (Unitless)
$R_g = 8.314$	Universal Gas Constant (J/mol K)
$T = 330.0$	Reactor Temperature (K)

The conversion of the component A is defined via the auxiliary variable:

$$X_A = \frac{C_{A0} - C_A}{C_{A0}} \times 100$$

The sensitivity functions of the components with respect to the reaction rate constants  $\{k_1, k_2\}$  are given by the first order differentials as indicated below (notice the Athena Visual Studio nomenclature):

$$\begin{bmatrix} U(1,1) & U(1,2) & U(1,3) \\ U(2,1) & U(2,2) & U(2,3) \\ U(3,1) & U(3,2) & U(3,3) \\ U(4,1) & U(4,2) & U(4,3) \end{bmatrix} = \begin{bmatrix} C_A & \frac{\partial C_A}{\partial k_1} & \frac{\partial C_A}{\partial k_2} \\ C_B & \frac{\partial C_B}{\partial k_1} & \frac{\partial C_B}{\partial k_2} \\ C_C & \frac{\partial C_C}{\partial k_1} & \frac{\partial C_C}{\partial k_2} \\ C_D & \frac{\partial C_D}{\partial k_1} & \frac{\partial C_D}{\partial k_2} \end{bmatrix}$$

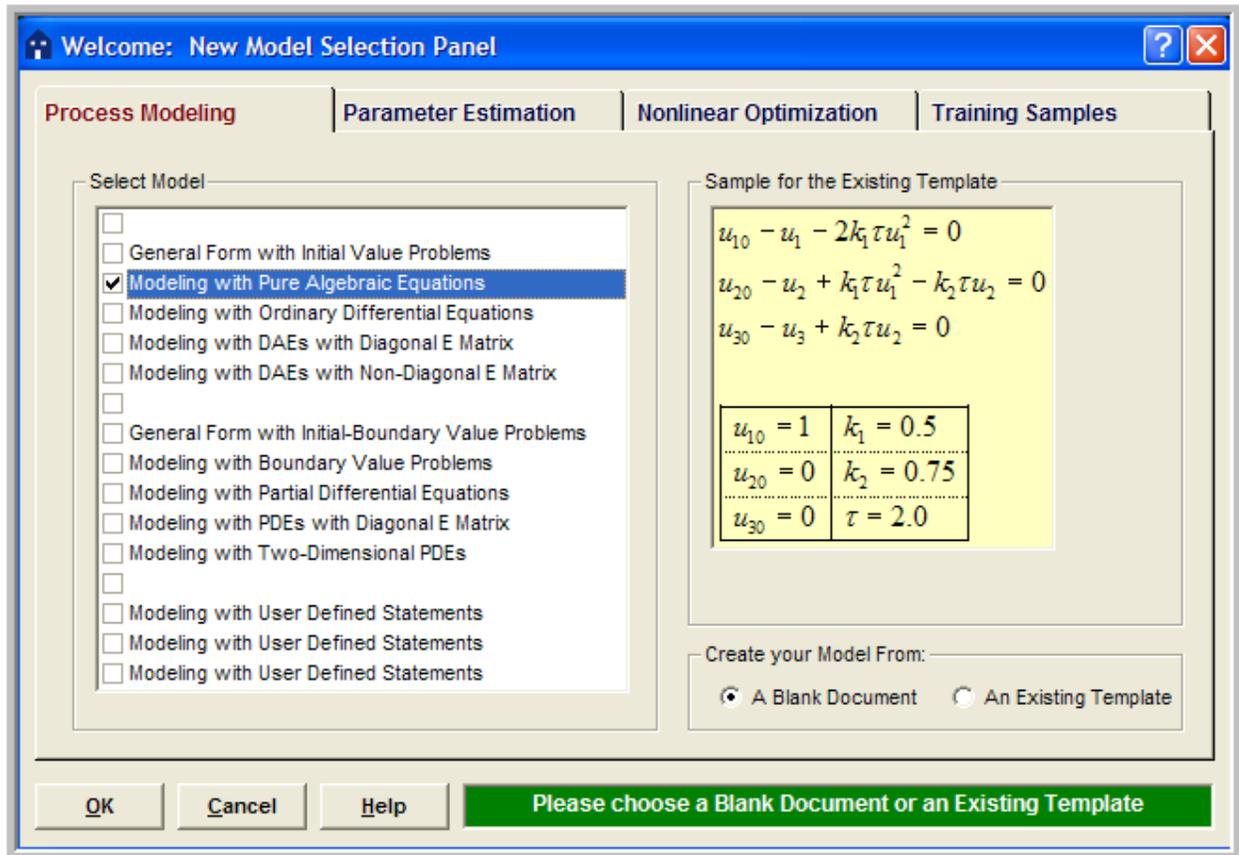
This example tutorial is already precoded in Athena Visual Studio. If you do not wish to type the code on your own you may access it by doing the following:

- ❖ Open **Athena Visual Studio**
- ❖ From the **File** menu click **New**
- ❖ Select the **Training Samples** tab
- ❖ Select the **Steady-State Isothermal CSTR** sample
- ❖ Click **OK**

## Implementation in Athena Visual Studio

The following step by step process describes the model implementation in Athena Visual Studio

- ❖ Open **Athena Visual Studio**.
- ❖ From the **File** menu, choose **New**.
- ❖ The *Welcome: New Model Selection Panel* window appears.



