

第七讲化工过程概念设计（2）



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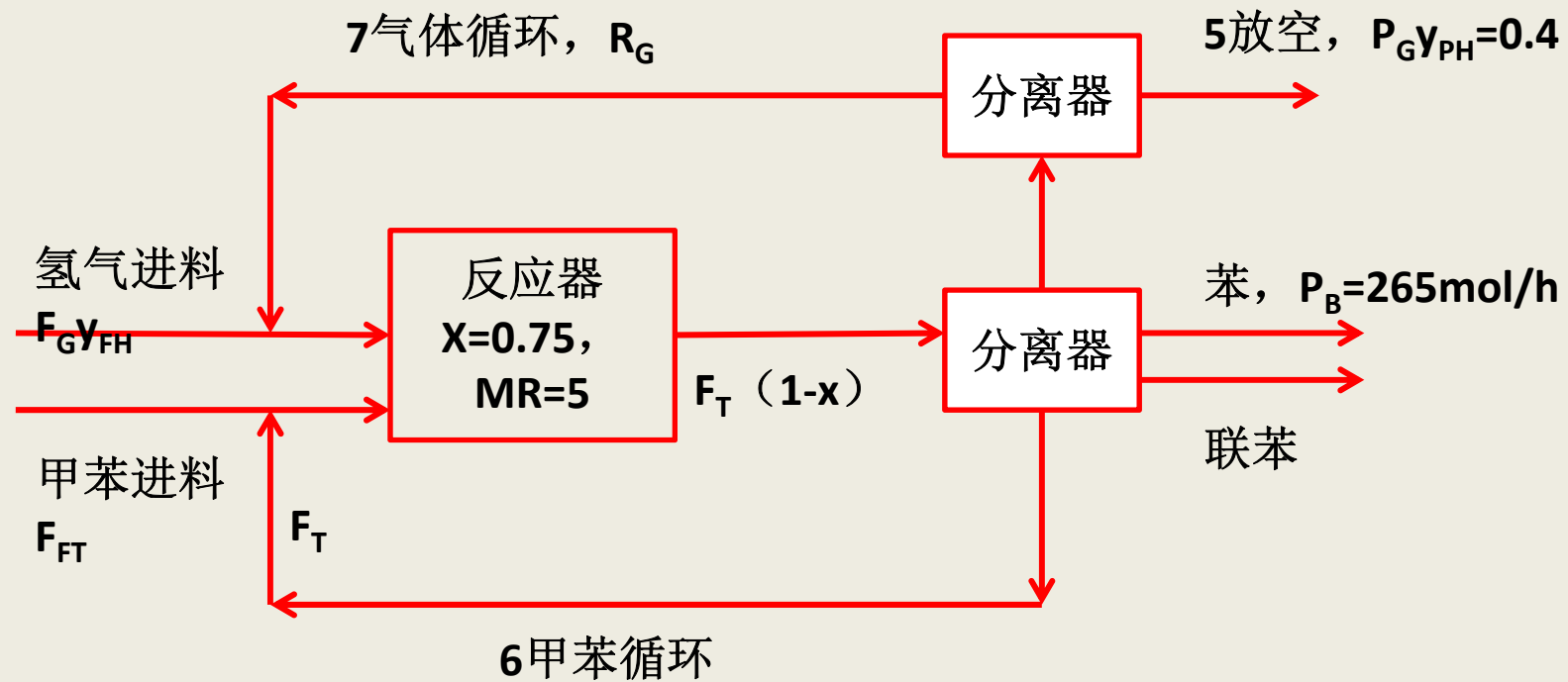
本节主要内容



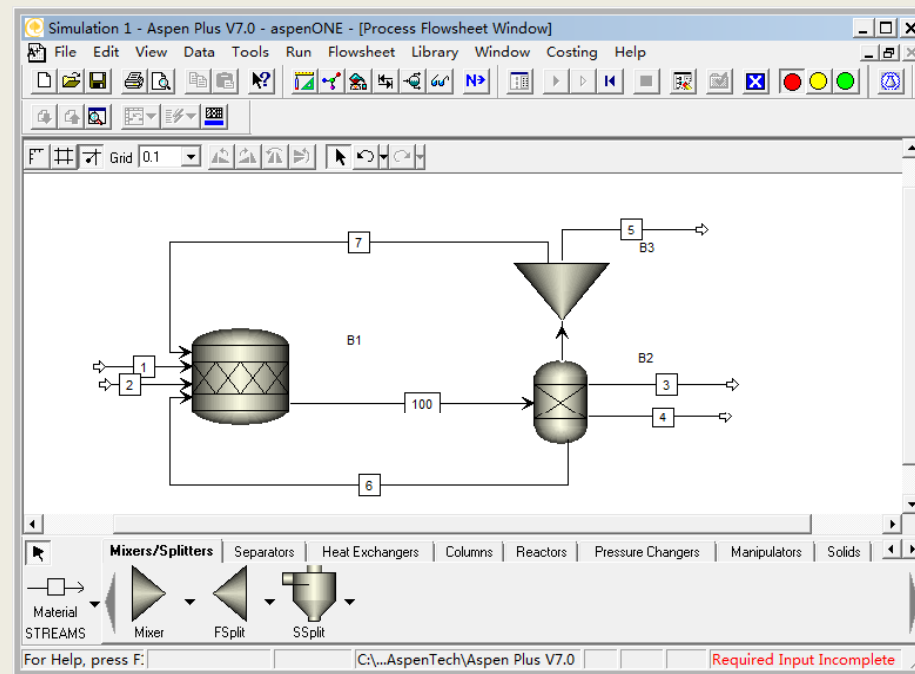
- ❖ 循环的物料衡算
- ❖ 反应器对循环结构的影响
- ❖ 循环的物料衡算优化
- ❖ 模拟实例

循环的物料衡算

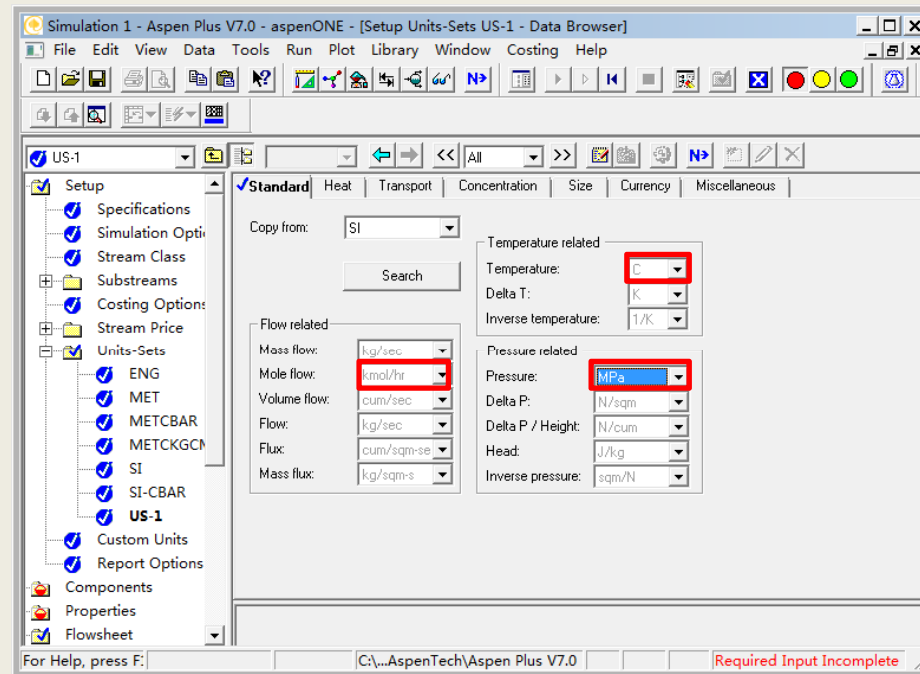
※ 循环结构，反应器进口处氢对甲苯的摩尔比 MR ，则可计算循环物流6、7的流量和组成，如图：



搭建流程图



指定单位制



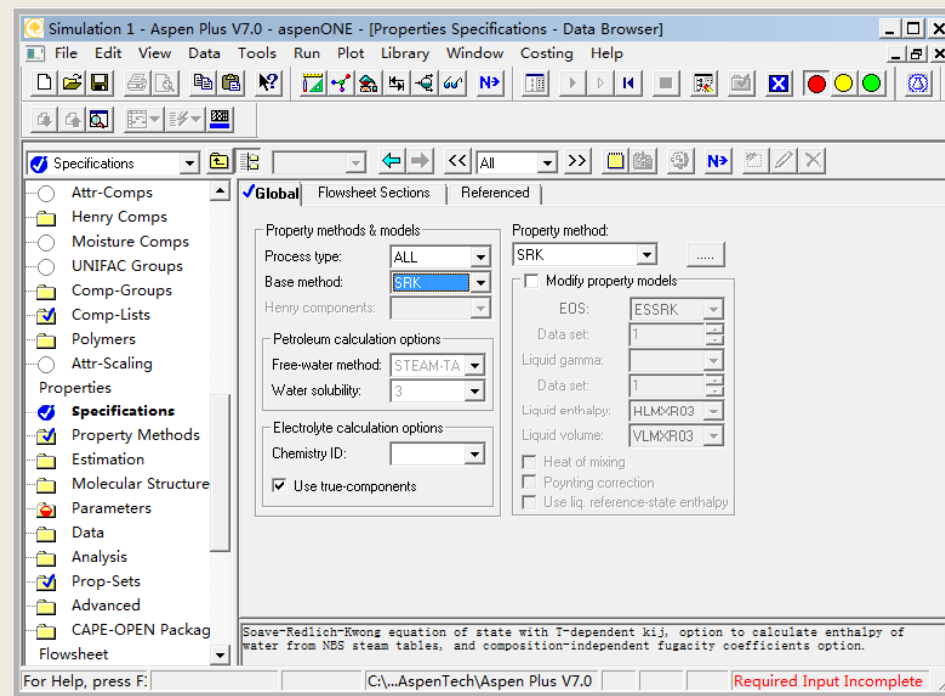
指定组分

The screenshot displays the 'Components Specifications - Data Browser' window in Aspen Plus V7.0. The window title is 'Simulation 1 - Aspen Plus V7.0 - aspenONE - [Components Specifications - Data Browser]'. The interface includes a menu bar (File, Edit, View, Data, Tools, Run, Plot, Library, Window, Costing, Help), a toolbar, and a navigation pane on the left. The 'Specifications' section is expanded, showing a tree view with 'Components' and 'Specifications' selected. The 'Define components' table is visible, listing several components with their IDs, types, names, and formulas. The table has columns for Component ID, Type, Component name, and Formula. The components listed are HYDRO-01 (Conventional, HYDROGEN, H2), METHA-01 (Conventional, METHANE, CH4), BENZE-01 (Conventional, BENZENE, C6H6), TOLUE-01 (Conventional, TOLUENE, C7H8), and DIPHE-01 (Conventional, DIPHENYL, C12H10). There is also an asterisk (*) in the Component ID column. Below the table are buttons for 'Find', 'Elec Wizard', 'User Defined', 'Reorder', and 'Review'. A status bar at the bottom indicates 'Required Input Incomplete'.

Component ID	Type	Component name	Formula
HYDRO-01	Conventional	HYDROGEN	H2
METHA-01	Conventional	METHANE	CH4
BENZE-01	Conventional	BENZENE	C6H6
TOLUE-01	Conventional	TOLUENE	C7H8
DIPHE-01	Conventional	DIPHENYL	C12H10
*			

指定热力学方法

※ 选择SRK热力学方法，如图：



输入进料物流数据

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Stream 1 (MATERIAL) Input - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Input US-1 All

Substream name: MIXED Ref Temperature

State variables: Temperature 38 C Pressure 3.8 MPa Total flow: 250 kmol/hr Mole Solvent

Component	Value
HYDRO-01	0.95
METHA-01	0.05
BENZE-01	
TOLUE-01	
DIPHE-01	

Total: 1

For Help, press F: C:\AspenTech\Aspen Plus V7.0 Required Input Incomplete

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Stream 2 (MATERIAL) Input - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Input US-1 All

Substream name: MIXED Ref Temperature

State variables: Temperature 25 C Pressure 0.1 MPa Total flow: 150 kmol/hr Mole Solvent

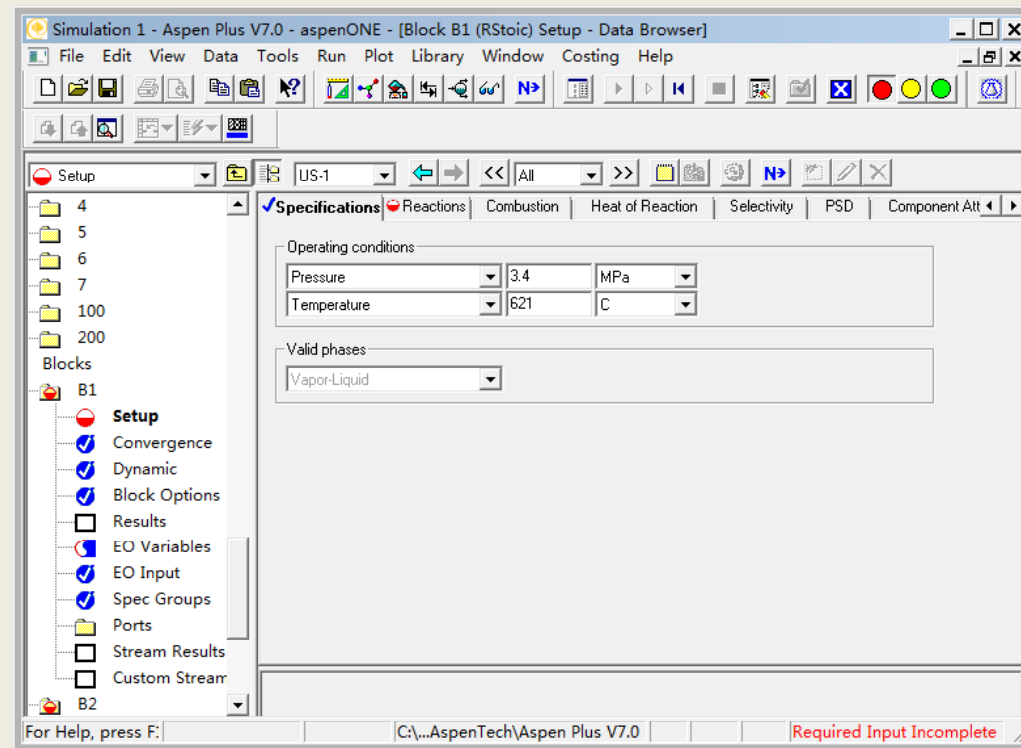
Component	Value
HYDRO-01	
METHA-01	
BENZE-01	
TOLUE-01	1
DIPHE-01	

Total: 1

For Help, press F: C:\AspenTech\Aspen Plus V7.0 Required Input Incomplete

输入反应器参数

✧ 输入反应器操作压力位**3.4Mpa**，温度为**621℃**，如图：



输入主反应方程式

Edit Stoichiometry

Reaction No.: 1

Reactants

Component	Coefficient
TOLUE-01	-1
HYDRO-01	-1
*	

Products

Component	Coefficient
BENZE-01	1
METHA-01	1
*	

Products generation

Molar extent: kmol/hr

Fractional conversion: of component

输入副反应方程式

Edit Stoichiometry

Reaction No.:

Reactants

Component	Coefficient
BENZE-01	-2
*	

Products

Component	Coefficient
DIPHE-01	1
HYDRO-01	1
*	

Products generation

Molar extent: kmol/hr

Fractional conversion: of component

输入的反应式列表

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Block B1 (RStoic) Setup - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Setup US-1

Specifications Reactions Combustion Heat of Reaction Selectivity PSD Component Att

Rxn No.	Specification type	Stoichiometry
1	Frac. conversion	TOLUE-01 + HYDRO-01 -> BENZE-01 + METHA-01
2	Frac. conversion	2 BENZE-01 -> DIPHE-01 + HYDRO-01

New... Edit Delete Copy Paste

Reactions occur in series

Use to specify if the reactions occur simultaneously or in series. The series reactions occur in the sequence of ascending order of the Rxn No. See Help.

For Help, press F: C:\...AspenTech\Aspen Plus V7.0 Required Input Incomplete

输入分离器参数 (1)

※ 物流3对苯的分割值为1，如图：

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Block B2 (Sep) Input - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Input US-1 All

Specifications Feed Flash Outlet Flash Utility

Outlet stream conditions

Outlet stream: 3

Substream: MIXED

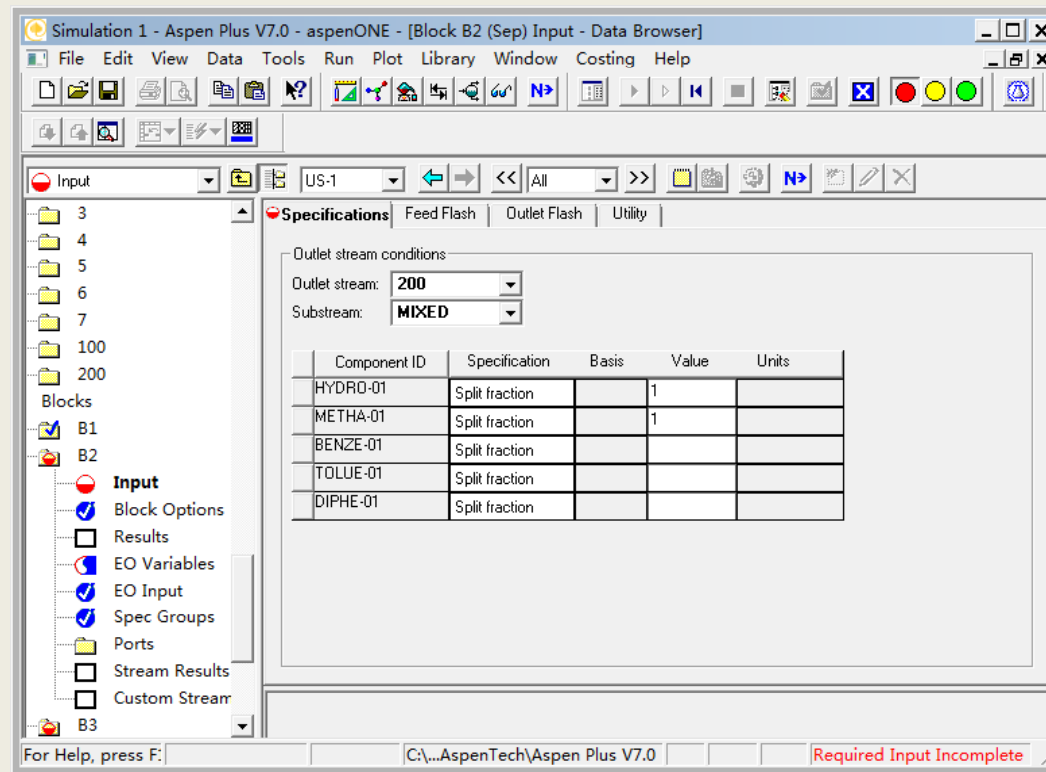
Component ID	Specification	Basis	Value	Units
HYDRO-01	Split fraction			
METHA-01	Split fraction			
BENZE-01	Split fraction		1	
TOLUE-01	Split fraction			
DIPHE-01	Split fraction			

Fraction of component in the inlet stream going to the outlet stream. If left blank, the value is set to 0 except for the last outlet stream.

For Help, press F: C:\...AspenTech\Aspen Plus V7.0 Required Input Incomplete

输入分离器参数 (2)

※ 物流200对氢气和甲烷的分割值均为1，如图：

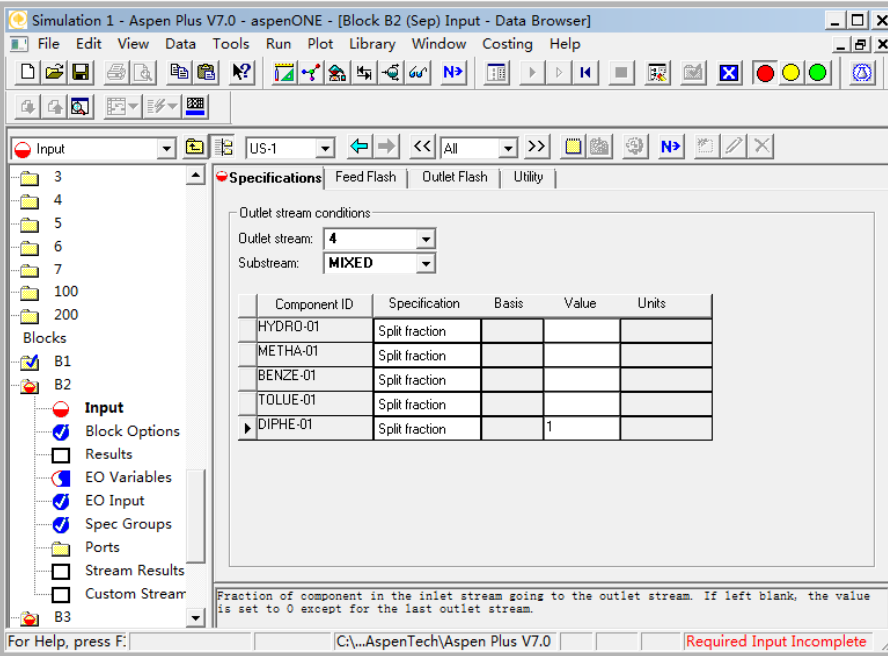


The screenshot displays the Aspen Plus V7.0 Data Browser interface for a simulation. The 'Specifications' tab is selected, showing the configuration for stream 200. The 'Outlet stream conditions' section indicates the outlet stream is 200 and the substream is MIXED. A table below lists the components and their specified split fractions.

Component ID	Specification	Basis	Value	Units
HYDRO-01	Split fraction		1	
METHA-01	Split fraction		1	
BENZE-01	Split fraction			
TOLUE-01	Split fraction			
DIPHE-01	Split fraction			

输入分离器参数 (3)

- ※ 由于分离器B2增加了一个甲苯出料6，所以需要制定物流4来分割联苯，物流4对联苯的分割值为1，如图：



Simulation 1 - Aspen Plus V7.0 - aspenONE - [Block B2 (Sep) Input - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Input US-1 All

Specifications Feed Flash Outlet Flash Utility

Outlet stream conditions:

Outlet stream: 4

Substream: MIXED

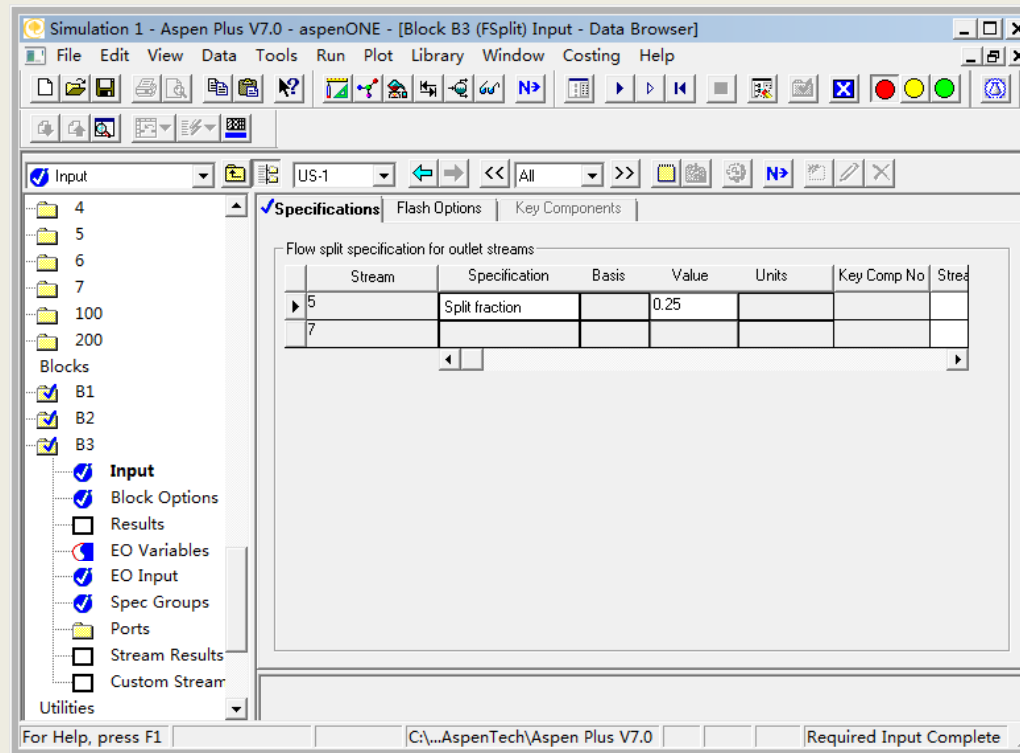
Component ID	Specification	Basis	Value	Units
HYDRO-01	Split fraction			
METHA-01	Split fraction			
BENZE-01	Split fraction			
TOLUE-01	Split fraction			
DIPHE-01	Split fraction		1	

Fraction of component in the inlet stream going to the outlet stream. If left blank, the value is set to 0 except for the last outlet stream.

For Help, press F1: C:\...AspenTech\Aspen Plus V7.0 Required Input Incomplete

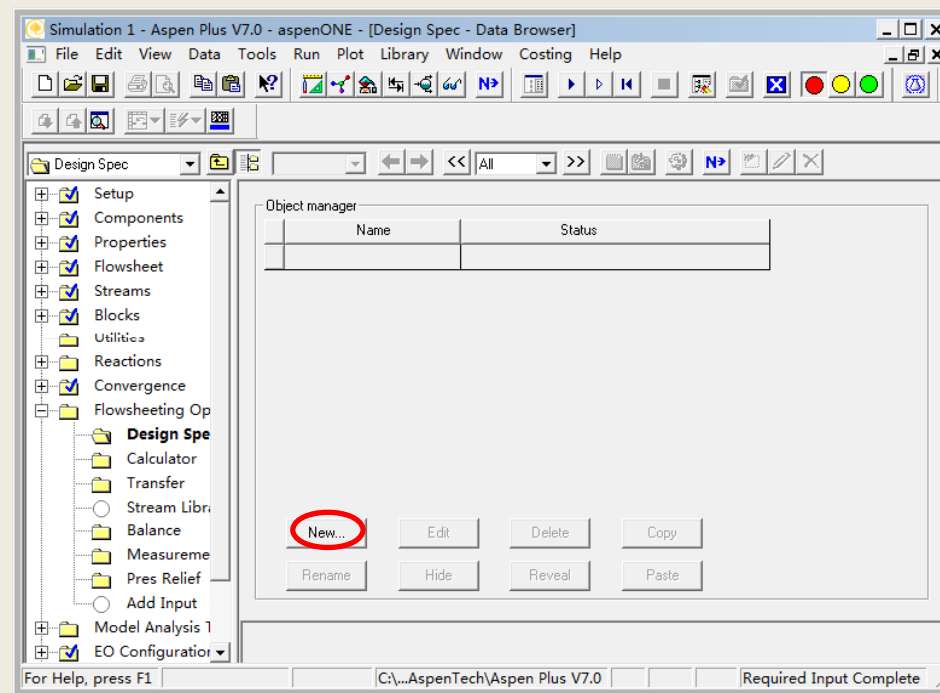
输入放空气与循环气的比例

※ 放空气与循环气的比例为**1:4**，如图：



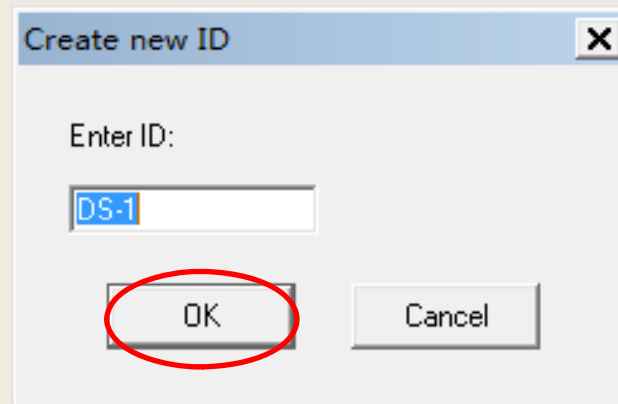
制定设计规定 (1)

✧ 在Data Browser的Flowsheeting Options/Design Spec中点击NEW创建一个新的设计规定：



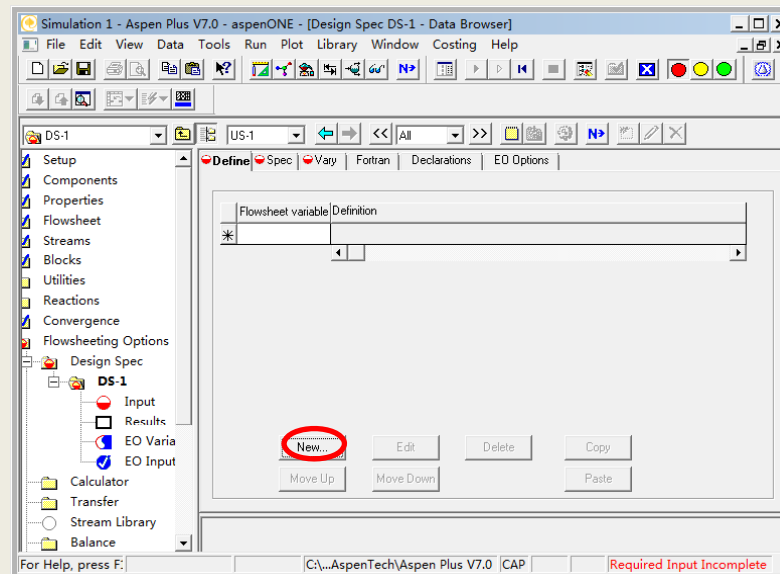
制定设计规定（2）

※ 创建的新的设计规定**DS-1**，如图：



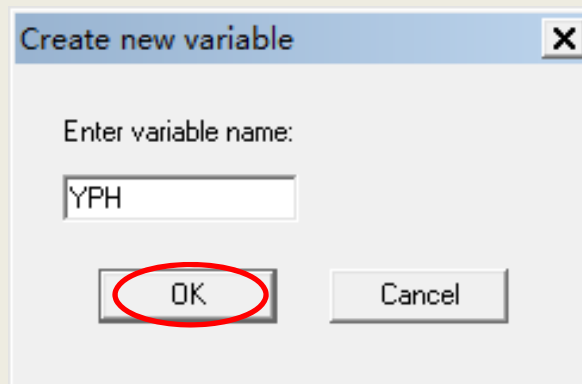
制定设计规定 (3)

※ 点击上图OK，弹出下图窗口，如图：



制定设计规定（4）

※ 点击上图**NEW**，弹出下图对话框，定义名为**YPH**的变量，如图：



制定设计规定 (5)

※ 变量定义完成，如图：

Variable Definition

Select a variable category and reference

Variable name: YPH

Category:

- All
- Blocks
- Streams
- Model Utility
- Physical Property Parameters
- Reactions

Reference

Type: Mole-Frac

Stream: 5

Substream: MIXED

Component: HYDRO-01

EO input

Open variable:

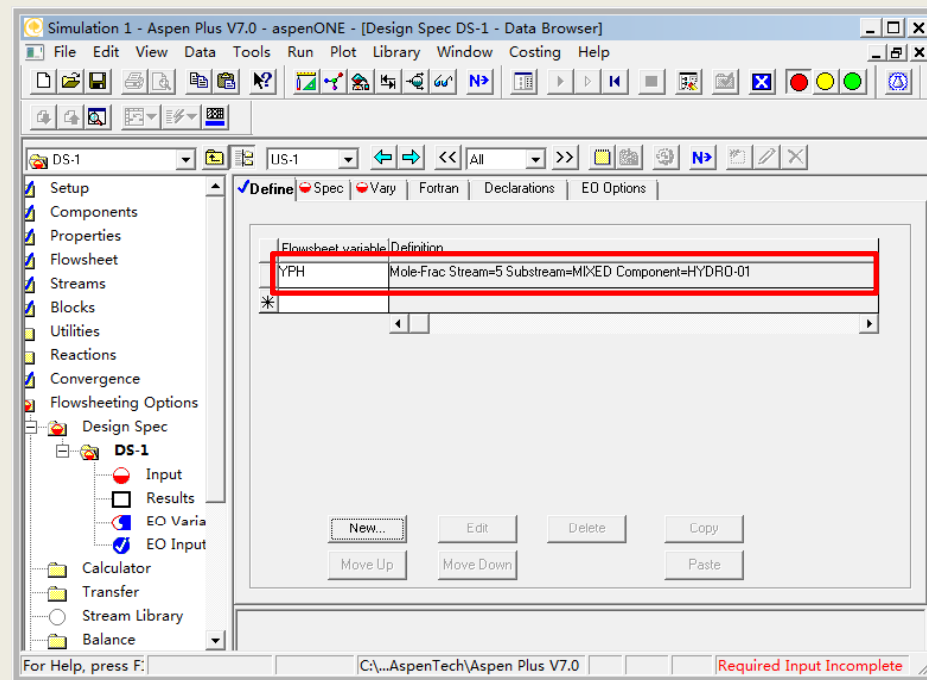
Description:

Next Close

Lets you select the component ID.

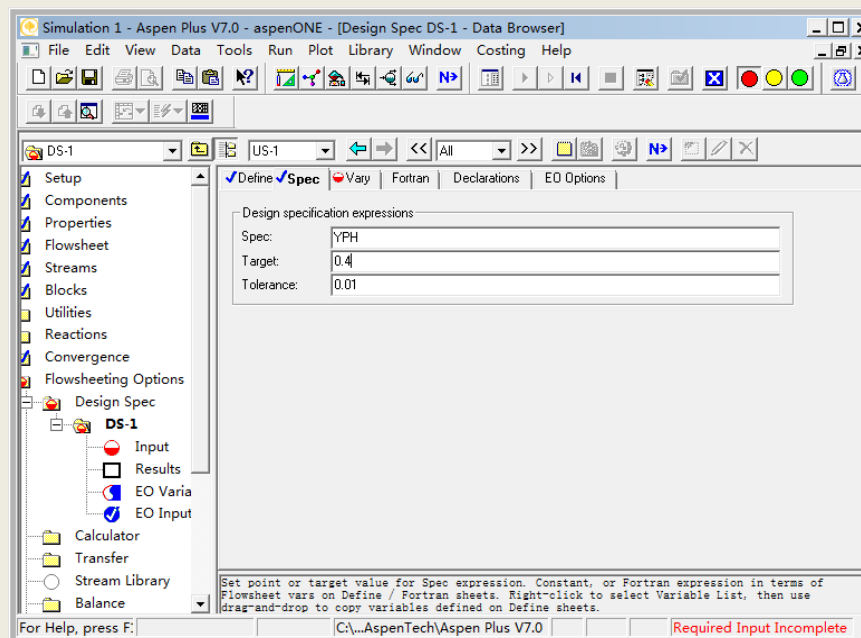
制定设计规定 (6)

✧ 图中显示已添加上YPH的变量，如图：



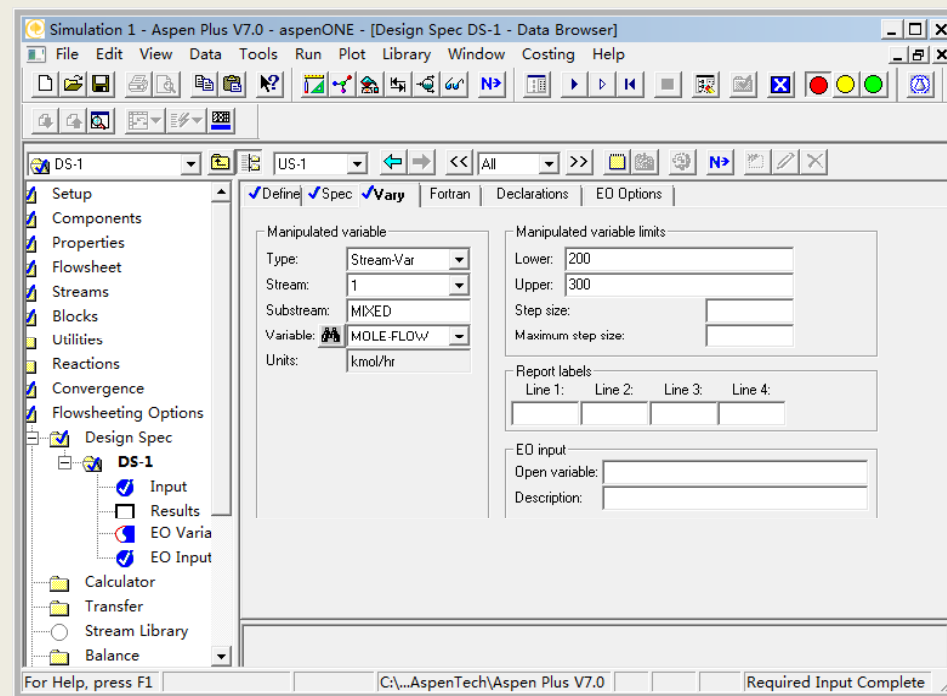
制定设计规定 (7)

✧ 在**Spec**标签中输入设计变量为前面定义好的**YPH**，其规定值为**0.4**，绝对误差为**0.01**，如图：



制定设计规定 (8)

✘ 在 **Vary** 标签中选择操作变量，如图：



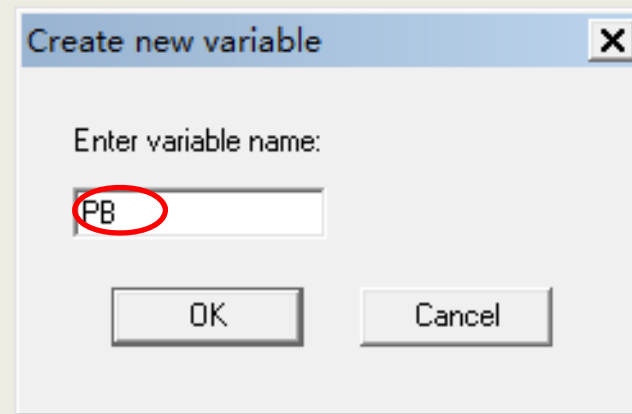
制定设计规定（9）



- ※ 该设计规定的**含义**是：在**200—300kmol/h**的范围内调节氢气进料物流**1**的摩尔流量，控制防空气物流**5**中氢气的含量在 **(0.4±0.01) kmol/h**。

制定设计规定（10）

※ 同样定义名为**PB**的变量，如图：



制定设计规定 (11)

※ 变量定义完成，如图：

Variable Definition

Select a variable category and reference

Variable name:

Reference

Type:

Stream:

Substream:

Variable:

Units:

Category

All

Blocks

Streams

Model Utility

Physical Property Parameters

Reactions

EO input

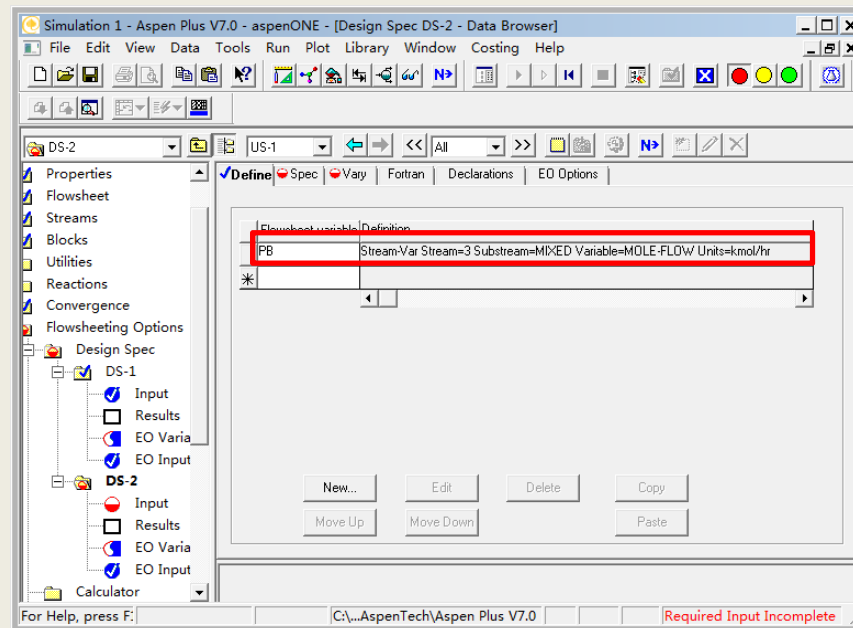
Open variable:

Description:

Lets you select the variable name. A sampled input variable must either have been previously entered as an input specification or have a default value.

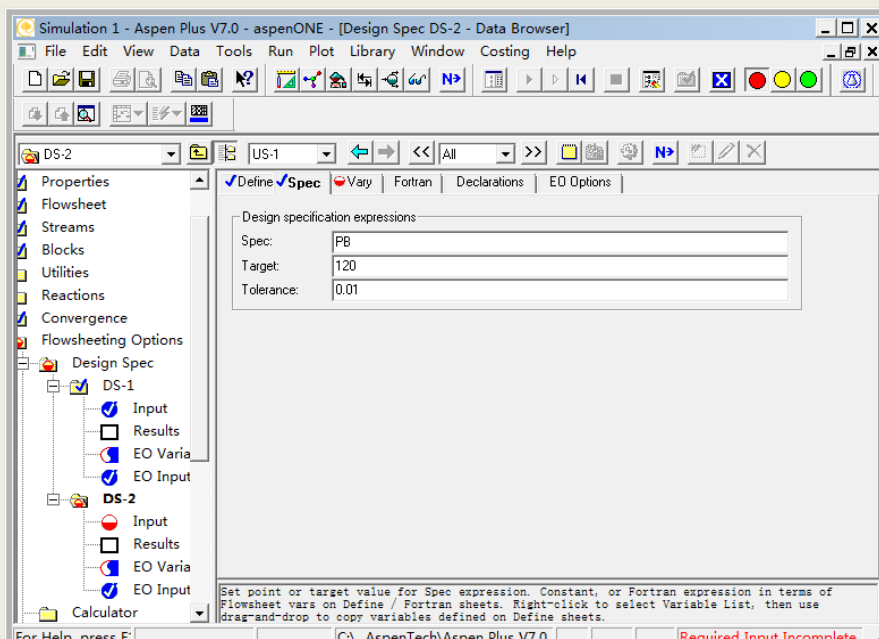
制定设计规定 (12)

✧ 图中显示已添加上PB的变量，如图：



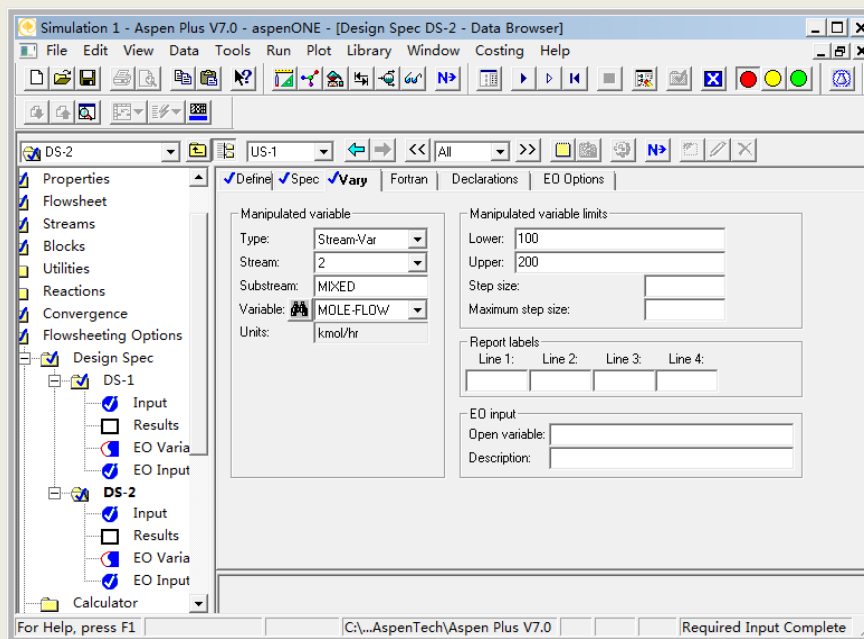
制定设计规定 (13)

在**Spec**标签中输入设计变量为前面定义好的**PB**，其规定值为**120**，绝对误差为**0.01**，如图：



制定设计规定 (14)