- ❖ You are in the *Process Modeling* tab
- ❖ Select the *Modeling with Pure Algebraic Equations* option.
- ❖ Choose *A Blank Document* and click **OK**.

Type your source code in the new window. The source code contains data and modeling sections (see detailed description below); it may also contain calls to the available Athena Visual Studio math and engineering procedures as well as user-defined subroutines and/or functions.

## Writing the Source Code

The user must enter a minimum of two sections in order to create the algebraic model. The first section labeled **@Initial Conditions** is used to insert initial guesses for the unknown vector. These initial guesses are used by the Newton method to start the iterative algorithm. The second section labeled **@Model Equations** is used to enter the model equations. A data section not labeled by Athena Visual Studio is used to enter all the data pertinent to the model. The data section also contains the declaration statements for all model variables, parameters and constants. This section, if used, must be the first one. The declaration of the model variables, parameters and constants must be done in accordance the Athena Visual Studio syntax rules detailed below:

### Data Section

In the data section the user simply enters the problem data and various constants. In this example the user enters values for residence time, reactor temperature, initial feed concentration and miscellaneous other reaction parameters. The Athena interpreter treats any line that begins with the exclamation mark ! as a comment. It is mandatory and strongly recommended that the users declare all the problem variables, parameters and constants. All variables in Athena are either real double or single precision or integer long. Character and Logical variables are also allowed. The following source code may be entered for this example (If you use the Windows Copy and Paste commands to enter this code into your Athena Visual Studio project, please beware that invisible format symbols may also be copied and cause the compilation of your code to fail):

```
! Declarations and Model Constants
!=====
Global k1,k2,k3,Keq1,Ka,Kb As Real
Global Temp,Rg,Tau As Real
Global CAo,CBo,CCo,CDo As Real
Global CA,CB,CC,CD As Real

Rg=8.314      ! Universal Gas Constant (J/mole K)
Tau=90.0     ! Residence Time (s)
Temp=330.0   ! Temperature (K)

CAo=0.35     ! Initial Concentration of A (mol/m3)
CBo=0.0      ! Initial Concentration of B (mol/m3)
CCo=0.0      ! Initial Concentration of C (mol/m3)
CDo=0.0      ! Initial Concentration of D (mol/m3)

k1=0.01      ! Reaction rate coefficient (mol/m3 s)
k2=0.01      ! Reaction rate coefficient (mol/m3 s)
k3=0.001     ! Reaction rate coefficient (mol/m3 s)

Ka=exp(35000.0/Rg/Temp-91.0/Rg)      ! Adsorption constant (m3/mol)
Kb=exp(20000.0/Rg/Temp-53.0/Rg)      ! Adsorption constant (m3/mol)
Keq1=4.29E-4*Ka/Kb*exp(30000.0/Rg/Temp) ! Equilibrium constant
```

## Declaration of Variables

**Global Variables:** To declare global variables in the Athena Visual Studio environment you must use the **Global** keyword as the examples below illustrate:

```
Global x, y, z, krate As Real  
Global Skount, Ncc As Integer  
Global myName As Character  
Global myDecision As Logical
```

In the above statements the variables *x, y, z, krate* will be treated as double precision and will be accessible by all modeling sections. Similarly the variables *Skount, Ncc* will be treated as integer and be accessible by all modeling sections. Character variables are assigned as Character\*132 from the Athena Visual Studio parser. Single precision variables cannot be declared **Global**.

Vectors and matrices can be declared in a similar manner. The array size, type and number of dimensions are declared with the **Global** statement. The elements of the array can be referenced by an integer index number, which runs from one (or zero) to the maximum number declared in the **Global** statement:

```
Global y(10), c(0:5), a(4,50), b(2,4,6) As Real  
Global istate(5) As Integer
```

**Local Variables:** To declare local variables in the Athena Visual Studio environment you must use the **Dim** keyword as the examples below illustrate:

```
Dim Temp, Pres As Real  
Dim TotalFlow As Single  
Dim i As Integer
```

In the above statements the variables *Temp, Pres* will be treated as double precision, where as the variable *TotalFlow* will be treated as single precision; these variables will be accessible only at the section where they have been declared. Similarly the variable *i* will be treated as integer and will be accessible only by the corresponding modeling section where it has been declared.

Vectors and matrices can be declared in a similar manner. The array size, type and number of dimensions are declared with the **Dim** statement. The elements of the array are referenced by an integer index, which runs from one(or zero) to the number declared in the **Dim** statement:

```
Dim c(10), p(4,50) As Real  
Dim streamEnthalpy(10) As Single  
Dim irow(5) As Integer
```

**Parameter Statement:** Use the **Parameter** keyword to define named constants as the examples below illustrate:

```
Parameter y=2.0, z=4.0 As Real  
Parameter Skount=1, Ncc=4 As Integer
```

In the above statements the variables  $y$ ,  $z$  will be treated as double precision and their numerical values will be accessible by all parts of the modeling code. Similarly the variables  $Skount, Ncc$  will be treated as integer and their numerical values will be accessible through out all the modeling sections. The **Parameter** keyword is only allowed in the data section of the Athena Visual Studio modeling code. If it is used in the other modeling sections it will be ignored. You may view the generated Fortran code to see how the parser interprets the **Parameter** keyword.