在 **Vary** 标签中选择操作变量，如图：



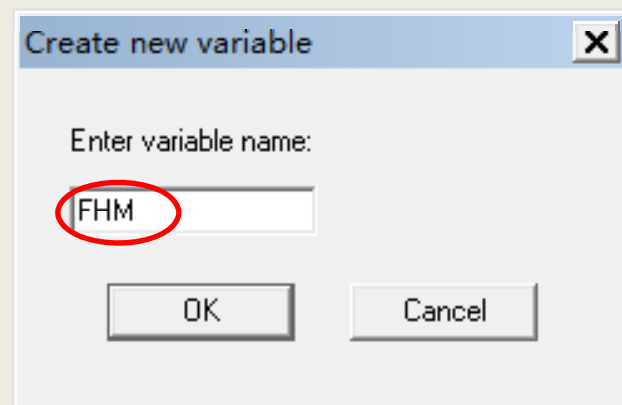
制定设计规定（15）



该设计规定的含义是：在100—200kmol/h的范围内调节甲苯进料物流2的摩尔流量，控制产品苯物流3的流量在（120±0.01） kmol/h。

制定设计规定 (16)

同样定义名为**FHM**（测量氢气进料1中的氢组分摩尔流量）的变量，如图：



制定设计规定 (17)

变量定义完成，如图：

The screenshot shows a dialog box titled "Variable Definition" with a close button (X) in the top right corner. The dialog is divided into several sections:

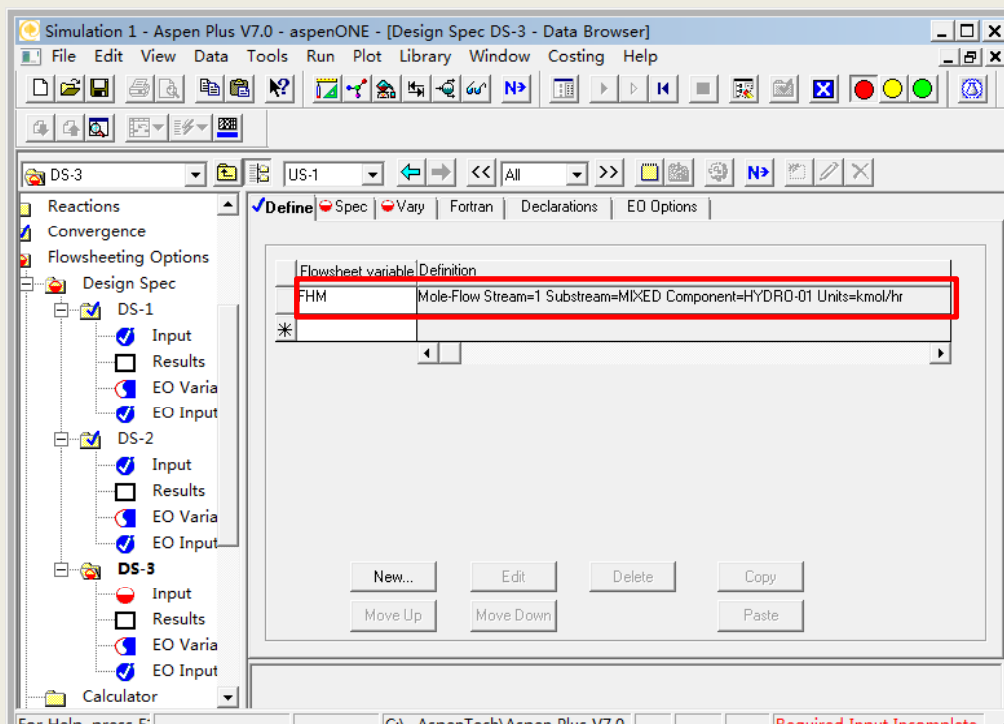
- Select a variable category and reference:**
 - Variable name:** A dropdown menu with "FHM" selected and a checkmark.
 - Category:** A list of radio buttons: "All", "Blocks", "Streams" (selected), "Model Utility", "Physical Property Parameters", and "Reactions".
 - Reference:** A group of dropdown menus: "Type" (Mole-Flow), "Stream" (1), "Substream" (MIXED), "Component" (HYDRO-01), and "Units" (kmol/hr).
- EO input:** Two text input fields labeled "Open variable:" and "Description:".

At the bottom of the dialog, there are two buttons: "Next" (with a right-pointing arrow) and "Close".

Below the dialog box, there is a small text note: "Lets you select the component ID."

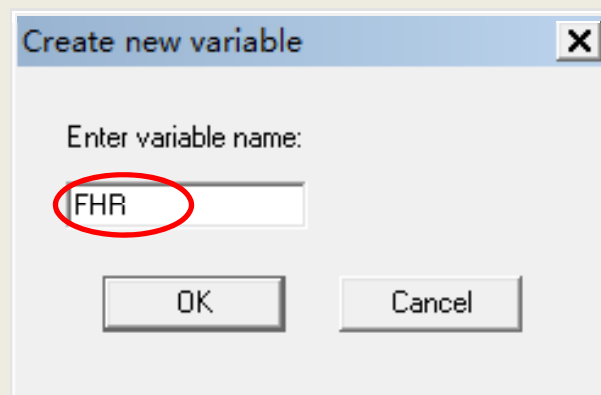
制定设计规定 (18)

※ 图中显示已添加上FHM的变量，如图：



制定设计规定 (19)

同样定义名为**FHR**（循环气7中氢组分摩尔流量）的变量，如图：



制定设计规定（20）

※ 变量定义完成，如图：

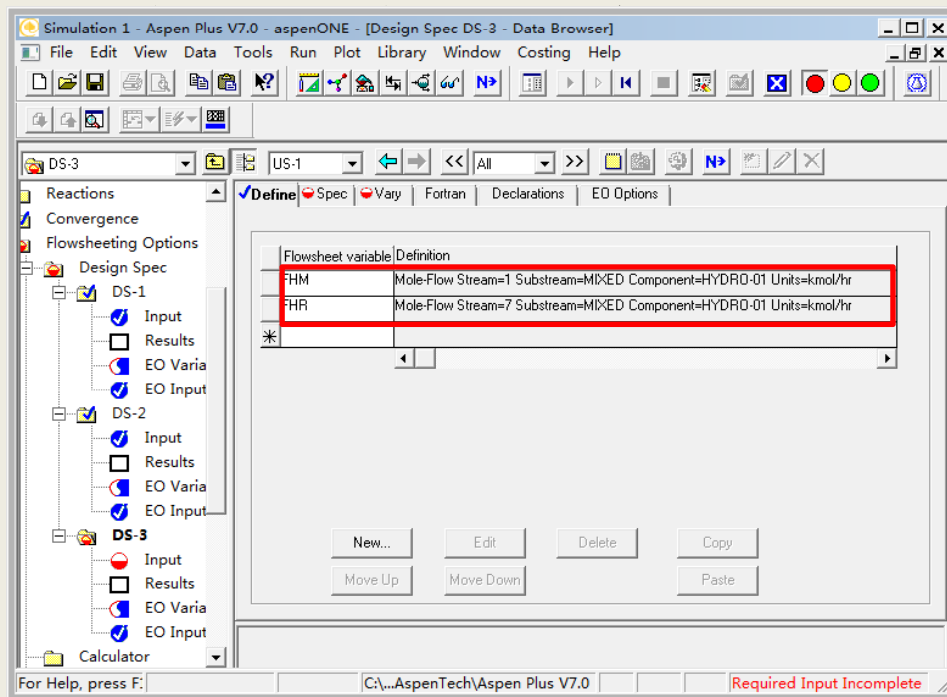
The screenshot shows a dialog box titled "Variable Definition" with a close button (X) in the top right corner. The dialog is divided into several sections:

- Select a variable category and reference:**
 - Variable name:** A dropdown menu with "FHR" selected and a checkmark.
 - Category:** A list of radio buttons: "All", "Blocks", "Streams" (selected), "Model Utility", "Physical Property Parameters", and "Reactions".
 - Reference:**
 - Type:** A dropdown menu with "Mole-Flow" selected.
 - Stream:** A dropdown menu with "7" selected.
 - Substream:** A dropdown menu with "MIXED" selected.
 - Component:** A dropdown menu with "HYDRO-01" selected.
 - Units:** A text field containing "kmol/hr".
- EO input:**
 - Open variable:** An empty text input field.
 - Description:** An empty text input field.

At the bottom of the dialog, there are two buttons: "N>" and "Close". Below the dialog box, the text "Lets you select the component ID." is visible.

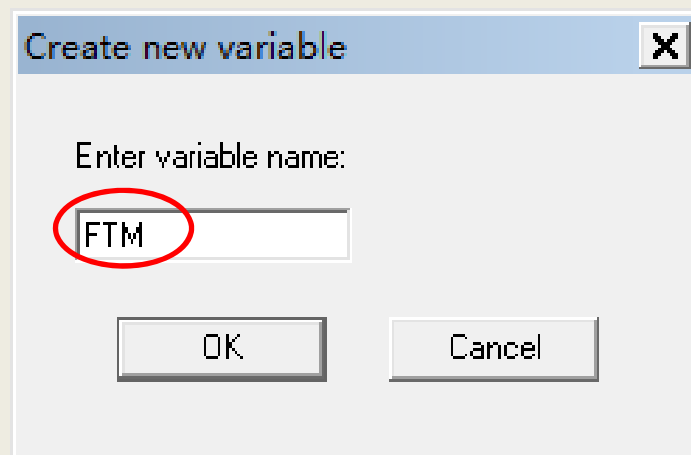
制定设计规定 (21)

✘ 图中显示已添加上**FHR**的变量，如图：



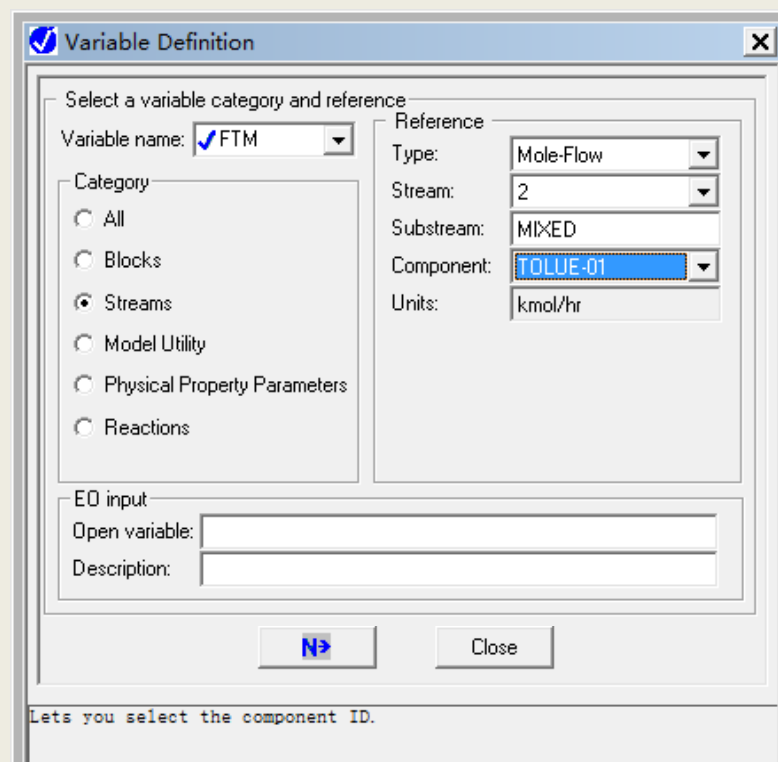
制定设计规定 (22)

同样定义名为**FTM**（进料甲苯中甲苯组分摩尔流量）的变量，如图：



制定设计规定 (23)

变量定义完成，如图：



The screenshot shows a dialog box titled "Variable Definition" with the following fields and options:

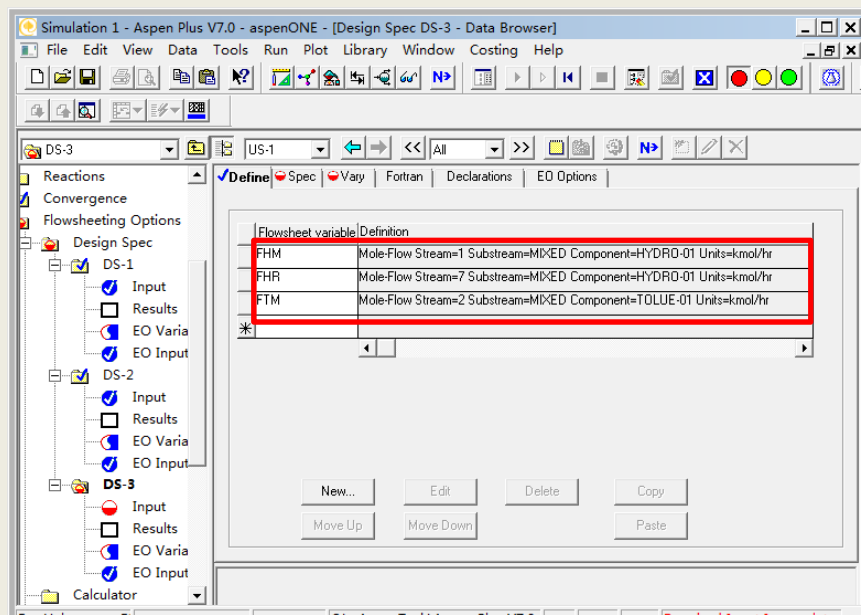
- Select a variable category and reference:**
 - Variable name:
 - Category:
 - All
 - Blocks
 - Streams
 - Model Utility
 - Physical Property Parameters
 - Reactions
 - Reference:
 - Type:
 - Stream:
 - Substream:
 - Component:
 - Units:
- EO input:**
 - Open variable:
 - Description:

Buttons:

Footer text: Lets you select the component ID.

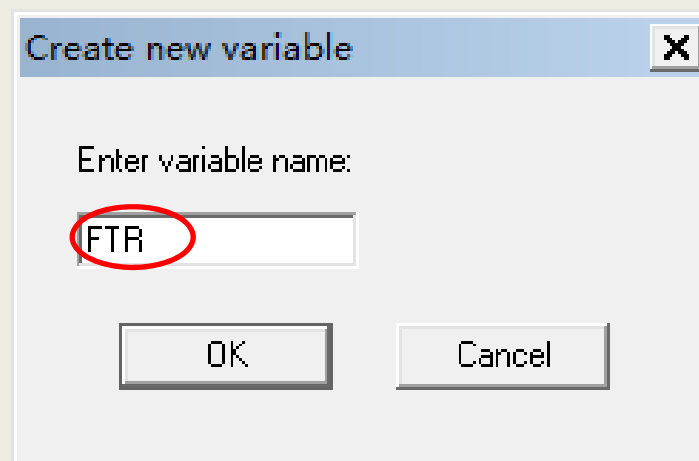
制定设计规定 (24)

图中显示已添加上**FTM**的变量，如图：



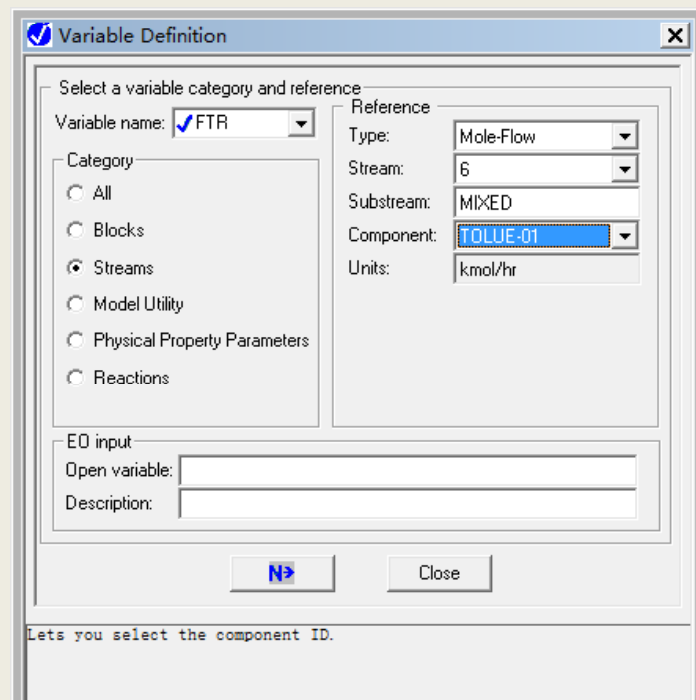
制定设计规定（25）

同样定义名为**FTR**（循环液中甲苯的摩尔流量）的变量，如图：



制定设计规定（26）

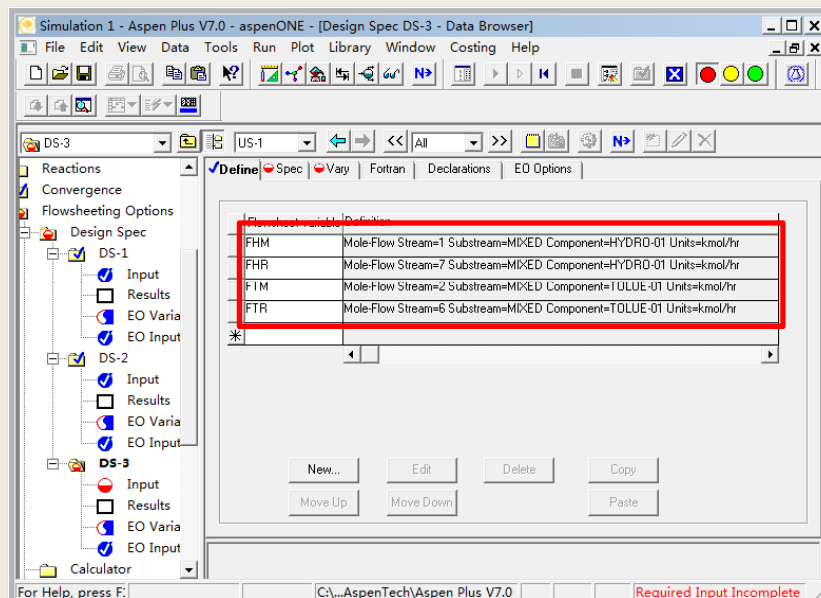
※ 变量定义完成，如图：



制定设计规定 (27)

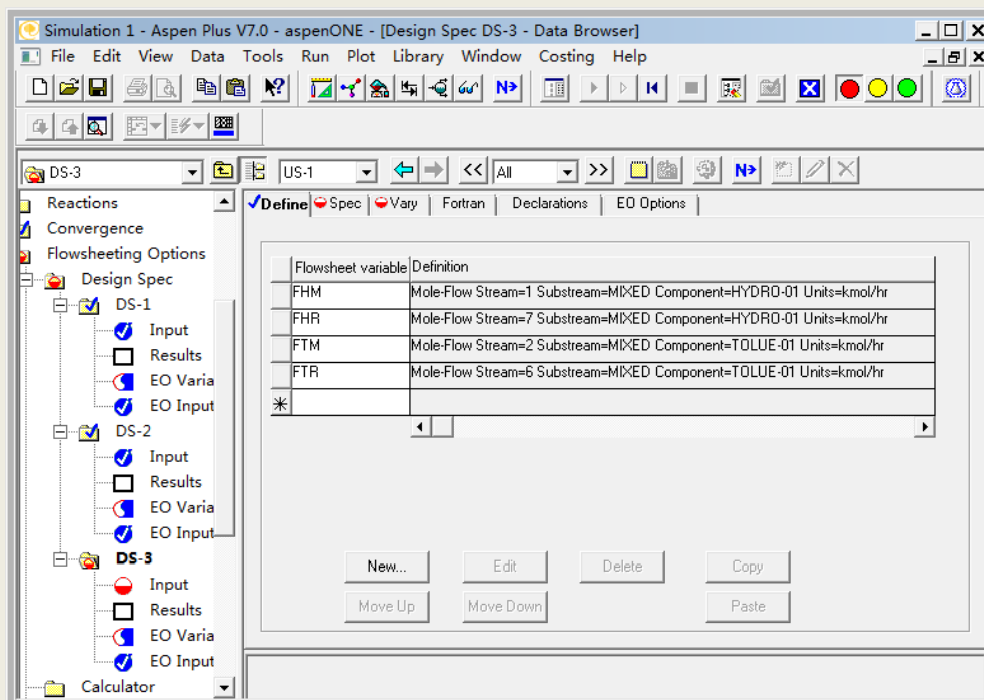


图中显示已添加上**FTR**的变量，如图：



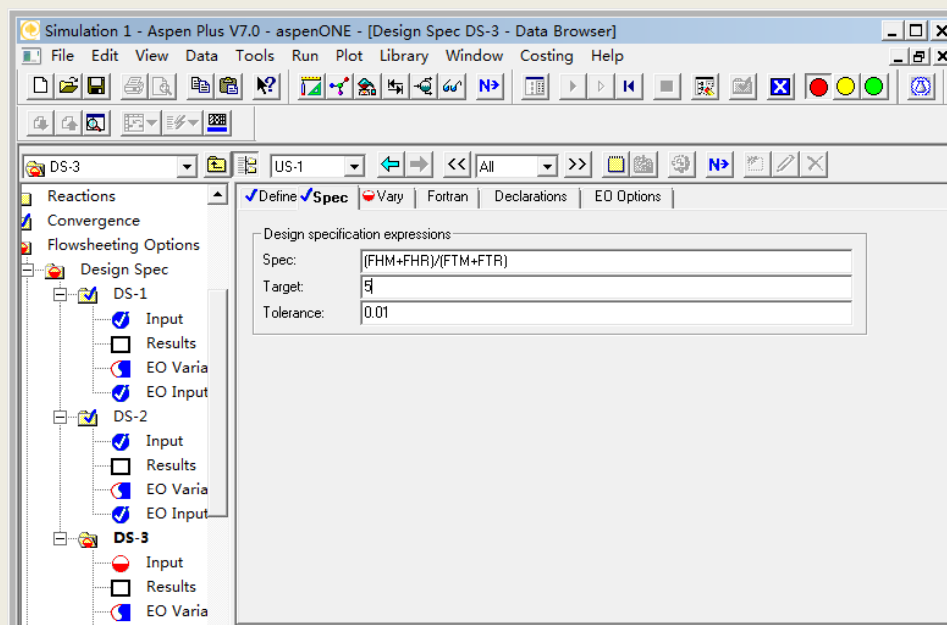
制定设计规定 (28)

所有变量定义完成，如图：



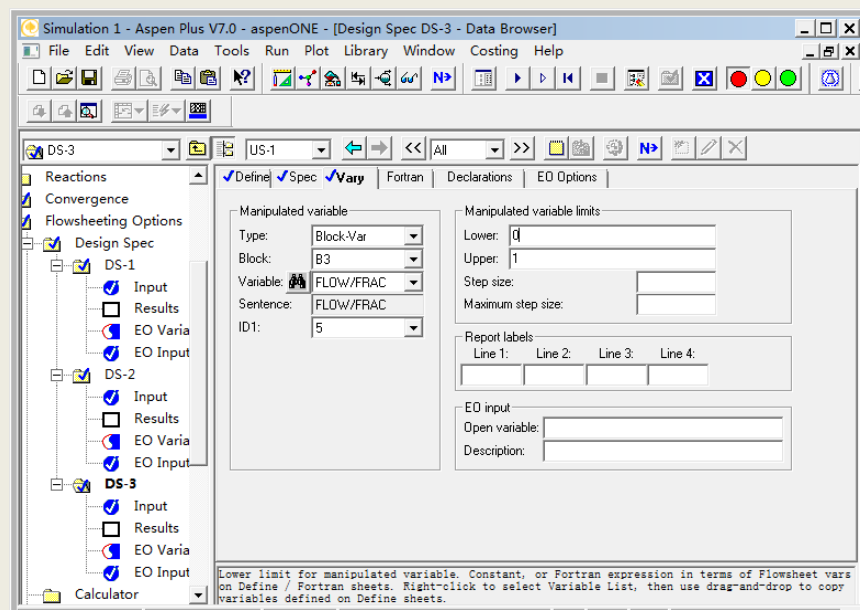
制定设计规定 (29)

在Spec标签中输入设计变量为 $(FHM+FHR) / (FTM+FTR)$ ，代表反应器进口处的氢和甲苯之比，并给定规定值为5，绝对误差为0.01，如图：



制定设计规定 (30)

✧ 在 **Vary** 标签中选择操作变量，如图：



运行模拟



Simulation 1 - Aspen Plus V7.0 - aspenONE - [Control Panel]

File Edit View Data Tools Run Library Window Costing Help

Solve

Calculation Sequence

- \$OLVER02
 - \$OLVER03
 - \$OLVER01
 - B2
 - \$OLVER04
 - B3
 - B1

```
>>> Loop #OLVER01 Method: WEGSTEIN      Iteration  14
# Converged           Max Err/Tol  -0.15677E+00

>>> Loop #OLVER03 Method: SECANT        Iteration   1
# Converged           Max Err/Tol   0.14211E-10

>>> Loop #OLVER02 Method: SECANT        Iteration   3
# Converged           Max Err/Tol  -0.83419E+00

-->Simulation calculations completed ...

*** Summary of Errors ***

Physical
Property      System      Simulation
Terminal Errors  0           0           0
Severe Errors   0           0           0
Errors          0           0           0
Warnings        0           0           9
```

More ▾

All blocks have been executed

Simulation run completed | C:\...AspenTech\Aspen Plus V7.0 | **Results Available**

查看模拟结果 (1)

查看所有物流结果，如图：

The screenshot shows the Aspen Plus V7.0 Results Summary Streams - Data Browser window. The window title is "Simulation 1 - Aspen Plus V7.0 - aspenONE - [Results Summary Streams - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Window, Costing, and Help. The toolbar contains various icons for file operations and simulation control. The left sidebar shows a tree view of the simulation components, with "Results Summary" expanded to show "Streams" checked. The main area displays a table of stream properties for "All streams" in "GEN_E" format. A red box highlights the "Stream Table" button. The table has columns for stream names and five data columns. The data rows include Temperature C, Pressure MPa, Vapor Frac, Mole Flow kmol/hr, Mass Flow kg/sec, Volume Flow cum/sec, Enthalpy MMBtu/hr, and Mole Flow kmol/hr for streams HYDRO-01 and METHA-01.

	1	2	3	4	5
Temperature C	38.0	25.0	621.0	621.0	6
Pressure MPa	3.80	0.10	3.40	3.40	3
Vapor Frac	1.000	0.000	1.000	1.000	1
Mole Flow kmol/hr	219.644	123.789	120.000	1.895	22
Mass Flow kg/sec	0.166	3.168	2.604	0.081	0
Volume Flow cum/sec	0.042	0.004	0.071	0.001	0
Enthalpy MMBtu/hr	-0.691	1.412	19.637	0.628	-4
Mole Flow kmol/hr					
HYDRO-01	208.662				86
METHA-01	10.982				13

查看模拟结果 (2)

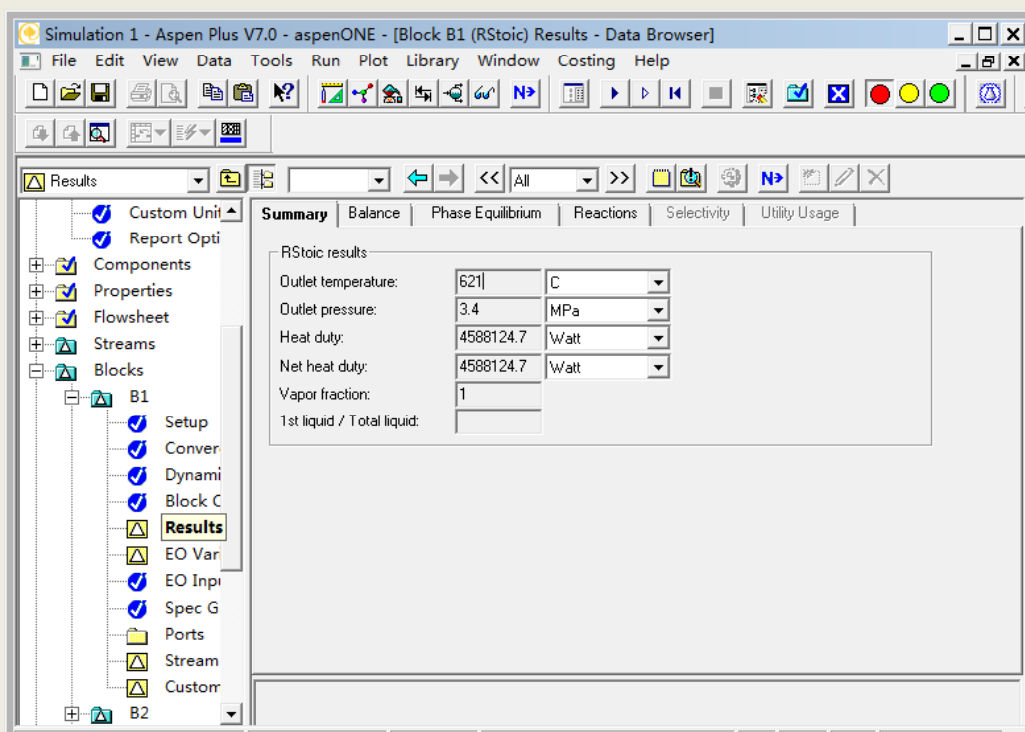


点击上图的**Stream table**，生成如下表格，如图：

Heat and Material Balance Table										
Stream ID		1	2	3	4	5	6	7	100	200
Temperature	C	38.0	25.0	621.0	621.0	621.0	621.0	621.0	621.0	621.0
Pressure	MPa	3.80	0.10	3.40	3.40	3.40	3.40	3.40	3.40	3.40
Vapor Frac		1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mole Flow	kmol/hr	219.644	123.789	120.000	1.895	221.539	41.263	1573.692	1958.389	1795.231
Mass Flow	kg/sec	0.166	3.168	2.604	0.081	0.649	1.056	4.611	9.002	5.261
Volume Flow	cum/sec	0.042	0.004	0.071	0.001	0.136	0.024	0.965	1.202	1.101
Enthalpy	MMBtu/hr	-0.691	1.412	19.637	0.628	-4.111	6.278	-29.201	-6.546	-33.312
Mole Flow	kmol/hr									
HYDRO-01		208.662				86.767		616.349	703.117	703.117
METHA-01		10.982				134.771		957.343	1092.114	1092.114
BENZE-01				120.000					120.000	
TOLUE-01			123.789				41.263		41.263	
DIBHE-01					1.895				1.895	

查看模拟结果 (3)

查看模块**B1**的结果，如图：



The screenshot displays the Aspen Plus V7.0 Data Browser interface for Block B1 (RStoic). The left sidebar shows a tree view with 'Results' selected under Block B1. The main window shows the 'Summary' tab with the following data:

RStoic results		
Outlet temperature:	621	C
Outlet pressure:	3.4	MPa
Heat duty:	4588124.7	Watt
Net heat duty:	4588124.7	Watt
Vapor fraction:	1	
1st liquid / Total liquid:		

查看模拟结果 (4)

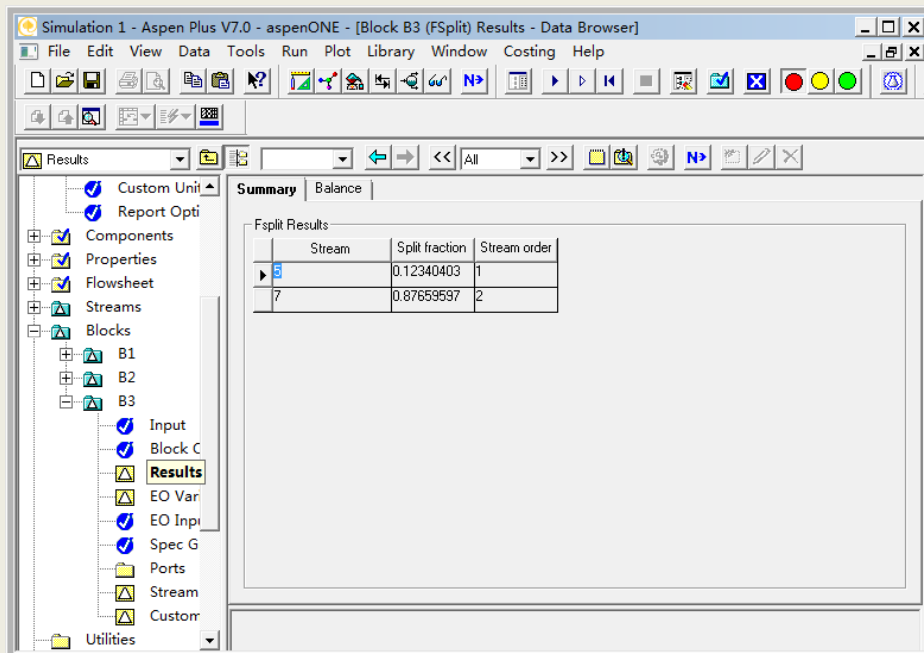
※ 查看模块**B2**的结果，如图：

The screenshot shows the Aspen Plus V7.0 Data Browser window for Block B2. The left-hand tree view shows the simulation hierarchy, with Block B2 selected. The main window displays the 'Summary' tab, showing a heat duty of -65410.19 Watt and a substream of MIXED. Below this, a table displays the split fractions for various components in the outlet streams.

Component ID	3	4	200	6
HYDRD-01	0	0	1	0
METHA-01	0	0	1	0
BENZE-01	1	0	0	0
TOLUE-01	0	0	0	1
DIPHE-01	0	1	0	0

查看模拟结果 (5)

物流5和7的模拟比例，如图：



Simulation 1 - Aspen Plus V7.0 - aspenONE - [Block B3 (FSplit) Results - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Results

Custom Unit
Report Opti

Components
Properties
Flowsheet
Streams
Blocks
B1
B2
B3
Input
Block C
Results
EO Var
EO Inpi
Spec G
Ports
Stream
Custom

Utilities

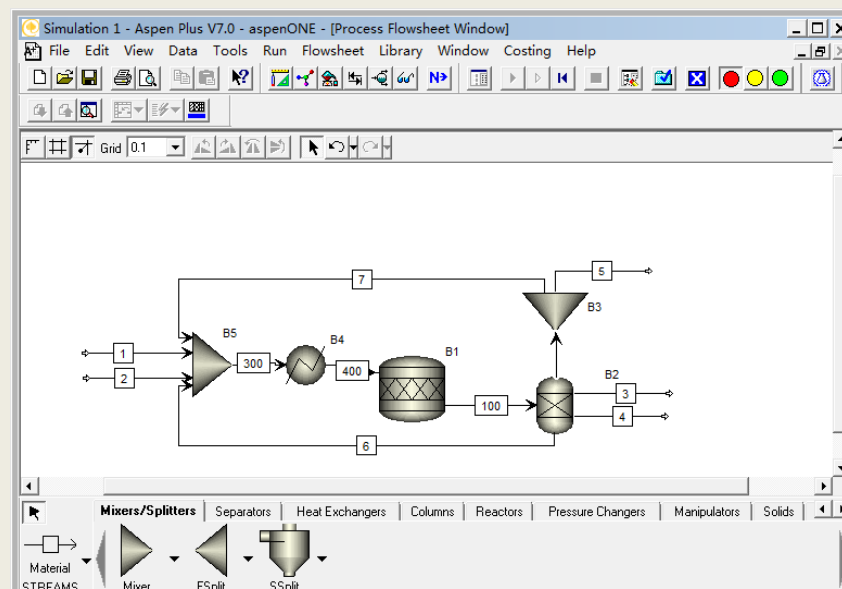
Summary | Balance

Fsplit Results

Stream	Split fraction	Stream order
5	0.12340403	1
7	0.87659597	2

反应器对循环结构的影响

向流程图添加一台换热器**B4**，其作用是保持进入反应
器**B1**的进料温度恒定，再向流程图添加一个汇合器**B5**，以便
反应器的新鲜进料和循环进料汇合在一起进入换热器**B4**，
图：



输入进料物流数据

1 - Aspen Plus V7.0 - aspenONE - [Stream 1 (MATERIAL) Input - Data Browser]

View Data Tools Run Plot Library Window Costing Help

Substream name: **MIXED**

State variables

Temperature: 38 C

Pressure: 3.8 MPa

Total flow: 250 kmol/hr

Composition

Component	Value
HYDRO-01	0.95
METHA-01	0.05
BENZE-01	
TOLUE-01	
DIPHE-01	

Total: 1

Required Input Incomplete

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Stream 2 (MATERIAL) Input - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Substream name: **MIXED**

State variables

Temperature: 25 C

Pressure: 0.1 MPa

Total flow: 150 kmol/hr

Composition

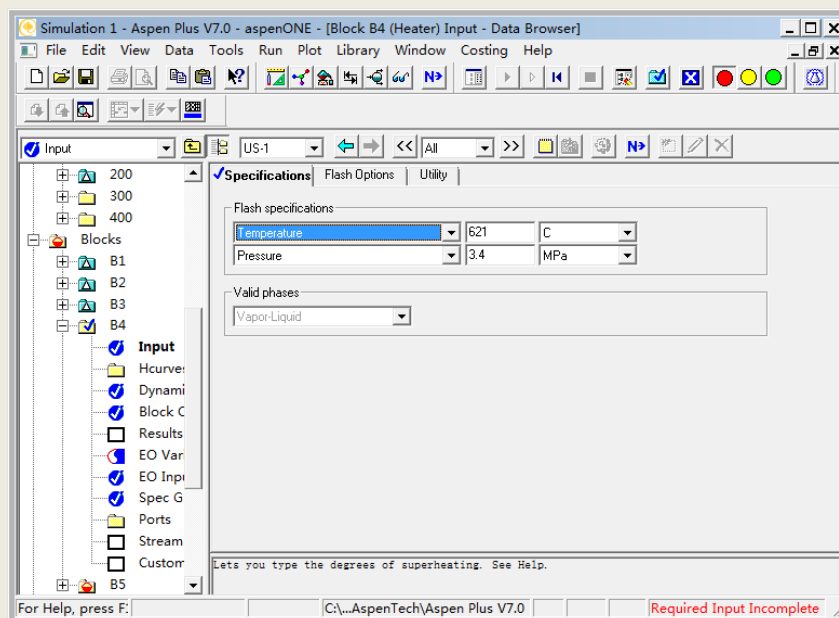
Component	Value
HYDRO-01	
METHA-01	
BENZE-01	
TOLUE-01	1
DIPHE-01	

Total: 1

Required Input Incomplete

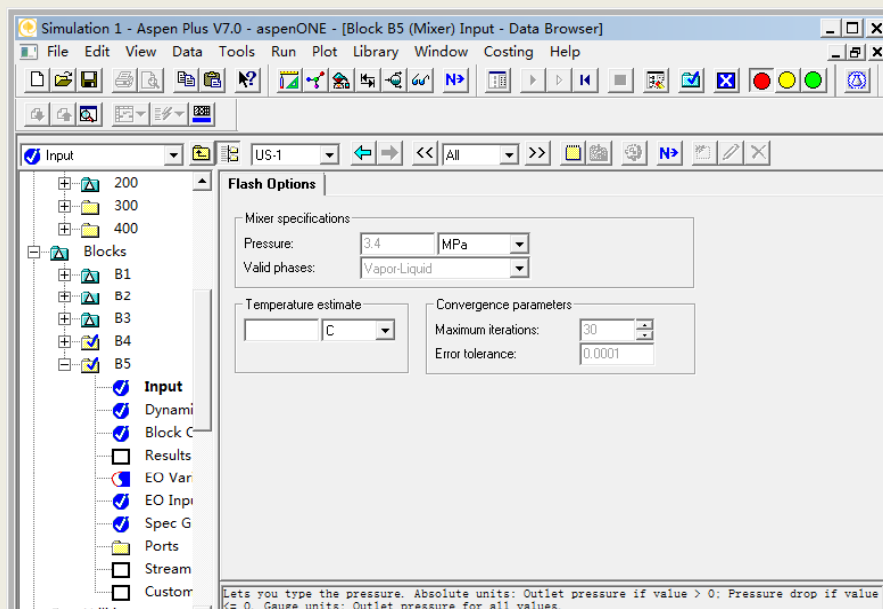
输入反应器参数 (1)

输入换热器B4操作压力位3.4Mpa，温度为621℃，如图：



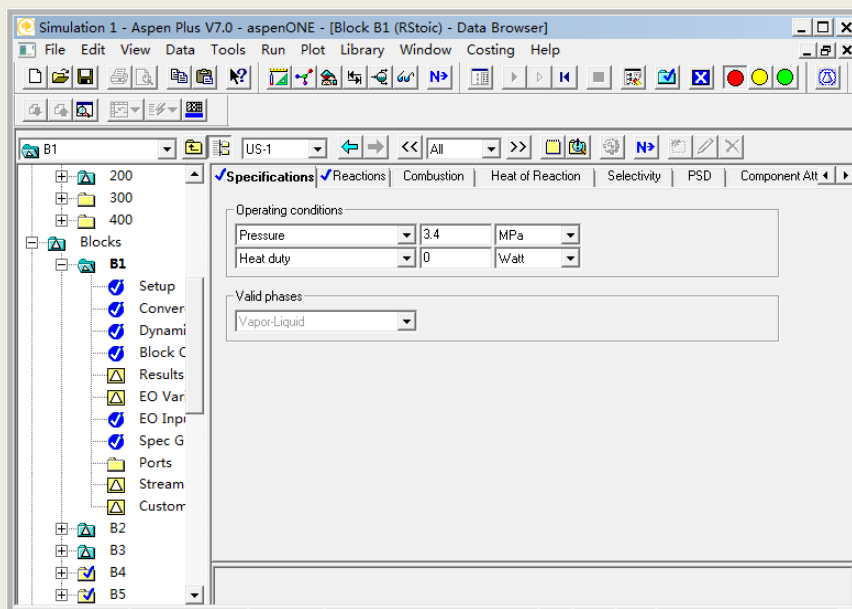
输入反应器参数 (2)

✘ 指定汇合器B5的操作参数，如图：



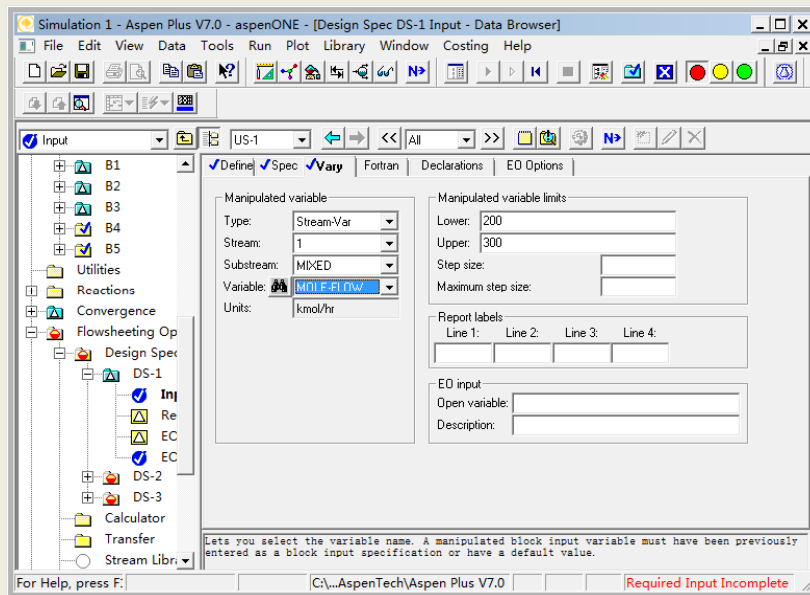
输入反应器参数 (3)