**Important Note:** Always remember to declare all of your variables. Athena treats **Real** variables as double precision, **Integer** variables as 4-byte integers, **Character** variables as `Character*132` and **Logical** variables as `.True.` or `.False.` Single precision variables are only allowed if are declared as local with the **Dim** keyword.

**Fortran 95 Declaration Statements:** You can insert Fortran 95 declaration statements by prefixing them with the double dollar sign. Below please see a list of Fortran 95 declaration statements that you can insert in your Athena code. Consult your Fortran 95 manual for the syntax rules of variable and constant declarations:

```
$$Integer, Parameter:: dp=Kind(1.0D0)  
$$Integer, Parameter:: sp=Kind(1.0)  
$$Real(Kind=dp):: v1,v2  
$$Real(Kind=sp), Dimension(3):: a1,a2  
$$Integer:: I1, I2  
$$Character(Len=3):: s2,s3  
$$Character(Len=10), Dimension(2):: s1  
$$Logical:: Done  
$$Real(Kind=dp), Dimension(:), Allocatable:: w
```

We are now going to describe in detail the various steps involved in writing the algebraic model for this example in the Athena Visual Studio environment. The modeling code is NOT case sensitive.

## Initial Conditions

In the Initial Conditions section the user must enter the initial guess for the unknown state vector. The initial guess is required by the Newton algorithm in **DDAPLUS** to start the iterations. The user must do the selection of the unknown state variables and make sure that he/she has a well-defined system where the number of equations is equal to the number of unknowns. The unknown state vector is represented by the variable  $\mathbf{U}()$  in Athena. For our example we choose  $\mathbf{U}(1)$  to represent the molar concentration of component  $A$ ,  $\mathbf{U}(2)$  to represent the molar concentration of component  $B$  and so forth. To enter the heading for the Initial Conditions section for our example:

- ❖ From the *Model* menu choose *Initial Conditions* (or **Hit F11**)
- ❖ Enter the source code as shown below for our example.

```
@Initial Conditions
U(1)=CAo  ! [Ca]
U(2)=CBo  ! [Cb]
U(3)=CCo  ! [Cc]
U(4)=CDo  ! [Cd]
```

Notice that we chose as the initial guess the reactor feed composition. If the reactions are very fast this might be a bad initial guess; that can cause the Newton method to fail. In that case you may try to come up with a better initial guess or use one of the continuation methods that are available in Athena Visual Studio. (see sections later in this tutorial)

## Model Equations

In the Model Equations section the user must enter the functions that describe the physical process. For example these functions may be simply the component balances. The value of these functions will eventually be driven to zero by the Newton algorithm. At the initial guess these functions will have values, which are indicative of how good our guess is. The closer to zero we are, the better our initial guess is. The vector  $\mathbf{F}(\ )$  is reserved in the Athena environment to represent the values of these functions (often know as residuals). For example  $\mathbf{F}(1)$  may be used to represent the component *A* material balance,  $\mathbf{F}(2)$  may be used to represent the component *B* material balance and so forth. In this section the user may make use of temporary variables to calculate intermediate variables such as, for example, the reaction rates. This facilitates the model writing process and it is also a sign of good programming skills. To enter the Model Equations section for our example

- ❖ From the *Model* menu choose *Model Equations* (or **Hit F11**)
- ❖ Enter the source code as shown below for our example.

```
@Model Equations
```

```
Dim R1, R2, R3, R4, Denom As Real
```

```
CA = U(1)
```

```
CB = U(2)
```

```
CC = U(3)
```

```
CD = U(4)
```

```
Denom = 1.0 + Ka * CA + Kb * CB
```

```
R1 = k1 * Ka * (CA - CB / Keq1) / Denom
```

```
R2 = k2 * Kb * CB / Denom
```

```
R3 = k3 * Ka * CA / Denom
```

```
F(1) = CAo - CA + (-R1 - R3) * Tau
```

```
F(2) = CBo - CB + (R1 - R2) * Tau
```