指定反应器**B1**操作参数，在绝热条件下操作，如图：



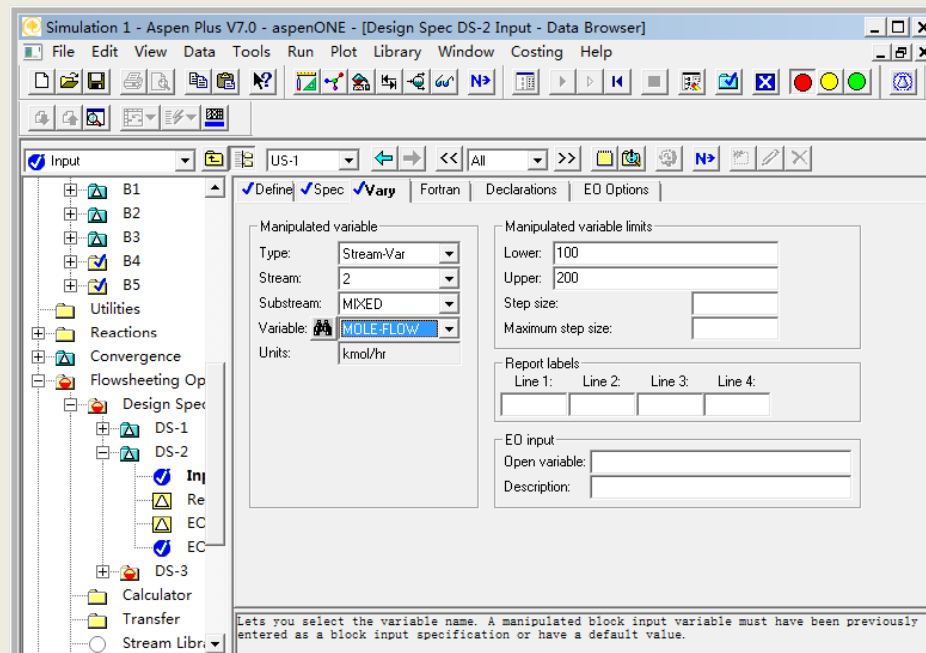
指定优化变量DS-1

定优化变量**DS-1**的选择变量，如图：



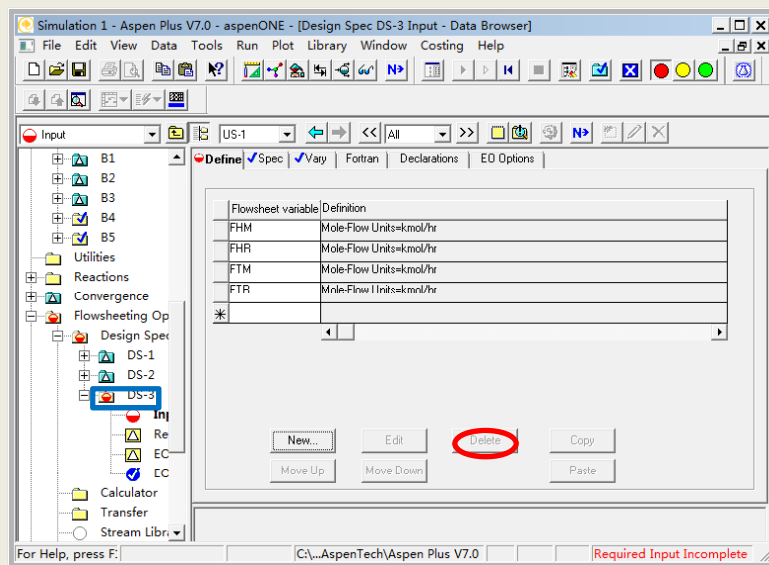
指定优化变量DS-2

指定优化变量DS-2的选择变量，如图：



指定优化变量DS-3

隐藏优化变量**DS-3**，选中图中蓝色框架所指，单击**Delete**，
如图：



运行模拟



Simulation 1 - Aspen Plus V7.0 - aspenONE - [Control Panel]

File Edit View Data Tools Run Library Window Costing Help

Solve

Calculation Sequence

- \$OLVER02
 - \$OLVER03
 - \$OLVER01
 - B2
 - B3
 - B5
 - B4
 - B1

```
# Converged          Max Err/Tol  -0.14001E-10
>> Loop $OLVER03 Method: SECANT   Iteration   1
# Converged          Max Err/Tol  0.14211E-10
> Loop $OLVER02 Method: SECANT   Iteration   2
# Converged          Max Err/Tol -0.83424E+00
->Simulation calculations completed ...

*** Summary of Errors ***

          Physical
          Property      System      Simulation
Terminal Errors      0           0           0
Severe Errors        0           0           0
Errors               0           0           0
Warnings            0           0           15
```

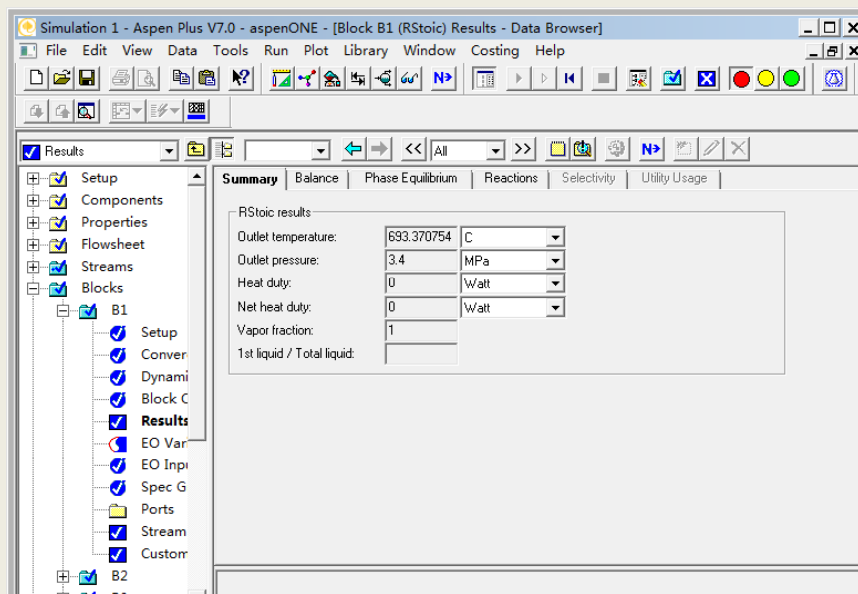
More ▾

All blocks have been executed

Simulation run completed | C:\...AspenTech\Aspen Plus V7.0 | **Results Available**

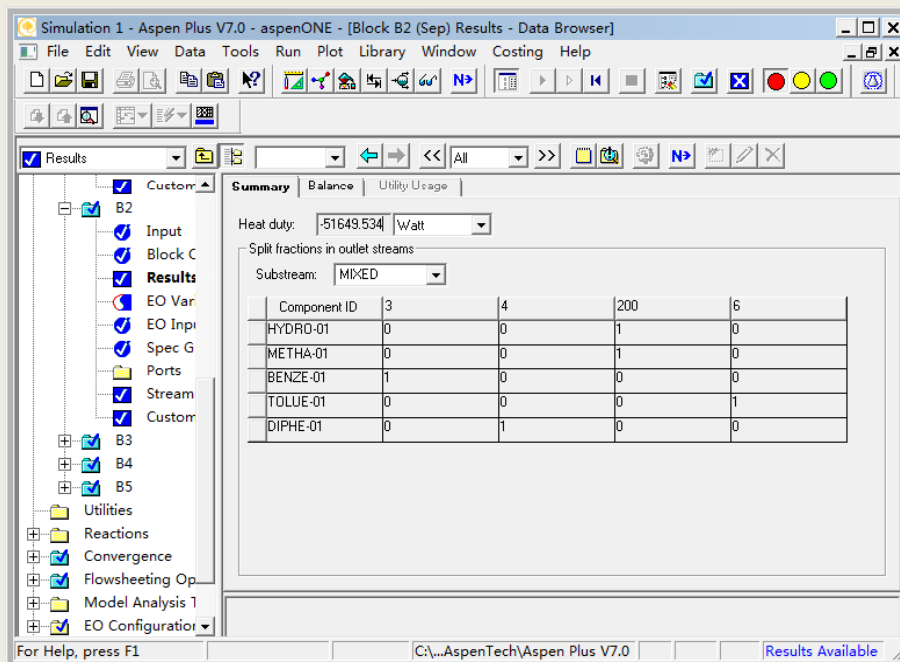
查看模拟结果 (1)

反应器**B1**的计算结果，如图：反应器的出口温度为**693°C**，
于反应器出口温度要求的上限704°C，所以使用一台绝热
反应器是可以接受的。



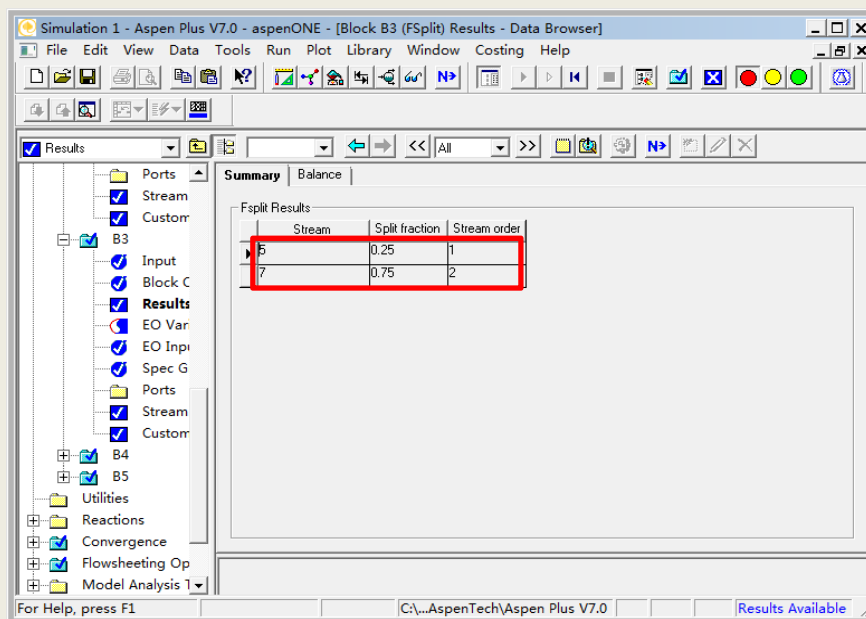
查看模拟结果 (2)

反应器B2的模拟结果，如图：



查看模拟结果 (3)

物流5和7的模拟比例为1/4，如图：



Simulation 1 - Aspen Plus V7.0 - aspenONE - [Block B3 (FSplit) Results - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Results

Summary Balance

Fsplit Results

Stream	Split fraction	Stream order
5	0.25	1
7	0.75	2

For Help, press F1

C:\AspenTech\Aspen Plus V7.0

Results Available

查看模拟结果 (4)



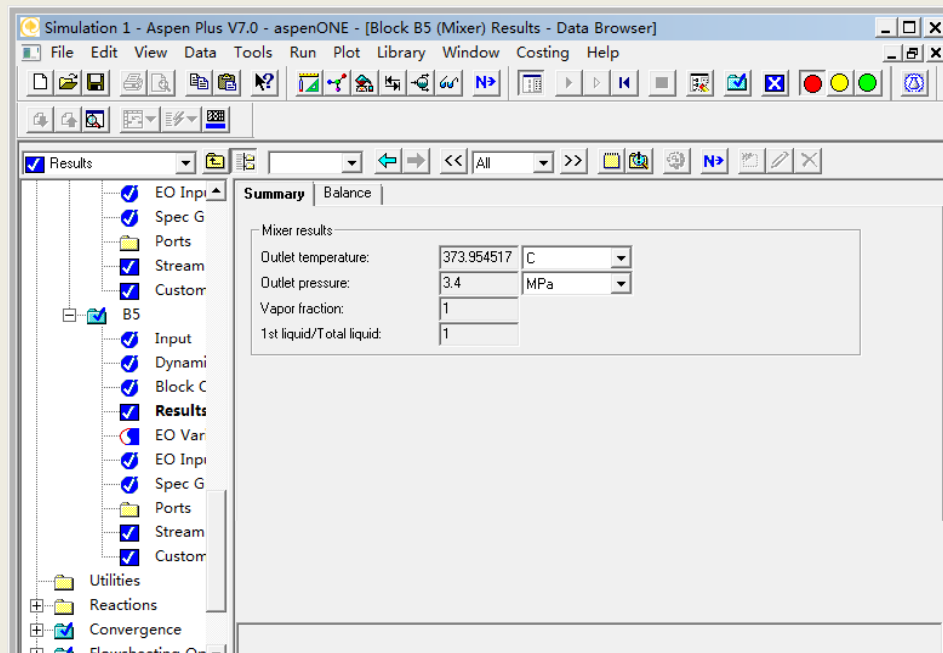
反应器B4的模拟结果，如图：

Block results summary		
Outlet temperature:	621	C
Outlet pressure:	3.4	MPa
Vapor fraction:	1	
Heat duty:	5335261.92	Watt
Net duty:	5335261.92	Watt
1st liquid / Total liquid:		
Pressure-drop correlation parameter:	0	

查看模拟结果 (5)

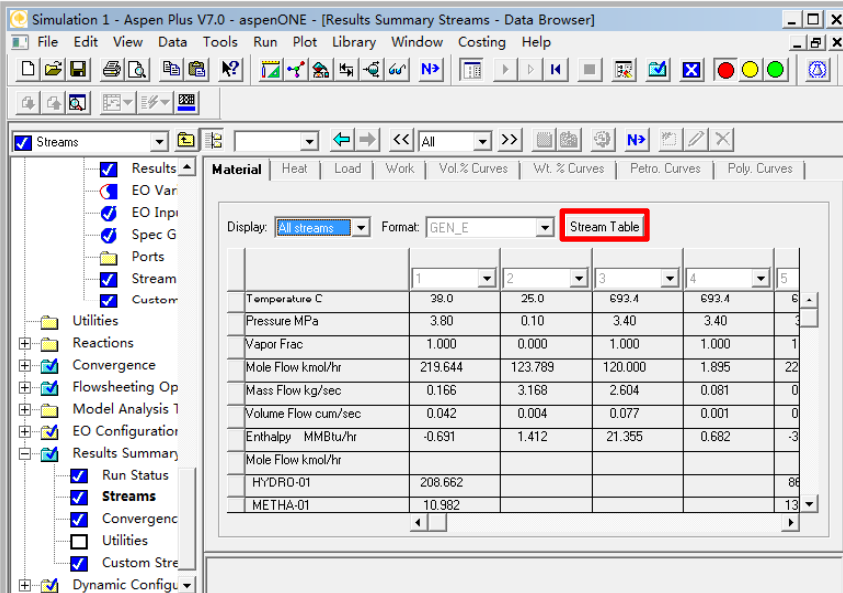


反应器**B5**的模拟结果，如图：



查看模拟结果 (6)

所有物流的结果，如图：



The screenshot shows the Aspen Plus 7.0 Results Summary Streams - Data Browser window. The window title is "Simulation 1 - Aspen Plus V7.0 - aspenONE - [Results Summary Streams - Data Browser]". The interface includes a menu bar (File, Edit, View, Data, Tools, Run, Plot, Library, Window, Costing, Help), a toolbar, and a left-hand navigation pane. The main area displays a table of stream properties for five streams (1, 2, 3, 4, 5). The table is titled "Stream Table" and has columns for various properties and stream numbers. The properties listed are Temperature C, Pressure MPa, Vapor Frac, Mole Flow kmol/hr, Mass Flow kg/sec, Volume Flow cum/sec, Enthalpy MMBtu/hr, and Mole Flow kmol/hr for specific components (HYDRD-01 and METHA-01). The "Stream Table" label is highlighted with a red box.

	1	2	3	4	5
Temperature C	39.0	25.0	693.4	693.4	6
Pressure MPa	3.80	0.10	3.40	3.40	3
Vapor Frac	1.000	0.000	1.000	1.000	1
Mole Flow kmol/hr	219.644	123.789	120.000	1.895	22
Mass Flow kg/sec	0.166	3.168	2.604	0.081	0
Volume Flow cum/sec	0.042	0.004	0.077	0.001	0
Enthalpy MMBtu/hr	-0.691	1.412	21.355	0.682	-3
Mole Flow kmol/hr					
HYDRD-01	208.662				88
METHA-01	10.982				13

查看模拟结果 (7)

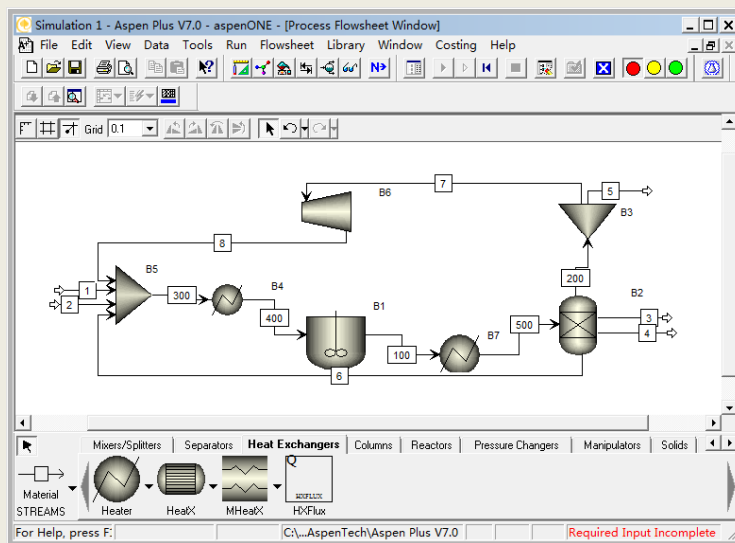


点击上图的**Stream table**，生成下图表格，如图：

Heat and Material Balance Table												
Stream ID		1	2	3	4	5	6	7	100	200	300	400
Temperature	C	38.0	25.0	693.4	693.4	693.4	693.4	693.4	693.4	693.4	374.0	621.0
Pressure	MPa	3.80	0.10	3.40	3.40	3.40	3.40	3.40	3.40	3.40	3.40	3.40
Vapor Frac		1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mole Flow	kmol/hr	219.644	123.789	120.000	1.895	221.539	41.263	664.617	1049.314	886.156	1049.314	1049.314
Mass Flow	kg/sec	0.166	3.168	2.604	0.081	0.649	1.056	1.948	6.338	2.597	6.338	6.338
Volume Flow	cum/sec	0.042	0.004	0.077	0.001	0.147	0.026	0.440	0.696	0.587	0.465	0.645
Enthalpy	MMBtu/hr	-0.691	1.412	21.355	0.682	-3.286	7.009	-9.859	16.076	-13.146	-2.128	16.076
Mole Flow	kmol/hr											
HYDRO-01		208.662				86.767		260.302	347.070	347.070	468.964	468.964
METHA-01		10.982				134.772		404.315	539.086	539.086	415.297	415.297
BENZE-01				120.000					120.000			
TOLUE-01			123.789				41.263		41.263		165.052	165.052
DIPHE-01					1.895				1.895			

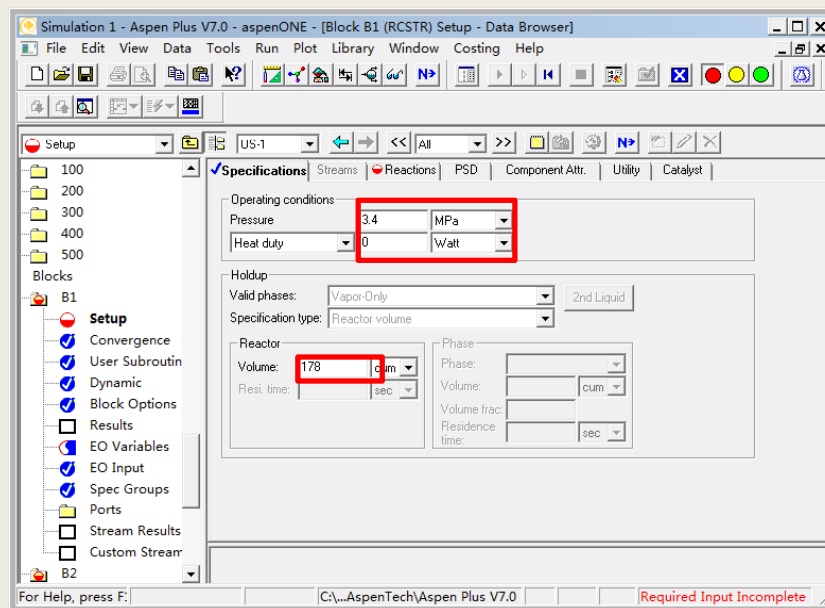
循环物料衡算优化

由于考虑了气相和液相循环对物料衡算的影响，所以压缩机和反应器的费用被包括进优化目的中，搭建流程图如图：



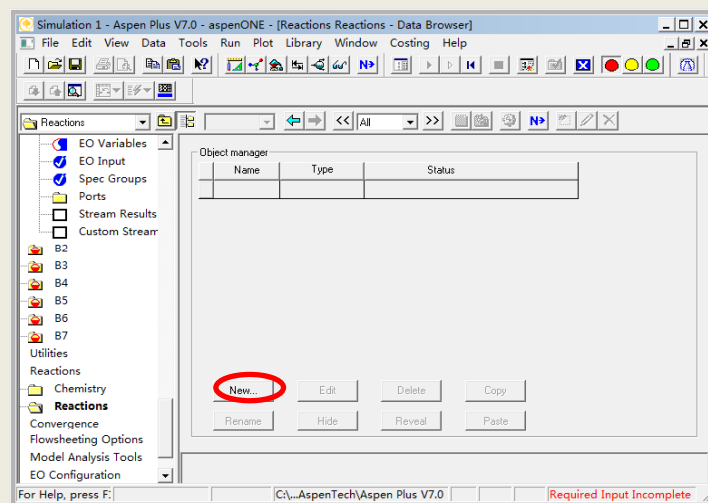
设置反应器B1参数

输入反应器**B1**的操作压力、热负荷及容积，
如图：



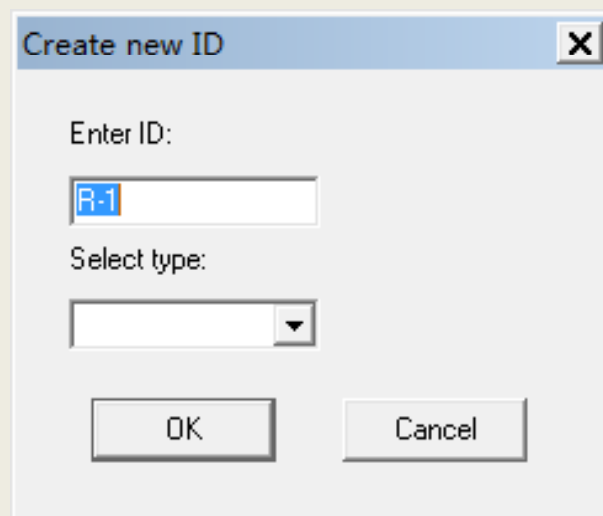
全混流反应器的反应需在模块外定义

点击**Data Browser**的**Reactions/Reactions**，出现
下图窗口，如图：



定义反应 (1)

※ 点击上图的**NEW**，出现下图对话框，如图：



Create new ID

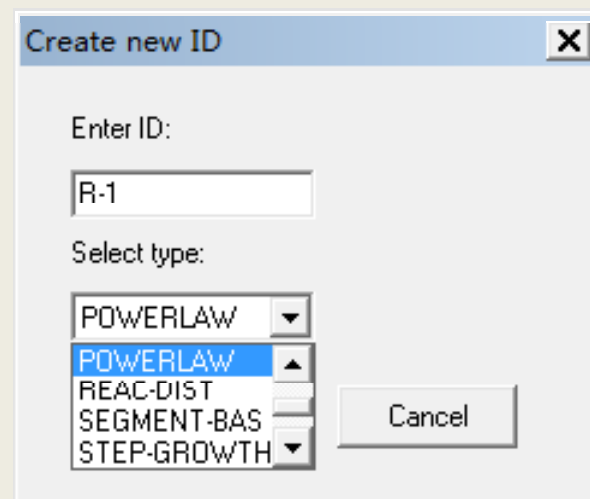
Enter ID:
R-1

Select type:
[Dropdown menu]

OK Cancel

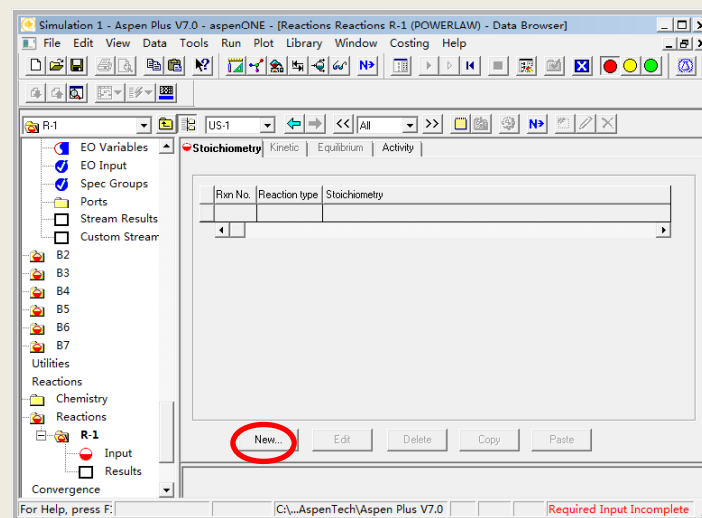
定义反应（2）

※ 通过下拉菜单那选择一个**POWERLAW**类型的反应集，如图：



定义反应 (3)

※ 点击上图的OK，出现下图窗口，如图：



定义反应 (4)

单击上图的**NEW**，出现下图对话框，在此对话框中输入反应方程式，该反应为**动力学型**，如图：

Reaction No.: 1

Reaction type: Kinetic

Reactants

Component	Coefficient	Exponent
TOLUE-01	-1	
HYDR0-01	-1	
*		

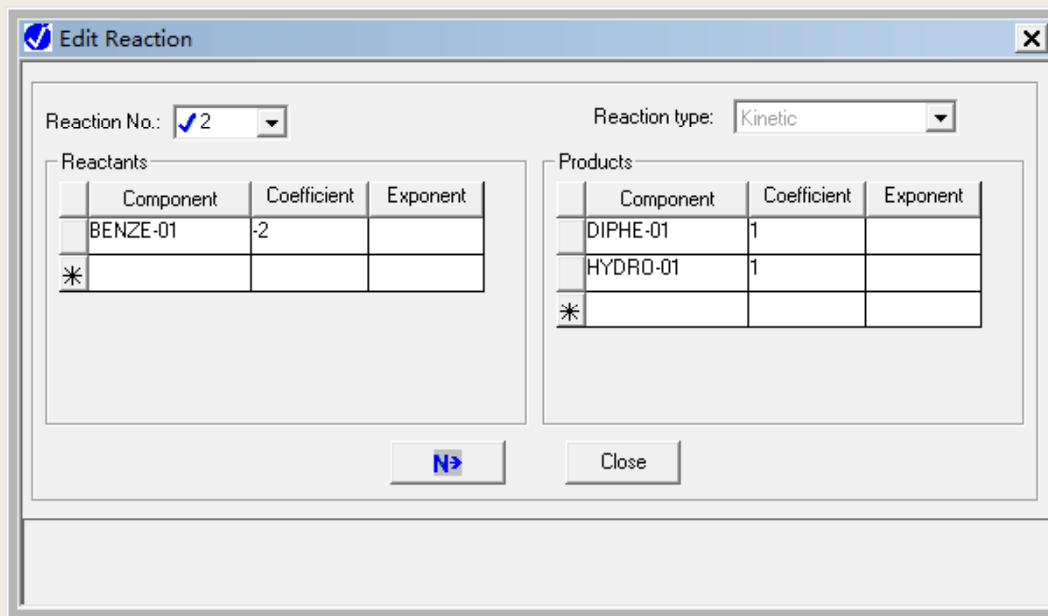
Products

Component	Coefficient	Exponent
BENZE-01	1	
METHA-01	1	
*		

Buttons: [Next] [Close]

定义反应 (5)

同样在对话框2中输入副反应方程式，如图：



The screenshot shows a software dialog box titled "Edit Reaction". It contains the following fields and tables:

- Reaction No.: 2
- Reaction type: Kinetic
- Reactants table:

	Component	Coefficient	Exponent
<input type="checkbox"/>	BENZE-01	-2	
*			

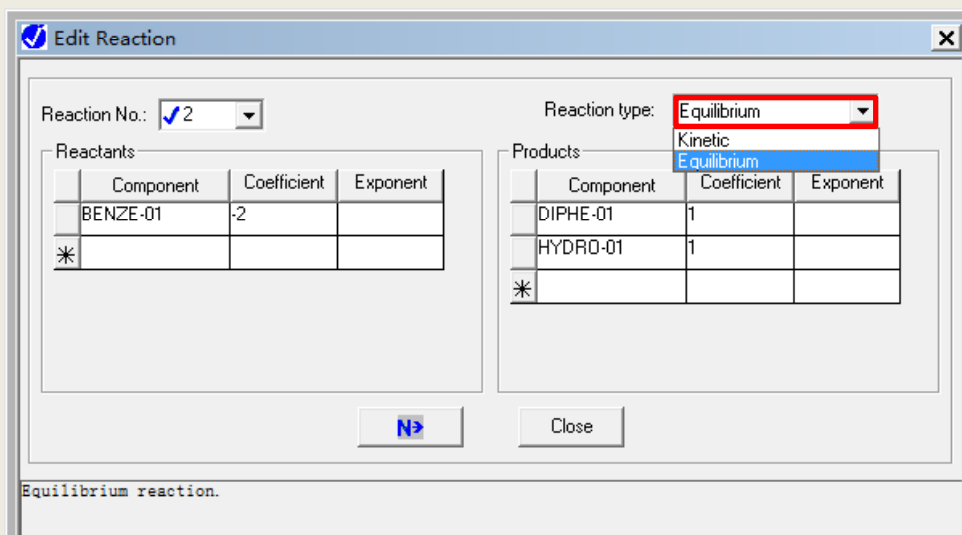
- Products table:

	Component	Coefficient	Exponent
<input type="checkbox"/>	DIPHE-01	1	
<input type="checkbox"/>	HYDRO-01	1	
*			

At the bottom of the dialog box, there are two buttons: "N" and "Close".

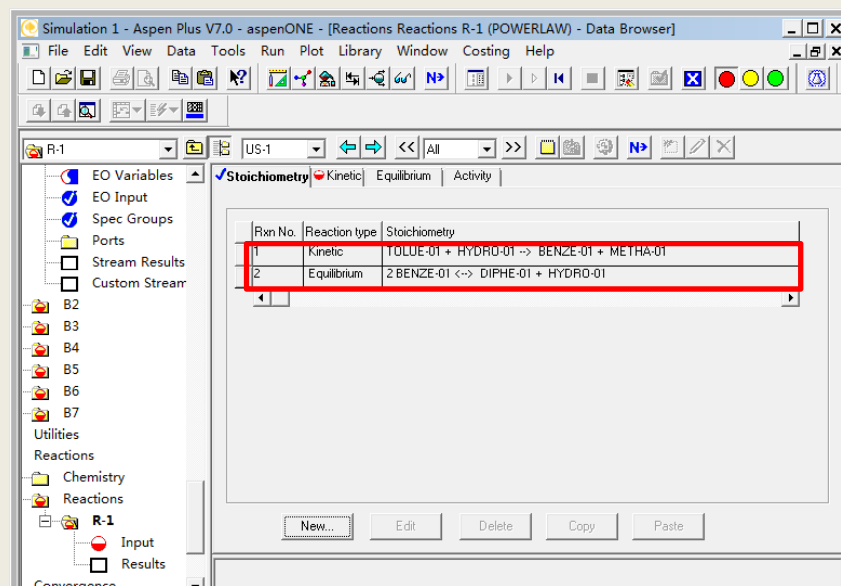
定义反应 (6)

※通过下拉菜单选择反应类型，该反应为平衡型反应，如图：



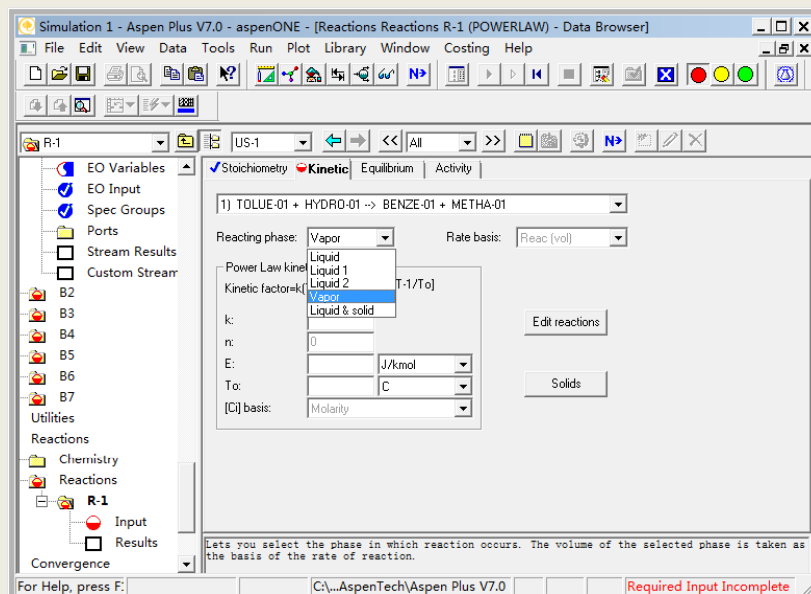
定义反应 (7)

※ 反应添加完毕，如图：



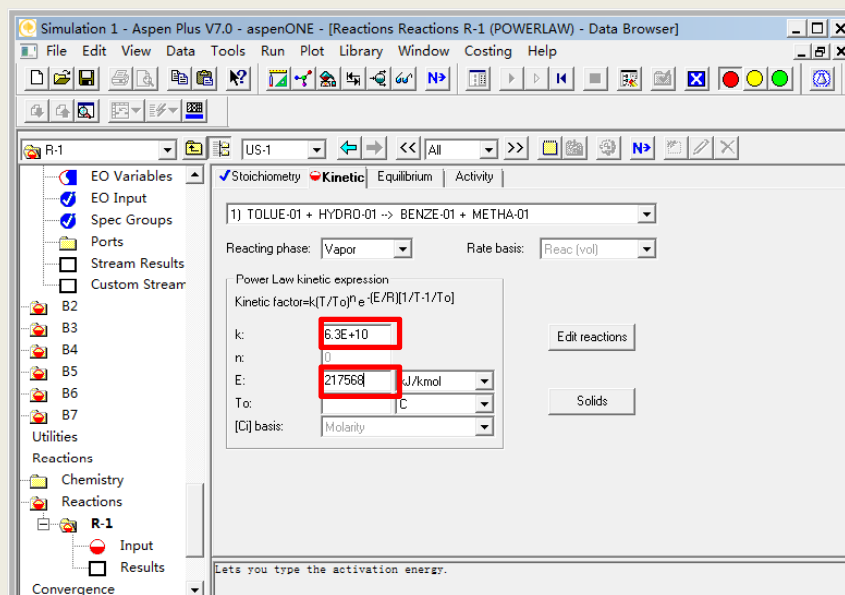
定义反应 (8)

※ 指定主反应相态为气相，如图：



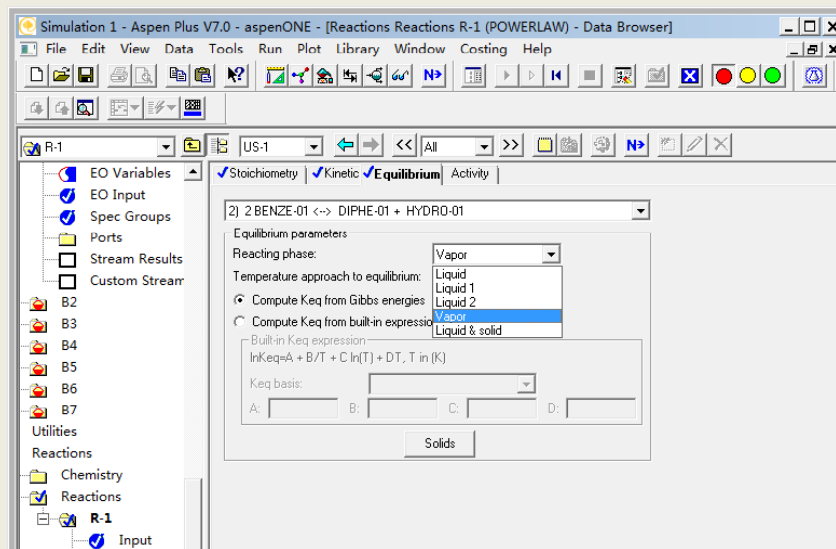
定义反应 (9)

输入主反应指前因子和活化能，如图：



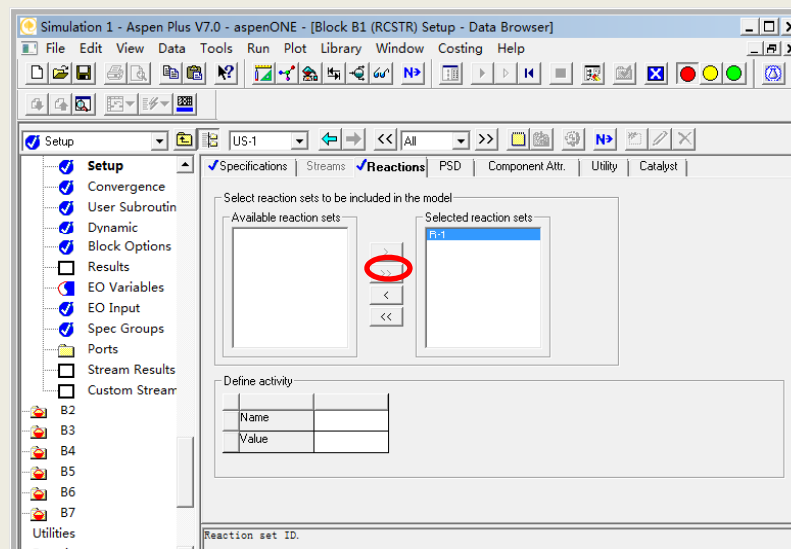
定义反应 (10)

指定副反应相态为气相，如图：



设置反应器B1参数

重新回到**Data Browser**的**Blocks/B1**，点击**Reactions**标签，
点击下图按钮，将反应集**R-1**由可用反应集移至选定反应集，
如图：



设置分离器B2参数

同样的物流3分割苯的值为1，物流4分割联苯的值为1，物流200分割氢气与甲烷的值均为1，完成后如图：

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Block B2 (Sep) Input - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Input US-1 All

Specifications Feed Flash Outlet Flash Utility

Outlet stream conditions

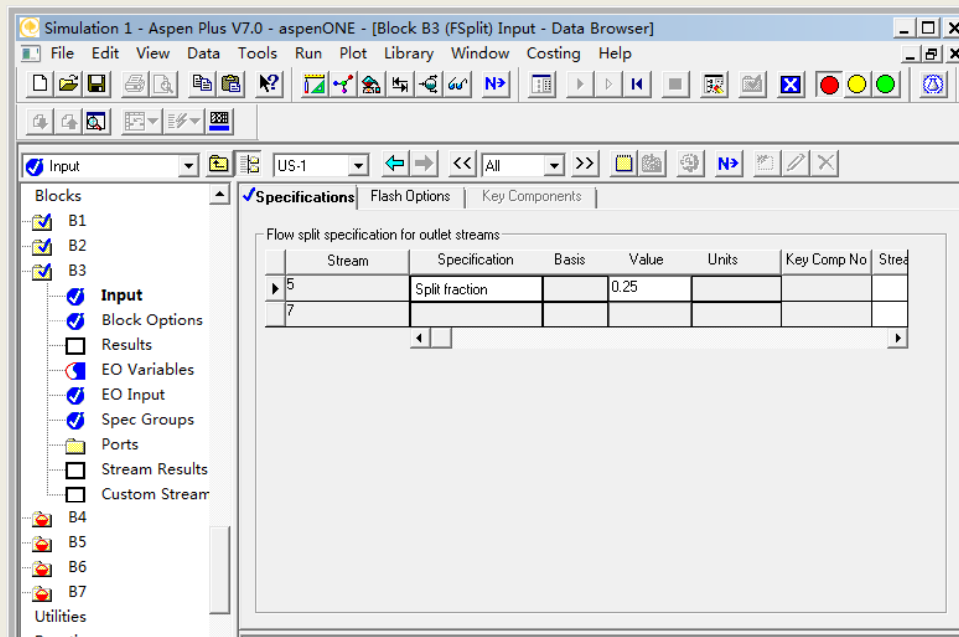
Outlet stream: 200

Substream: MIXED

Component ID	Specification	Basis	Value	Units
HYDRO-01	Split fraction		1	
METHA-01	Split fraction		1	
BENZE-01	Split fraction			
TOLUE-01	Split fraction			
DIPHE-01	Split fraction			

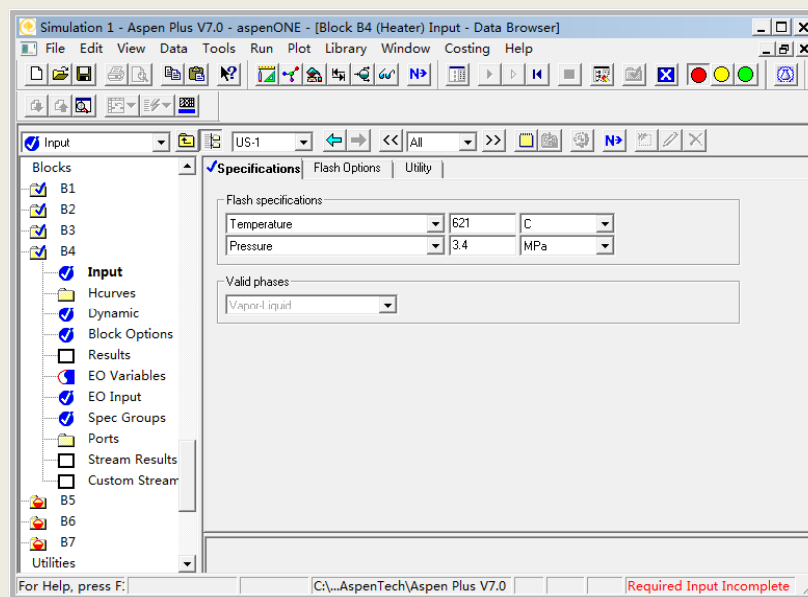
设置分离器B3参数

设置放空空气与循环气的比例为1:4，如图：



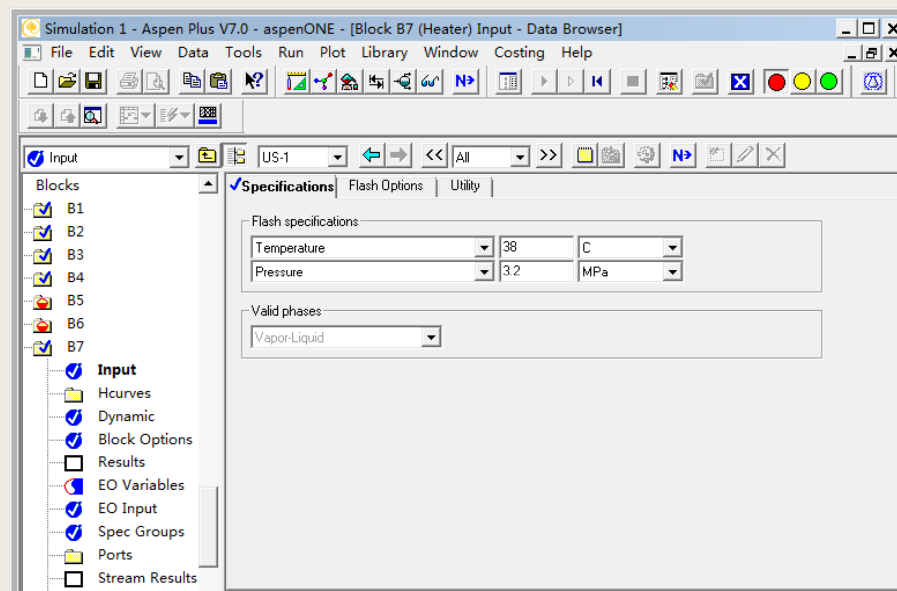
设置换热器B4参数

✘ 设置换热器的操作温度与操作压力，如图：



设置换热器B7参数

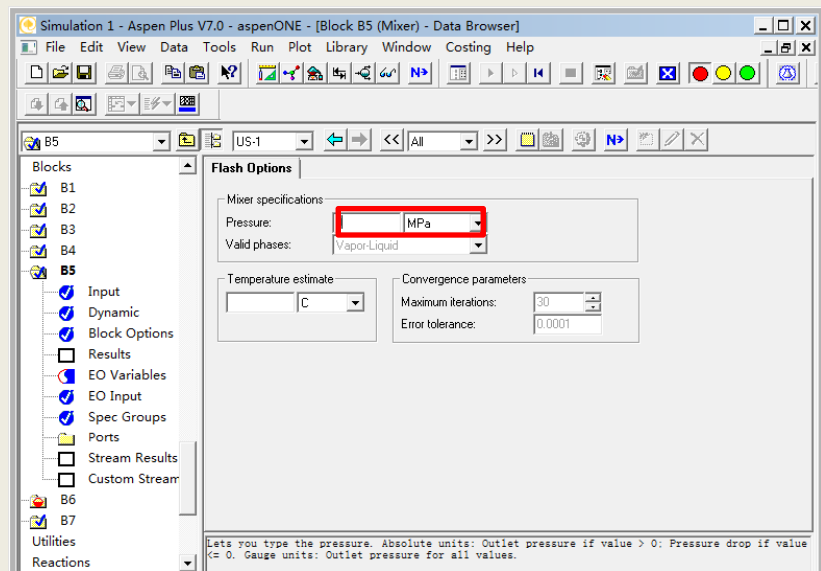
※ 设置换热器的操作温度与操作压力，如图：



查看混合器B5的操作参数

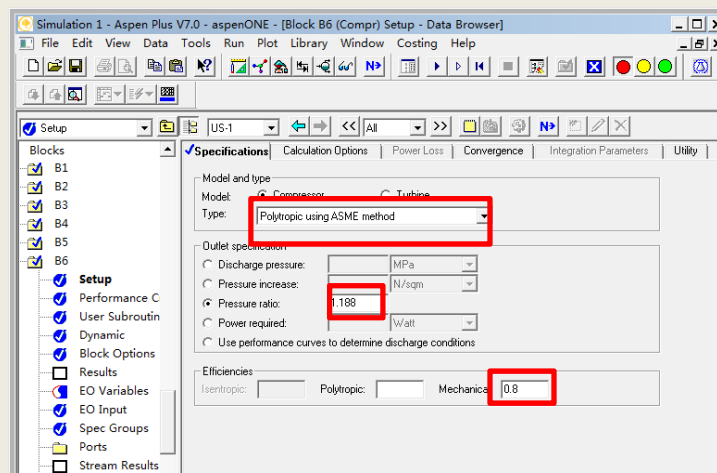


混合器B5是绝热操作，如图：



设置压缩机B6参数

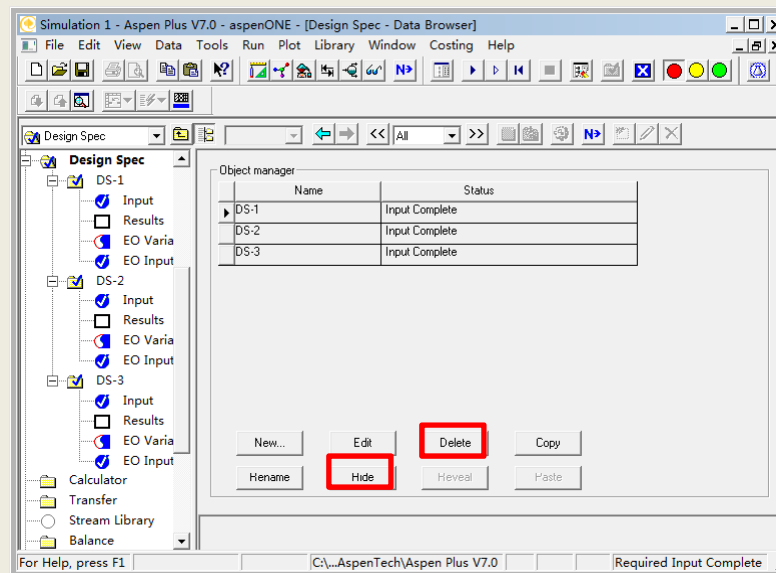
压缩机B6的模型为压缩机，类型为**多变压缩**，**压缩比**为**1.188**，**机械效率**为**0.8**，如图：