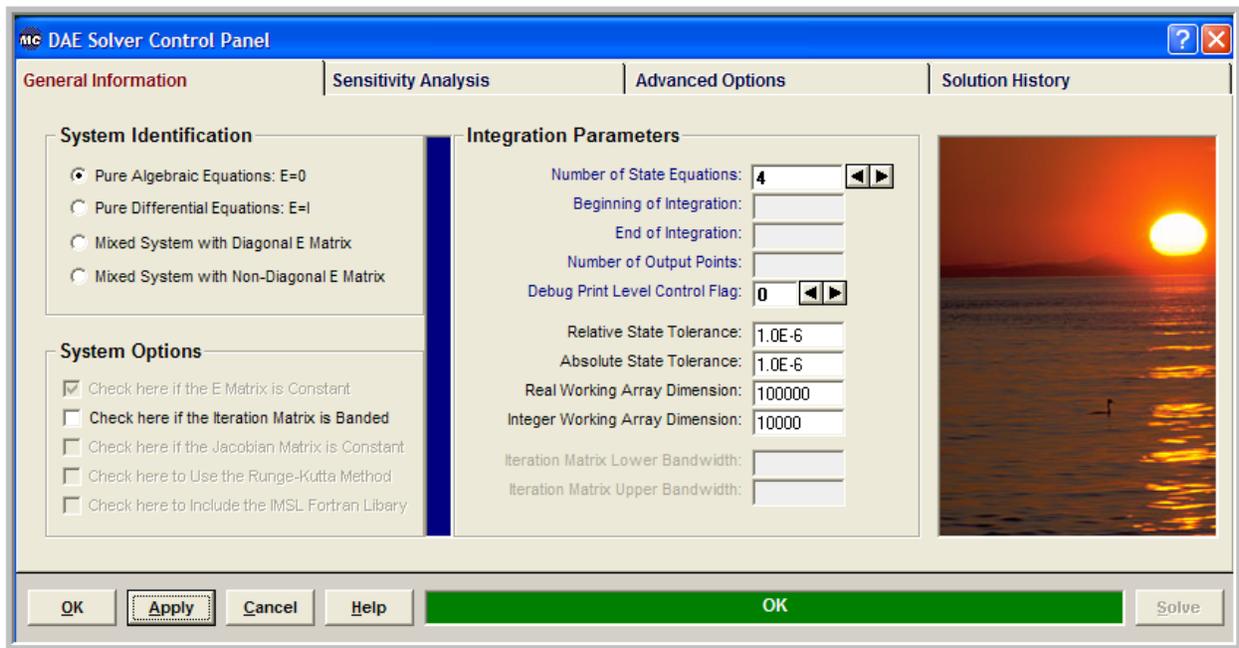
```
F(3) = CCo - CC + R2 * Tau
```

```
F(4) = CDo - CD + R3 * Tau
```

## The DDAPLUS Solver

It is now time to access the Athena Visual Studio solver for Differential/Algebraic Equations in order to enter information about the system of equations we wish to solve and various other parameters that control the Newton algorithm. To do that:

- ❖ From the *Model* menu choose *Load Solver* (or **Hit F12**)
- ❖ The *DAE Solver Control Panel* window appears
- ❖ Enter the solver parameters as shown below for our example



In the **System Identification** group you will see that the option *Pure Algebraic Equations E=0* has already been selected for you. From the **Integration Parameters** group enter the *Number of State Equations* and optionally change *Debug Print Level Control Flag*, and the *Relative* and *Absolute State Tolerance* fields. The *Real* and *Integer Working Array Dimension* fields are indicative of the size of the problem. If the default values are not large enough the solver will return with the message indicating the space requirements for your problem. You may also need to examine if your model has a banded structure in which case you will have to check the appropriate options in the **System Options** group. Then choose **OK** or click **Apply**.

## Saving and Running

You are now ready to save your model and run it. New files are labeled **UNTITLED** until they are saved. Keep in mind that the maximum number of characters in a line is 132; the maximum number of lines in a file is infinity. In order to save your project:

- ❖ From the **File** menu, choose **Save**. The *Save As* dialog box appears. This action saves your model and creates the Fortran code.
- ❖ In the Directories box, double-click a directory where you want to store the source file.
- ❖ Type a filename (a filename cannot contain the following characters: \ / : \* ? “ < > |) in the File Name box, then choose **OK**. The default extension is **avw**
- ❖ To view the Fortran code that you have just created from the **View** menu choose **Fortran Code**.

You may now choose to compile, build and execute your project; to do that:

- ❖ From the **Build** menu choose **Compile** (or **Hit F2**)
- ❖ From the **Build** menu choose **Build EXE** (or **Hit F4**)
- ❖ From the **Build** menu choose **Execute** (or **Hit F5**)

## Numerical Results

If everything goes well the results window will appear. In this window you can see the solution of your problem as well as various statistics pertaining to the solution process:

```
Number of Algebraic Equations..... 4
Number of Sensitivity Parameters..... 0
Number of User Specified Iterations..... 30
```

```
EXIT DDAPLUS: SOLUTION FOUND
```

VARIABLE	INITIAL GUESS	RESIDUALS	FINAL VALUE
U(1)	3.50000E-01	3.02720E-15	8.00051E-02
U(2)	0.00000E+00	-5.91150E-15	1.07519E-01
U(3)	0.00000E+00	3.10212E-15	1.37412E-01
U(4)	0.00000E+00	-2.59450E-16	2.50643E-02