去除设计规定，加入约束（1）

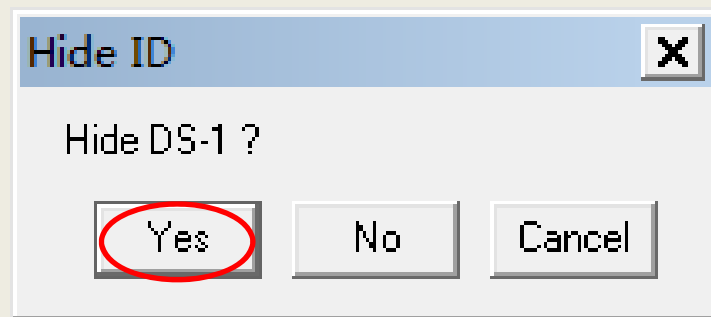


点击**Hide**隐藏所选的规定，**Delete**为删除所选的规定，如图：



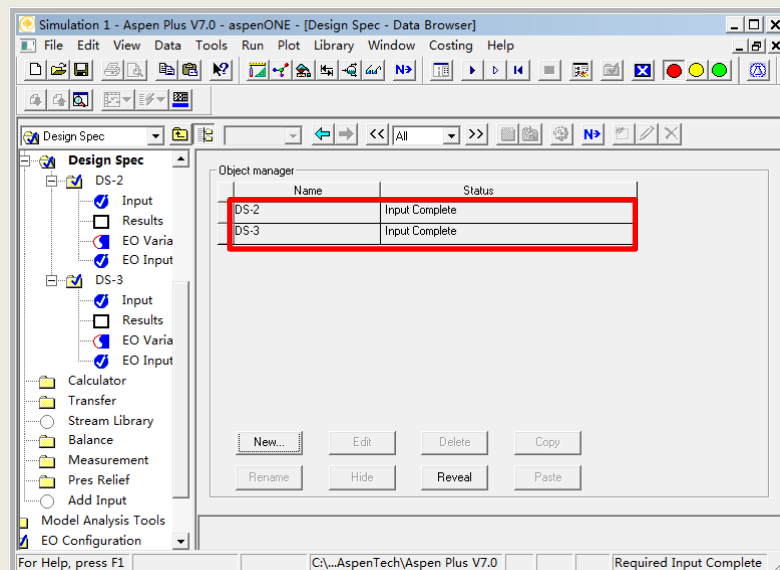
去除设计规定，加入约束（2）

选中上图DS-1，点击Hide，出现c下图对话框，如图：



去除设计规定，加入约束（3）

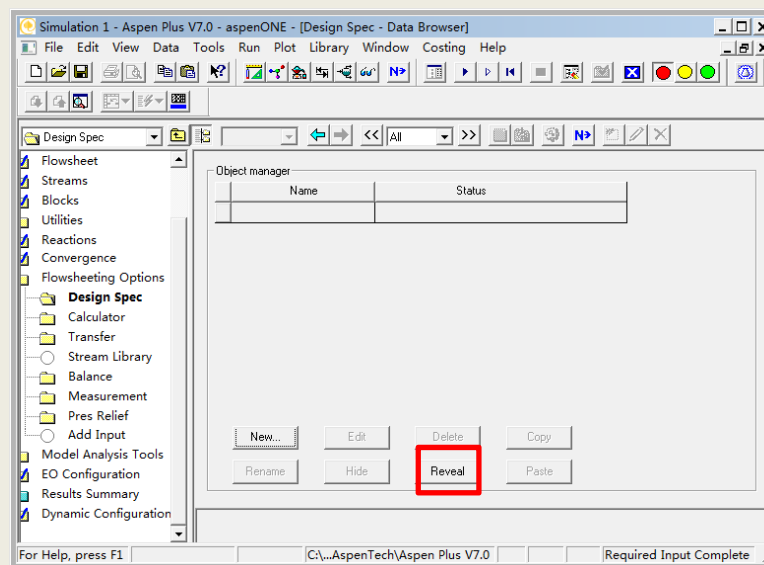
※ DS-1已被删除，如图：



去除设计规定，加入约束（4）

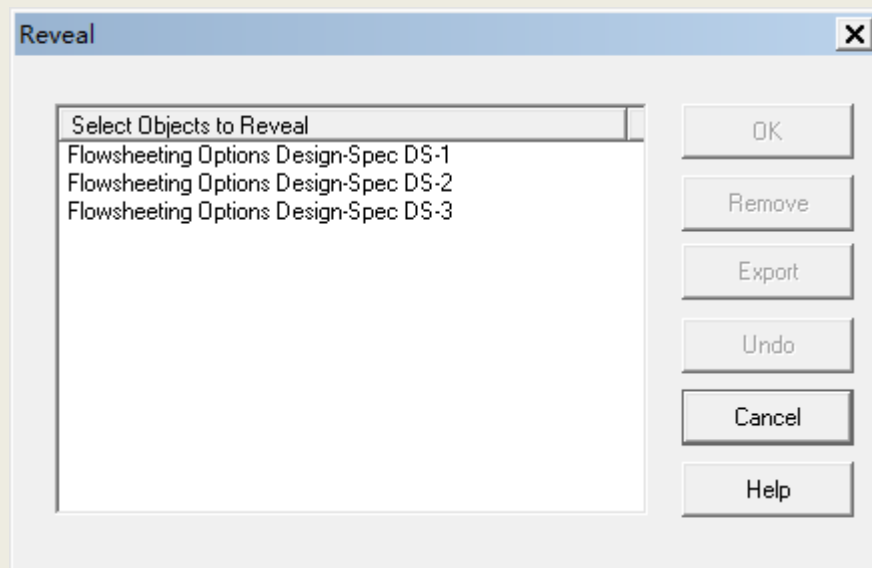


同理DS-2、DS-3也被删除，删除完成后如图：



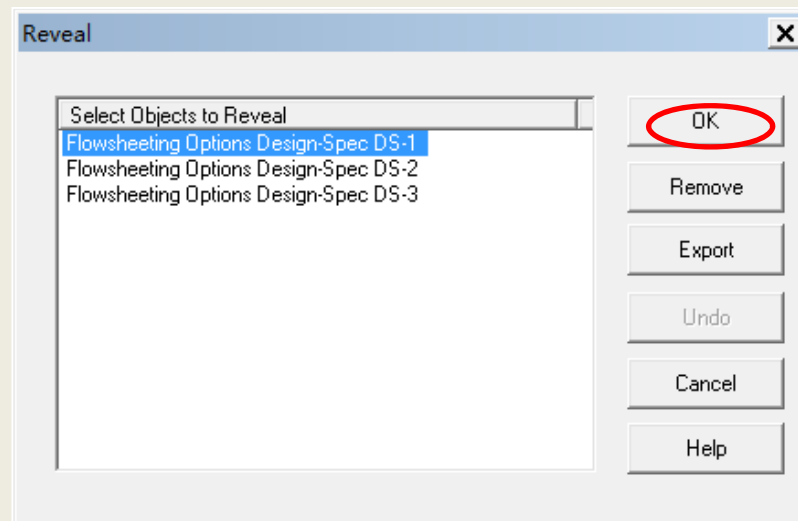
恢复设计规定 (1)

◀ 点击上图 **Reveal**，出现下图对话框，如图：



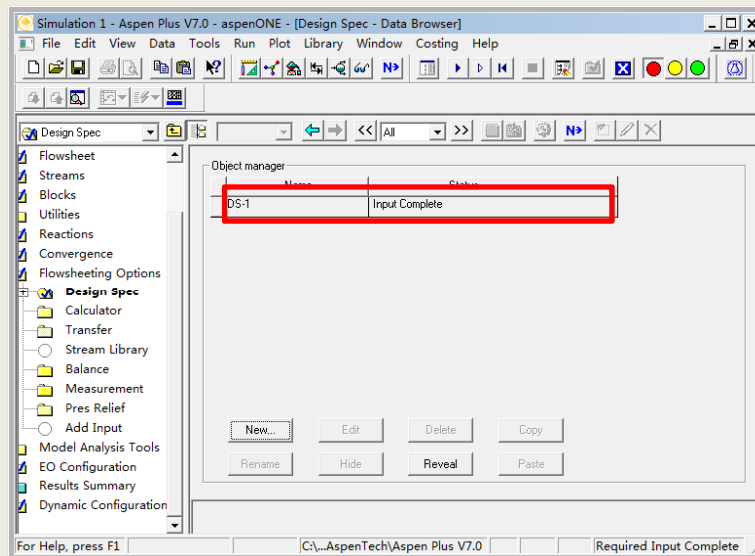
恢复设计规定 (2)

※ 选中 **DS-1** 并点击 **OK**，如图：



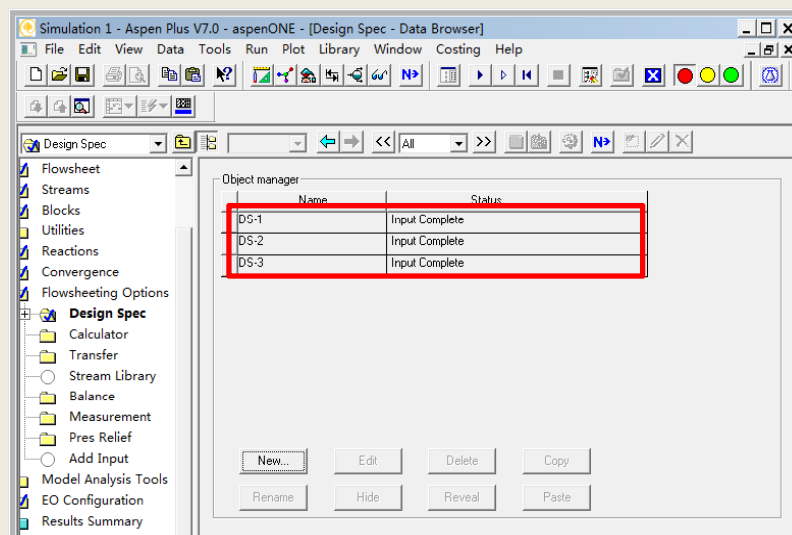
恢复设计规定 (3)

DS-1恢复完成，如图：



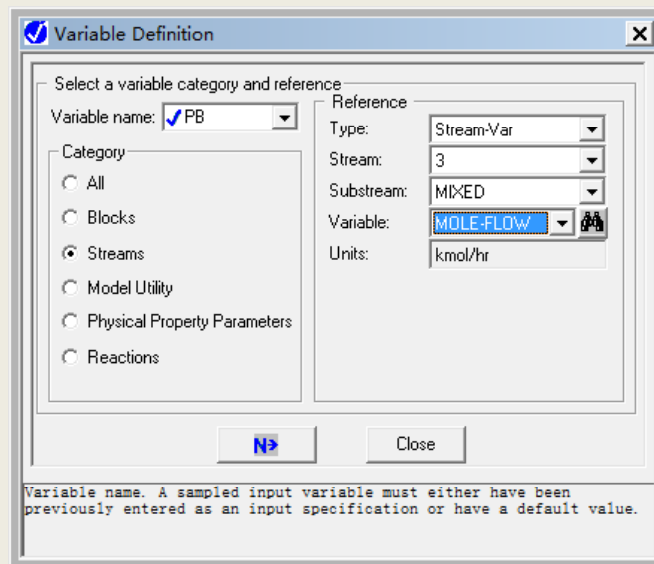
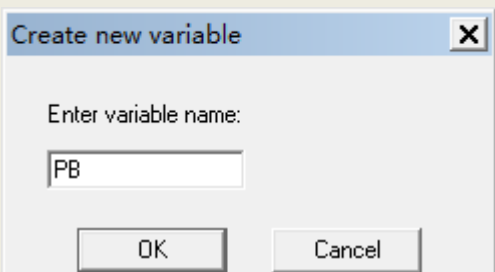
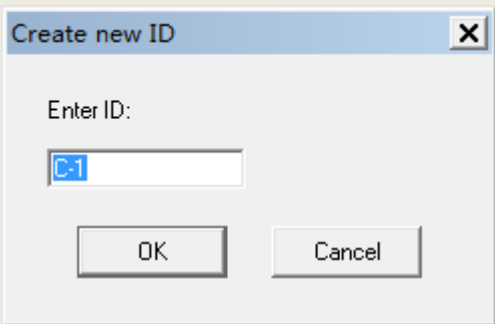
恢复设计规定 (4)

DS-1, DS-2, DS-3均恢复完成, 如图:

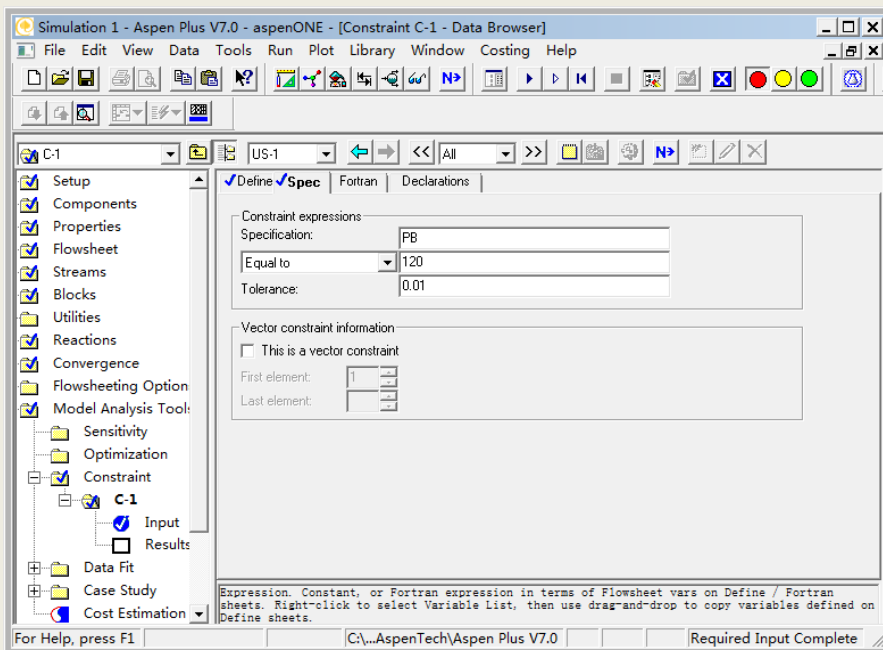


加入约束 (1)

※ 约束C-1, 如图:

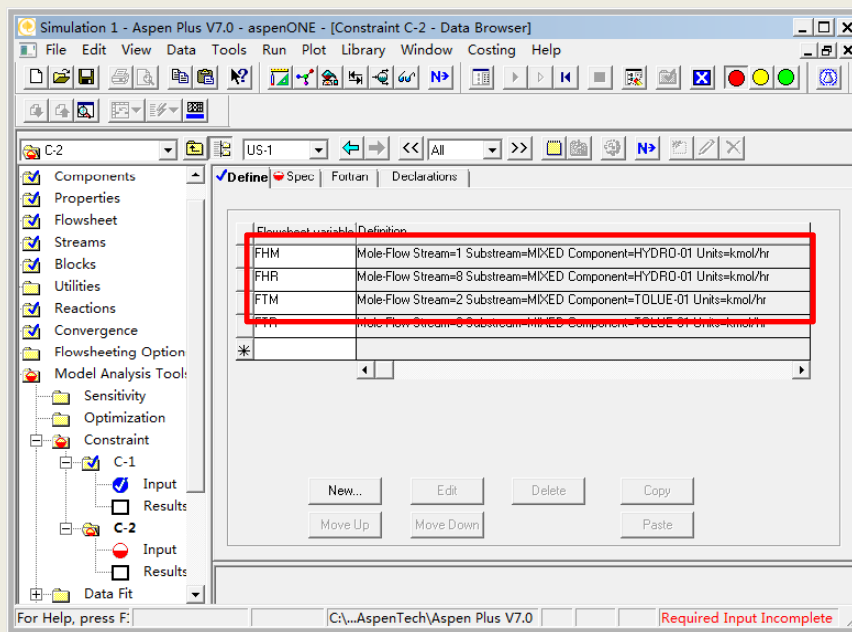
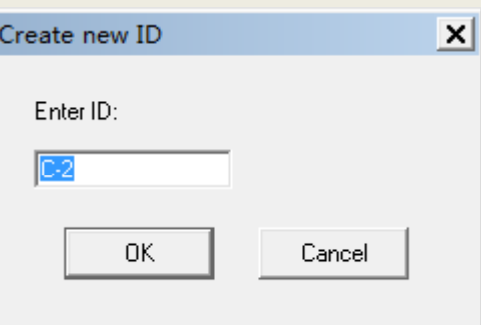


加入约束 (2)



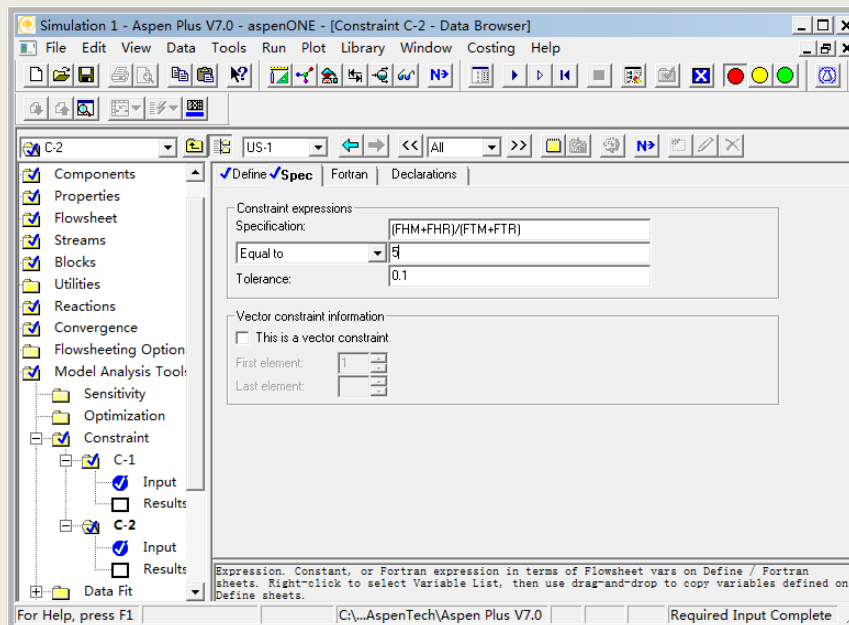
加入约束 (3)

约束C-2, 如图:



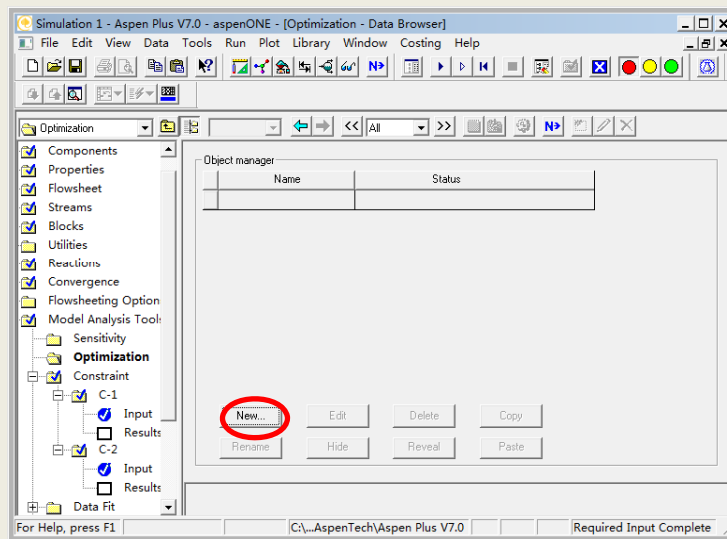
加入约束 (4)