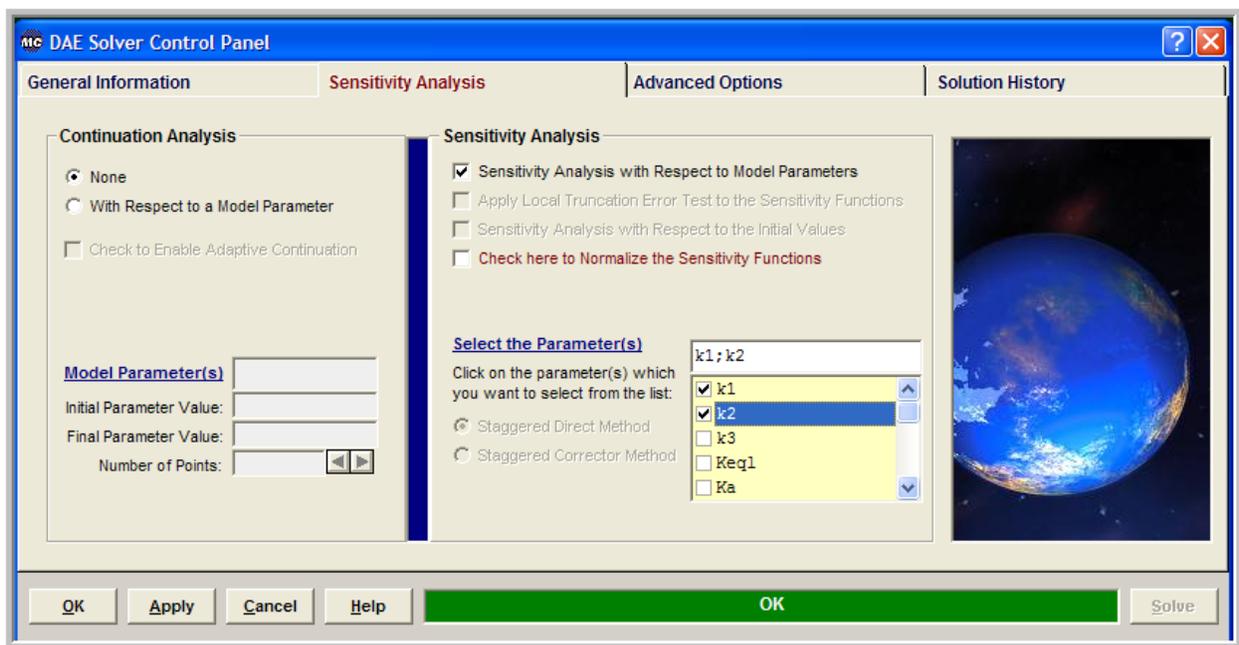
```
Number of Newton Iterations..... 5
Number of Function Evaluations..... 26
Number of Jacobian Evaluations..... 5
Number of Jacobian Factorizations..... 5
```

## Sensitivity Analysis

Athena Visual Studio allows for convenient and efficient calculation of the first order sensitivity functions given by:

$$\mathbf{W}(\boldsymbol{\theta}) = \frac{\partial \mathbf{u}}{\partial \boldsymbol{\theta}}$$

Suppose that we wish to investigate the sensitivity of the reactor effluent composition to small perturbations in the reaction rate constants  $k_1$  and  $k_2$ . In order to do that, first we must load the solver (**Hit F12**), and click the *Sensitivity Analysis* tab.



In the **Sensitivity Analysis** group click *Sensitivity Analysis with respect to Model Parameters* and subsequently select the parameters  $k_1, k_2$  from the drop down list; optionally you may wish to click on the *Check here to Normalize the Sensitivity Functions* in which case the following first order coefficients will be calculated:

$$\mathbf{W}(\boldsymbol{\theta}) = \frac{\partial \mathbf{u}}{\partial \ln \boldsymbol{\theta}}$$

Now choose **OK** or click **Apply**. From the *Build* menu select *Execute* (or **Hit F5**). You should see the following results:

```
Number of Algebraic Equations..... 4
Number of Sensitivity Parameters..... 2
Number of User Specified Iterations..... 30
```

**EXIT DDAPLUS: SOLUTION FOUND**

VARIABLE	INITIAL GUESS	RESIDUALS	FINAL VALUE	SENSITIVITY MATRIX	
U(1)	3.50000E-01	3.02720E-15	8.00051E-02	-6.68166E+00	-7.99267E-01
U(2)	0.00000E+00	-5.91150E-15	1.07519E-01	2.44028E+00	-6.41993E+00
U(3)	0.00000E+00	3.10212E-15	1.37412E-01	5.83854E+00	7.17137E+00
U(4)	0.00000E+00	-2.59450E-16	2.50643E-02	-1.59715E+00	4.78335E-02

```
Number of Newton Iterations..... 5
Number of Function Evaluations..... 28
Number of Jacobian Evaluations..... 5
Number of Jacobian Factorizations..... 5
```

An interpretation of these results is given in the following table using the nomenclature in our example:

$C_A = 0.080005$	$\frac{\partial C_A}{\partial k_1} = -6.68166$	$\frac{\partial C_A}{\partial k_2} = -0.799267$
$C_B = 0.107519$	$\frac{\partial C_B}{\partial k_1} = 2.44028$	$\frac{\partial C_B}{\partial k_2} = -6.41993$
$C_C = 0.137412$	$\frac{\partial C_C}{\partial k_1} = 5.83854$	$\frac{\partial C_C}{\partial k_2} = 7.17137$
$C_D = 0.025064$	$\frac{\partial C_D}{\partial k_1} = -1.59715$	$\frac{\partial C_D}{\partial k_2} = 0.047833$

## Implicit Auxiliary Variables

Athena Visual Studio allows for convenient and efficient calculation of derived quantities by the introduction of auxiliary variables. Assume for example that we wish to estimate the conversion of the component *A* in the continuous stirred tank reactor. We introduce an auxiliary variable  $U(5) = X_A$  that represents the conversion and the associated equation that is obviously the definition of the conversion, i.e.

$$F(5) = U(5) - \frac{C_{A0} - C_A}{C_{A0}} \times 100$$

We can implement this in Athena in a very straightforward manner. First we load the DDAPLUS solver (**Hit F12**) and increase the *Number of State Equations* to 5. Then we write the source code that corresponds to the introduction of the new variable and its associated equation. The new source code might look like the code displayed below:

```

! Declarations and Model Constants
!=====
Global k1,k2,k3,Keq1,Ka,Kb As Real
Global Temp,Rg,Tau As Real
Global CAo,CBo,CCo,CDo As Real
Global CA,CB,CC,CD As Real

Rg=8.314      ! Universal Gas Constant (J/mole K)
Tau=90.0      ! Residence Time (s)
Temp=330.0    ! Temperature (K)

CAo=0.35      ! Initial Concentration of A (mol/m3)
CBo=0.0       ! Initial Concentration of B (mol/m3)
CCo=0.0       ! Initial Concentration of C (mol/m3)
CDo=0.0       ! Initial Concentration of D (mol/m3)

k1=0.01       ! Reaction rate coefficient (mol/m3 s)
k2=0.01       ! Reaction rate coefficient (mol/m3 s)
k3=0.001      ! Reaction rate coefficient (mol/m3 s)

Ka=exp(35000.0/Rg/Temp-91.0/Rg)      ! Adsorption constant (m3/mol)
Kb=exp(20000.0/Rg/Temp-53.0/Rg)      ! Adsorption constant (m3/mol)
Keq1=4.29E-4*Ka/Kb*exp(30000.0/Rg/Temp) ! Equilibrium constant

@Initial Conditions
U(1)=CAo  ! [Ca]
U(2)=CBo  ! [Cb]
U(3)=CCo  ! [Cc]
U(4)=CDo  ! [Cd]
U(5)=0.0  ! Conversion

@Model Equations
Dim R1, R2, R3, R4, Denom As Real

CA = U(1)
CB = U(2)
CC = U(3)
CD = U(4)

Denom = 1.0 + Ka * CA + Kb * CB
R1 = k1 * Ka * (CA - CB / Keq1) / Denom
R2 = k2 * Kb * CB / Denom
R3 = k3 * Ka * CA / Denom

F(1) = CAo - CA + (-R1 - R3) * Tau
F(2) = CBo - CB + (R1 - R2) * Tau
F(3) = CCo - CC + R2 * Tau
F(4) = CDo - CD + R3 * Tau
F(5) = U(5) - (CAo - CA)/CAo * 100.0

```

Now from the *Build* menu select *Execute* (or **Hit F5**). You should see the following:

```
Number of Algebraic Equations..... 5
Number of Sensitivity Parameters..... 0
Number of User Specified Iterations..... 30
```

**EXIT DDAPLUS: SOLUTION FOUND**

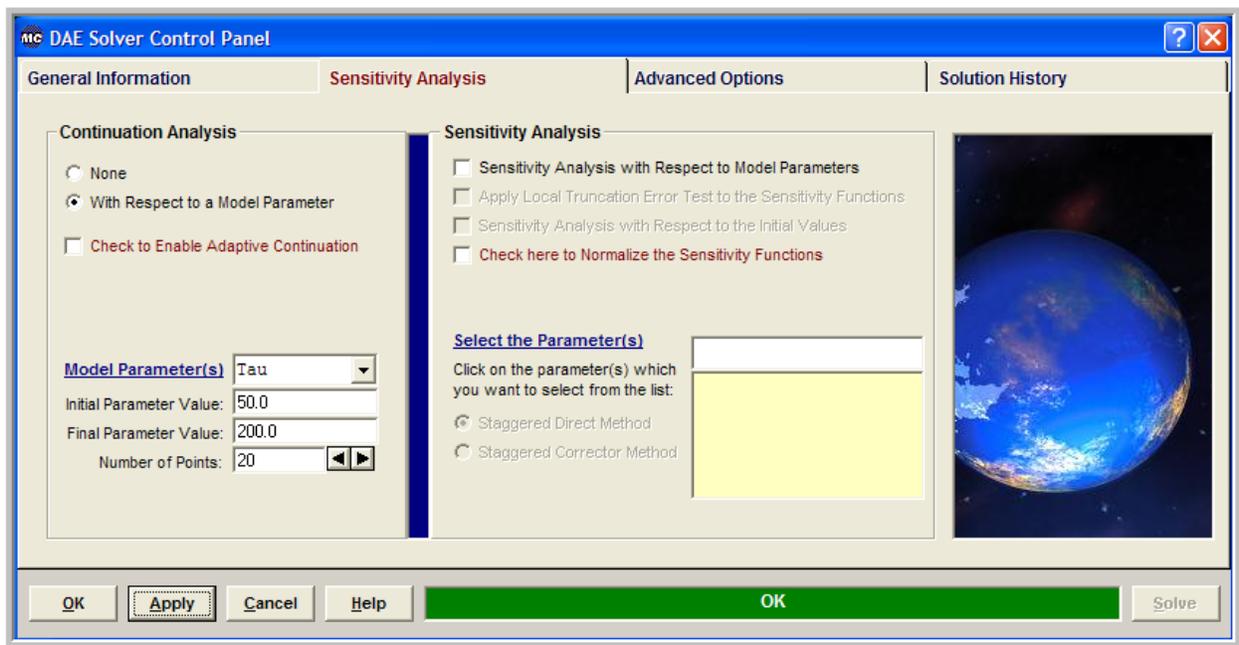
VARIABLE	INITIAL GUESS	RESIDUALS	FINAL VALUE
U(1)	3.50000E-01	3.02720E-15	8.00051E-02
U(2)	0.00000E+00	-5.91150E-15	1.07519E-01
U(3)	0.00000E+00	3.10212E-15	1.37412E-01
U(4)	0.00000E+00	-2.59450E-16	2.50643E-02
U(5)	0.00000E+00	-8.27047E-14	7.71414E+01

```
Number of Newton Iterations..... 5
Number of Function Evaluations..... 31
Number of Jacobian Evaluations..... 5
Number of Jacobian Factorizations..... 5
```