输入约束规定，如图：



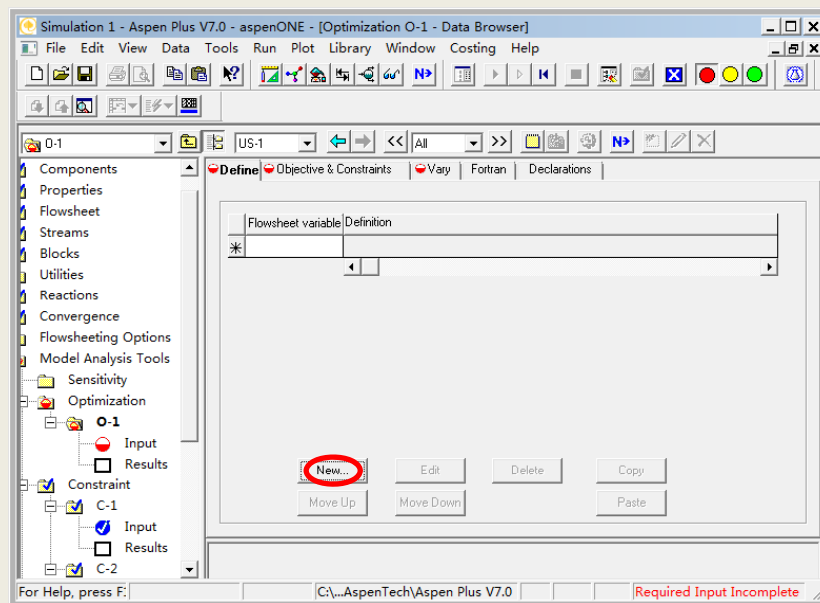
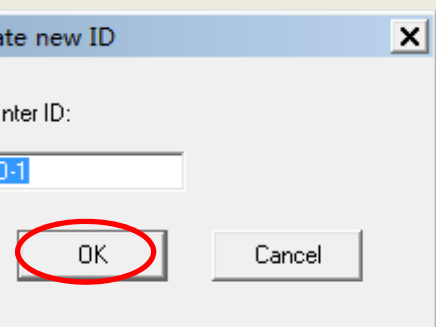
添加优化模块 (1)

点击**Data Browser**的**Model Analysis Tools/Optimization**出现下图窗口，如图：



添加优化模块 (2)

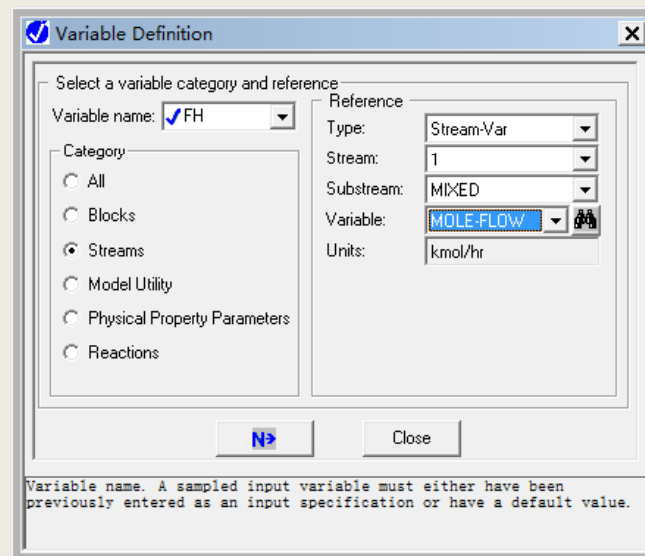
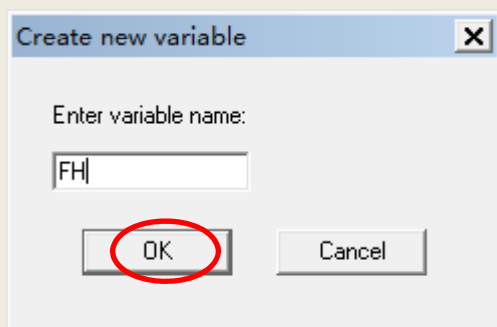
单击上图**NEW**，定义**O-1**优化模块，如图：



添加优化模块 (3)

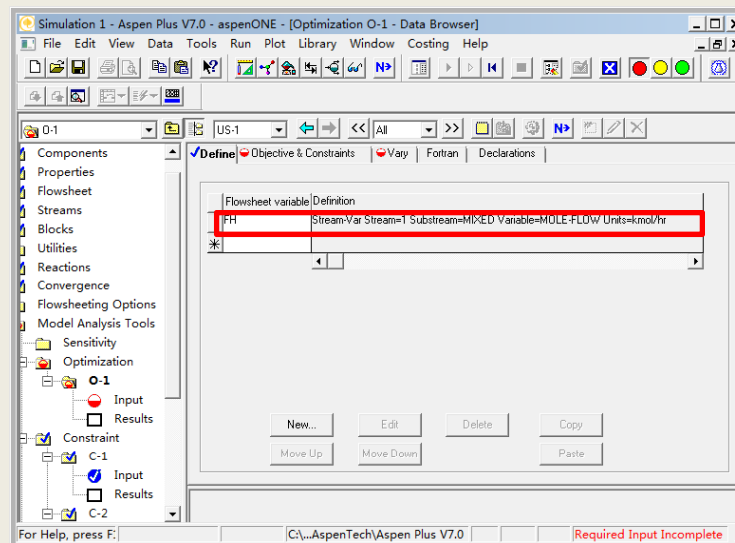


点击上图**NEW**，定义**FH**（进料氢气流量）变量，如图：



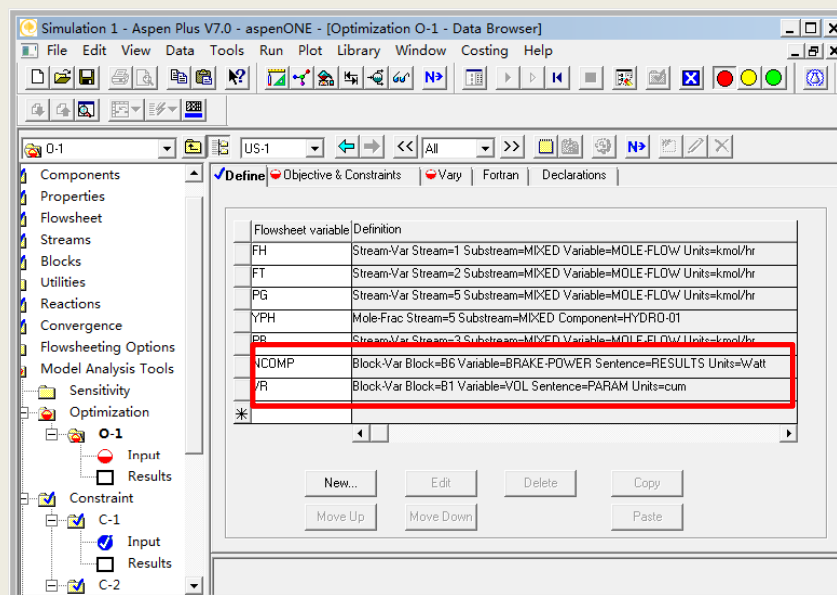
添加优化模块（4）

FH变量定义完成后，如图：



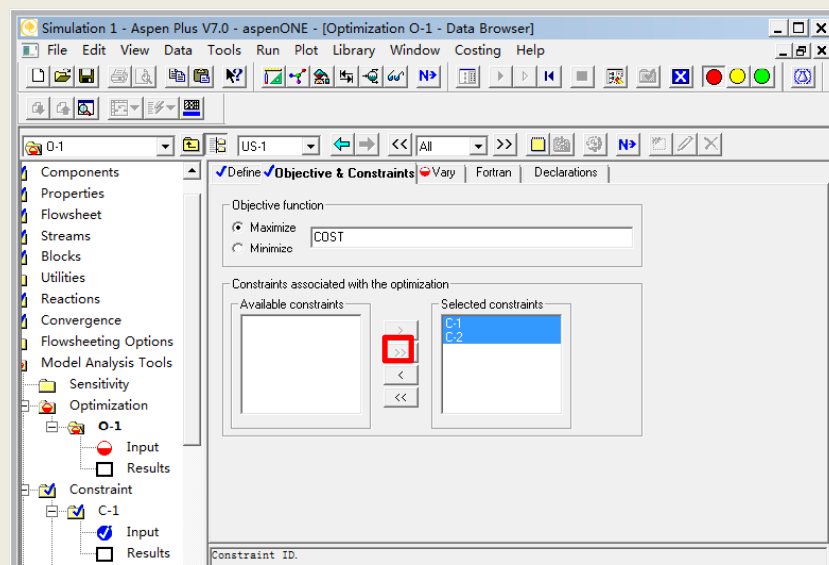
添加优化模块 (5)

同理定义其他变量，**FT**（进料甲苯流量）、**PG**（放空气流量）、**YPH**（放空气中氢含量）、**PB**（产品苯流量）、**PD**（副产物联苯流量）、**NCOMP**代表压缩机**B6**的轴功率、**VR**代表反应器**B1**的体积，变量定义完成后，如图：



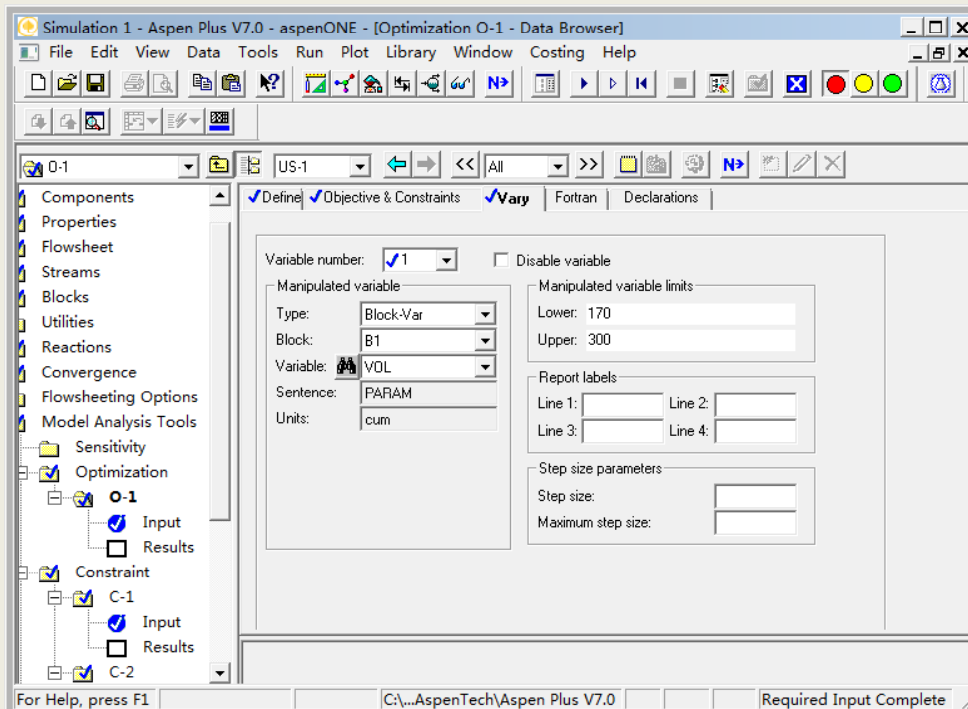
添加优化模块 (6)

※ 指定优化目标与约束，如图：



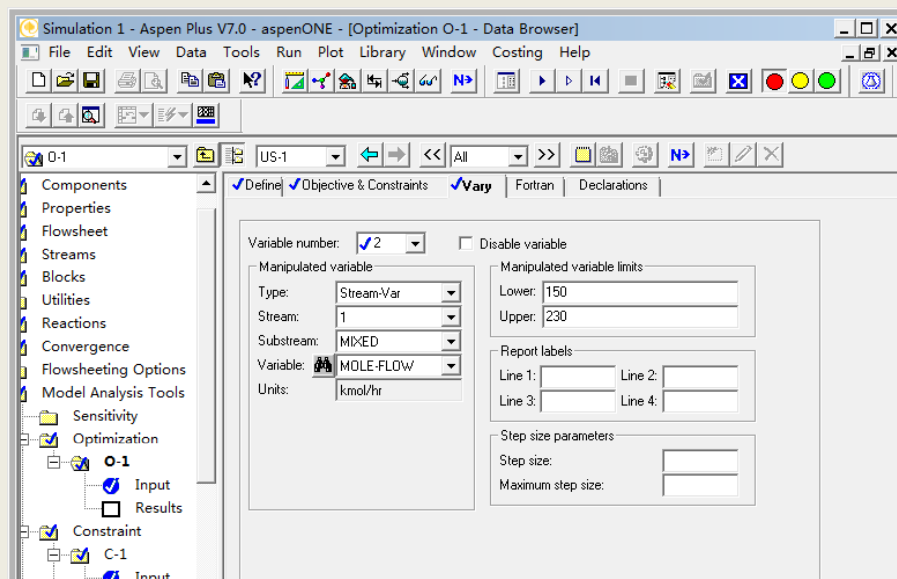
添加优化模块（7）

在0-0.1的范围内调节反应器B1中副反应的转化率，如图：



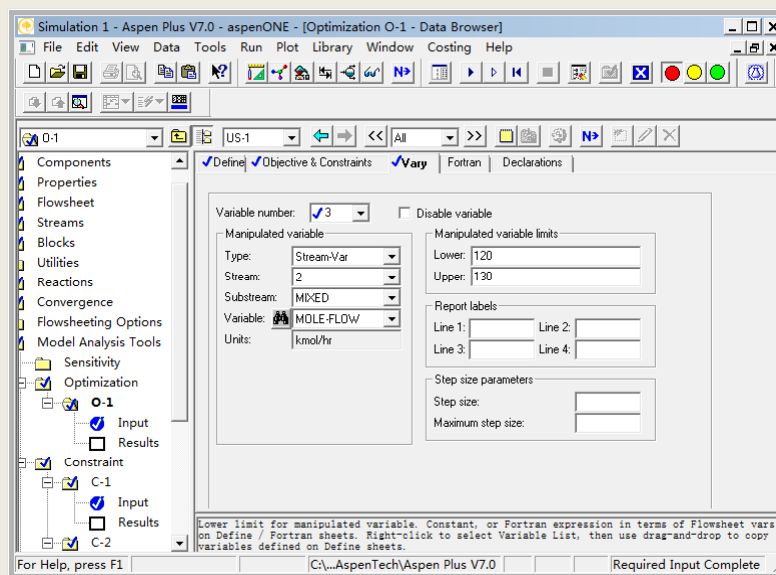
添加优化模块（8）

※ 在100-200kmol/h的范围内调节氢气进料流量的，如图：



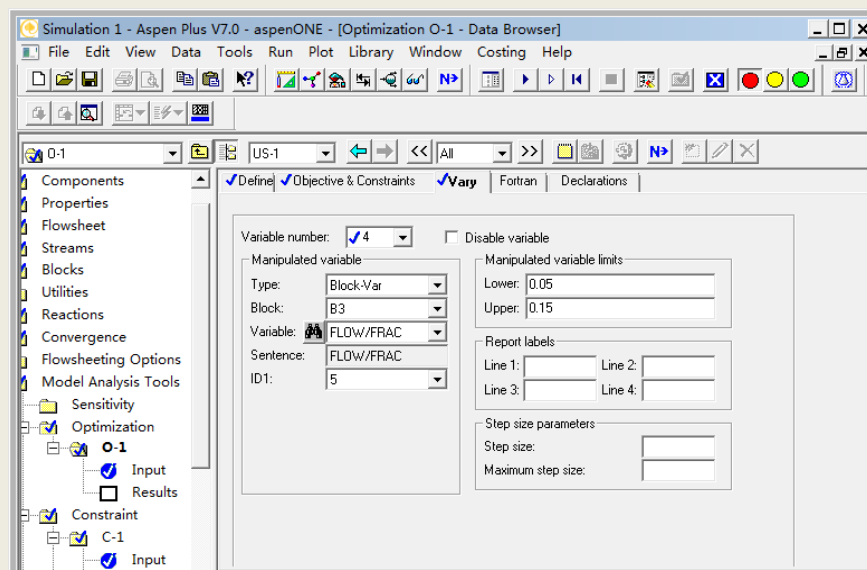
添加优化模块 (9)

※ 在100-200kmol/h的范围内调节甲苯进料流量的，如图：



添加优化模块（10）

✘ 在0.05-0.15的范围内调节分割器B3中物流5的流出比例，如图：



运行模拟

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Control Panel]

File Edit View Data Tools Run Library Window Costing Help

Solve

Calculation Sequen

- \$OLVER01
 - B4
 - B1
 - B7
 - B2
 - B3
 - B6
 - B5

** ERROR
Convergence block \$OLVER01 did not converge normally in the final pass

->Generating block results ...

Block: B4 Model: HEATER

->Simulation calculations completed ...

*** Summary of Errors ***

	Physical Property	System	Simulation
Terminal Errors	0	0	0
Severe Errors	0	0	21
Errors	0	0	292
Warnings	0	0	261

More

All blocks have been executed

Simulation run c C:\...AspenTech\Aspen Plus V7.0 Results Available with Errors

查看模拟结果 (1)



在**Data Browser**中的**Convergence**查看优化计算结果，
如图：

Simulation 1 - Aspen Plus V7.0 - aspenONE - [Convergence Convergence \$OLVER02 (SQP) Results - Data Browser]

File Edit View Data Tools Run Plot Library Window Costing Help

Results

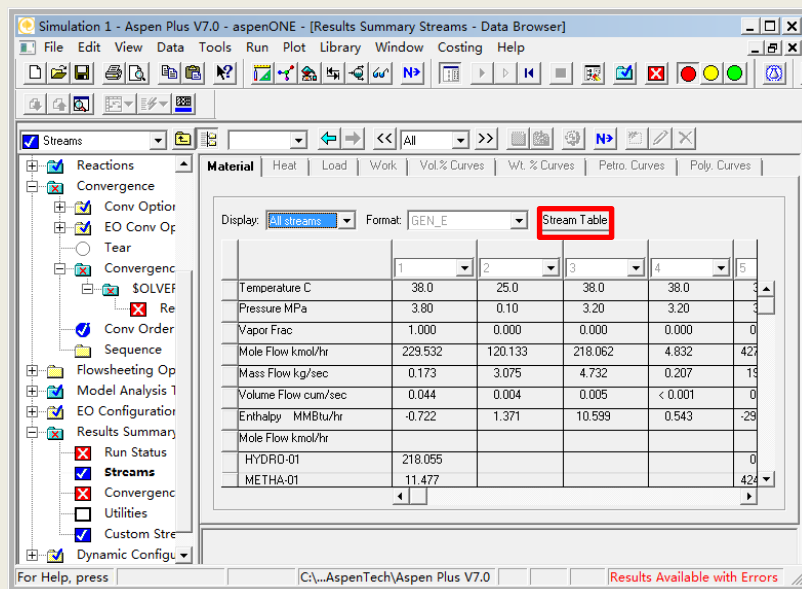
Summary | Manipulated Variables | Constraints | Tear Variables | **Iterations**

Iteration history

Iteration	OBJECTIVE FUNCTION	KUHN-TUCKER ERROR	CMAX	LAGRANGIAN FUNCTION	CONSTRAINT 1	CONSTRAINT 2	VARY 1
1	0	0.84421857	6930.91693		69.3091693	-3.3651103	176.305127
2	0	0.11041066	9848.94993	0.07358025	98.4894993	-3.1994997	183.577692
3	0	0.01579726	7534.00935	0.07189379	75.3400935	-3.1849234	183.98133
4	0	0.00150477	9806.15213	0.01602297	98.0615213	-3.1847747	183.979744
5	0	0.00150477	9806.15213	0.00127754	98.0615213	-3.1847747	183.979744

查看模拟结果 (2)

※ 查看全部物流结果，如图：



The screenshot shows the Aspen Plus V7.0 Results Summary Streams - Data Browser window. The 'Streams' section is selected in the left-hand tree. The 'Material' tab is active, and the 'Stream Table' is displayed. The table shows data for five streams (1-5) across various properties. The 'Stream Table' label is highlighted with a red box.

	1	2	3	4	5
Temperature C	38.0	25.0	38.0	38.0	38.0
Pressure MPa	3.80	0.10	3.20	3.20	3.20
Vapor Frac	1.000	0.000	0.000	0.000	0.000
Mole Flow kmol/hr	229.532	120.133	218.062	4.832	422.000
Mass Flow kg/sec	0.173	3.075	4.732	0.207	15.000
Volume Flow cum/sec	0.044	0.004	0.005	< 0.001	0.000
Enthalpy MMBtu/hr	-0.722	1.371	10.599	0.543	-29.000
Mole Flow kmol/hr					
HYDRO-01	218.055				0.000
METHA-01	11.477				422.000

查看模拟结果 (3)



点击上图 **Stream table** 生成如下表格，如图：

Heat and Material Balance Table														
Stream ID	1	2	3	4	5	6	7	8	100	200	300	400	500	
Temperature	C	38.0	25.0	38.0	38.0	38.0		38.0	52.2	621.0	38.0	32.1	621.0	38.0
Pressure	MPa	3.80	0.10	3.20	3.20	3.20		3.20	3.80	3.40	3.20	0.10	3.40	3.20
Vapor Frac		1.000	0.000	0.000	0.000	0.996		0.996	1.000	1.000	0.996	1.000	1.000	0.991
Mole Flow	kmol/hr	229.532	120.133	218.062	4.832	4278.682	0.000	24384.405	24384.405	28885.980	28663.087	28881.146	28881.146	28885.980
Mass Flow	kg/sec	0.173	3.073	4.732	0.207	19.769	0.000	112.663	112.663	137.370	132.432	132.554	132.554	137.370
Volume Flow	cm ³ /sec	0.044	0.004	0.005	< 0.001	0.915	0.000	5.212	4.604	17.745	6.127	199.078	17.741	6.140
Enthalpy	MMBtu/hr	-0.722	1.371	10.599	0.543	-298.995		-1703.987	-1689.986	-1176.094	-2002.982	-2008.950	-1134.897	-1989.289
Mole Flow	kmol/hr													
HYDRO-01		218.055				0.002		0.013	0.013	0.015	0.015	218.074	218.074	0.015
METHA-01		11.477				4245.491		24195.248	24195.248	28440.739	28440.739	28440.739	28440.739	28440.739
BENZE-01				218.062						218.062				218.062
TOLUE-01			120.133			33.189		189.144	189.144	222.333	222.333	222.333	222.333	222.333
DIPHE-01					4.832					4.832				4.832

结束