From these results we observe that the conversion is  $X_A = 77.14\%$

## Continuation Analysis

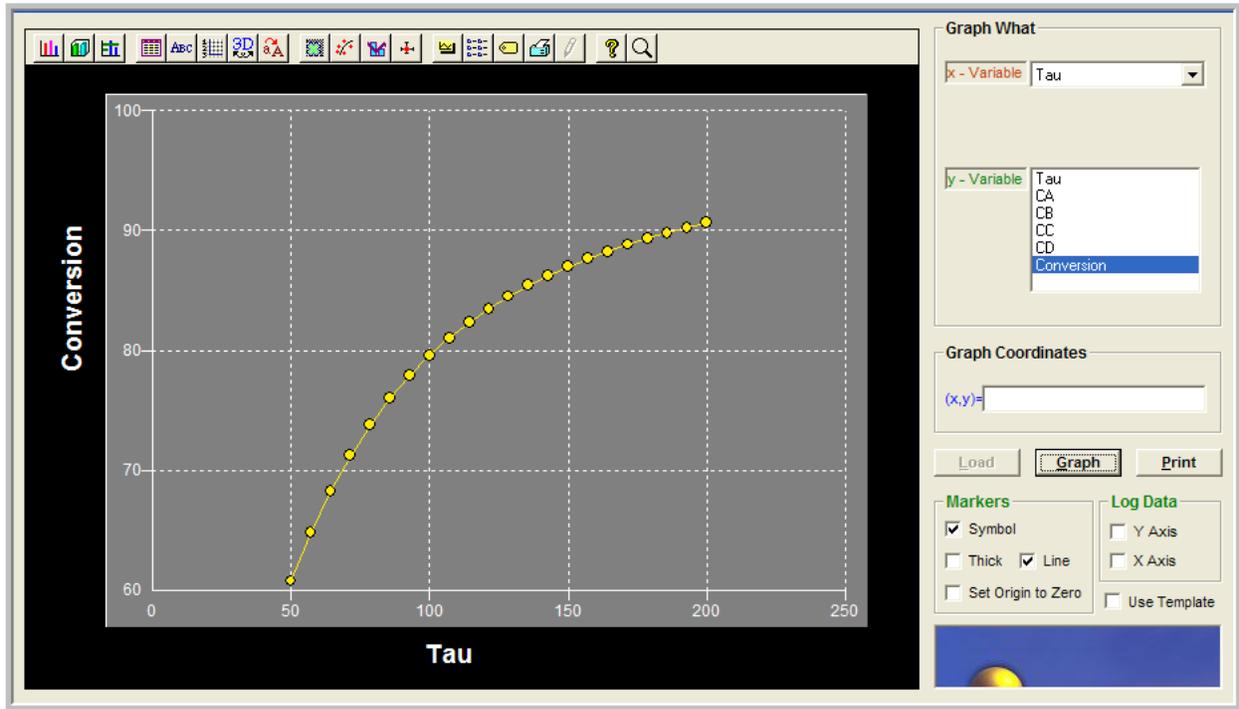
Now we can use Athena to conduct a continuation study. Our goal is to investigate the variation of conversion with respect to the reactor residence time. To do that we load the solver (**Hit F12**),



and click on the *Sensitivity Analysis* tab. In the **Continuation Analysis** group we click the option with caption *With respect to a Model Parameter* and select the parameter **Tau** from the drop

down list. We then input the *Initial Parameter Value* and the *Final Parameter Value* as well as the *Number of Points* and click **OK**.

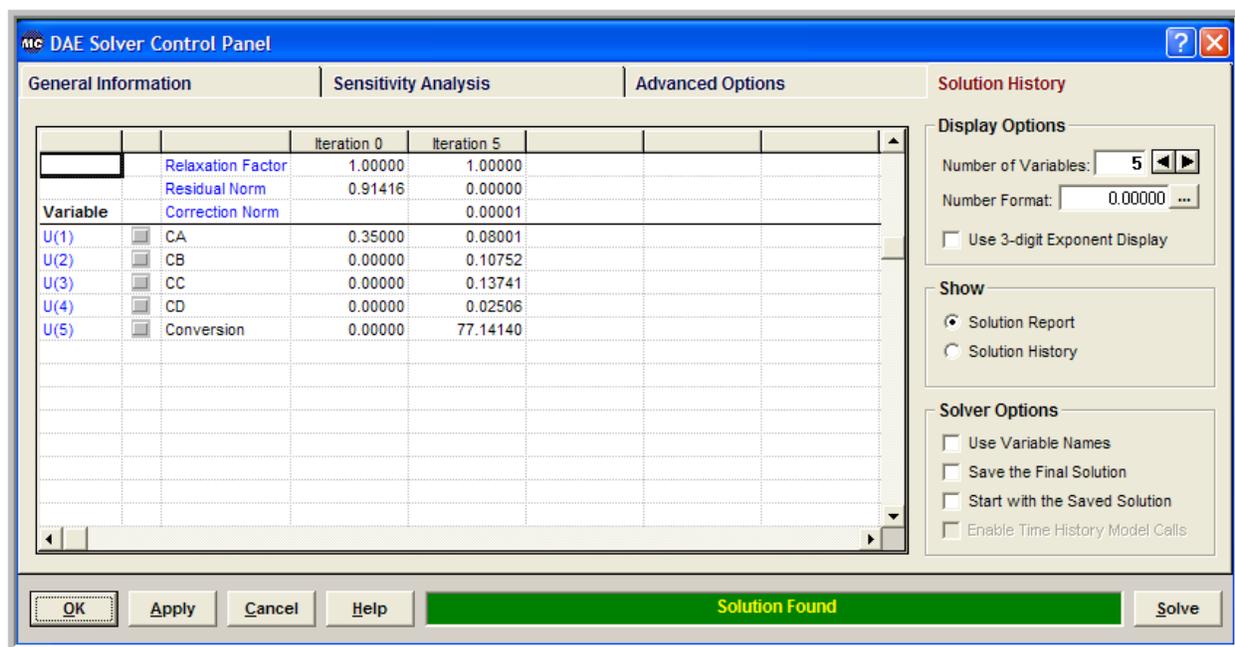
Now from the **Build** menu select **Execute** (or **Hit F5**). Instead of looking at the file with the large number of numerical results from the **View** menu we select **Solution Graphs** and the following panel is displayed:



In this window first we click **Load** to load the numerical results. Then in the **Graph What** group we select the **x-variable** (here **Tau**) and the **y-variable** (here **Conversion**) and click **Graph**. You should see the graph that appears above. You may now click on the graph toolbar and modify the type, title, symbol, the style and miscellaneous other properties of the graph

## State Variable Names

You might have noticed from the Graphics Control Panel shown above, the names of the independent variables being, CA, CB, CC, CD and Conversion. In order to enter these names as well as modify them, you must load the solver (**Hit F12**). Now, first disable the continuation analysis option (you can always enable it again) by selecting the *Sensitivity Analysis* tab, and then in the **Continuation Analysis** group by clicking the option with caption *None*. After you do that, select the *Solution History* tab:



In the **Display Options** group enter the *Number of Variables* using the spin control and then, in the adjacent spreadsheet change the names of the state variables. Also from the **Show** group select *Solution Report*. Then click *Apply* and then *Solve*. You should see the results as shown in the image above. Notice also, other types of solution information appearing in the spreadsheet. If you wish to enter analytical derivatives with respect to one of the independent variables you must click the corresponding cell in the **CheckBox** column. This can be helpful especially for the auxiliary variables, such as the conversion in our example, since the derivatives of all functions with respect to conversion are exactly equal to zero, except the last equation, in which of course the derivative with respect to conversion is equal to one. Should you decide to do that for the auxiliary variable, you just enter the following segment of code in your project:

#### @Model Equations

```
Dim R1, R2, R3, R4, Denom As Real
```

```
CA = U(1)
```

```
CB = U(2)
```

```
CC = U(3)
```

```
CD = U(4)
```

```
Denom = 1.0 + Ka * CA + Kb * CB
```

```
R1 = k1 * Ka * (CA - CB / Keq1) / Denom
```

```
R2 = k2 * Kb * CB / Denom
```

```
R3 = k3 * Ka * CA / Denom
```

```
F(1) = CAo - CA + (-R1 - R3) * Tau
```

```
F(2) = CBo - CB + (R1 - R2) * Tau
```

```
F(3) = CCo - CC + R2 * Tau
```

```
F(4) = CDo - CD + R3 * Tau
```

```
F(5) = U(5) - (CAo - CA)/CAo * 100
```

#### @Jacobian Matrix

```
dF(5,5) = 1.0
```