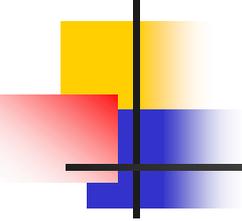


反应器单元的仿真设计

Simulation Design (二) *of Chemical Reactors*

化学动力学类反应器



化学动力学反应器

根据流动状况不同，有三种：

1、全混釜反应器 (RCSTR)

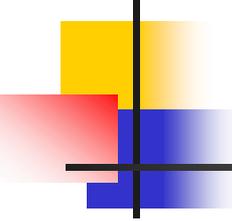
Continuous Stirred Tank Reactor

2、平推流反应器 (RPlug)

Plug Flow Reactor

3、间歇釜反应器 (RBatch)

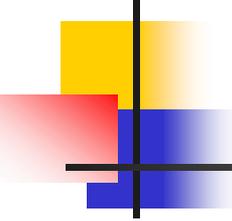
Batch Stirred Tank Reactor



一、*RCSTR*—全混釜反应器

性质：

釜内达到理想混合，即反应物料和出口物流有相同的组成和性质。
可模拟单、两、三相的体系，可同时处理动力学控制和平衡控制两类反应以及包含固体的反应。



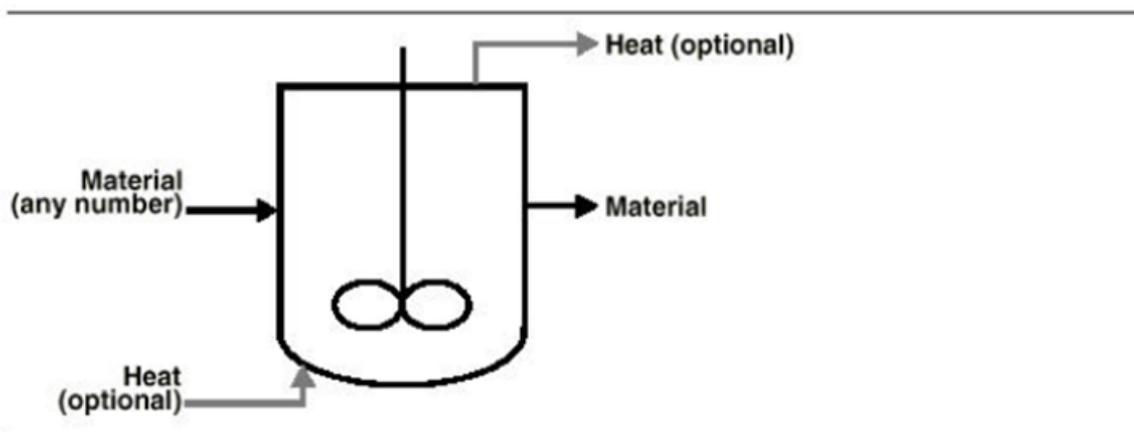
一、*RCSTR*—全混釜反应器

用途：

已知化学反应式、动力学方程和平衡关系，计算所需的反应器体积和反应时间，以及反应器热负荷。

一、RCSTR—全混釜反应器

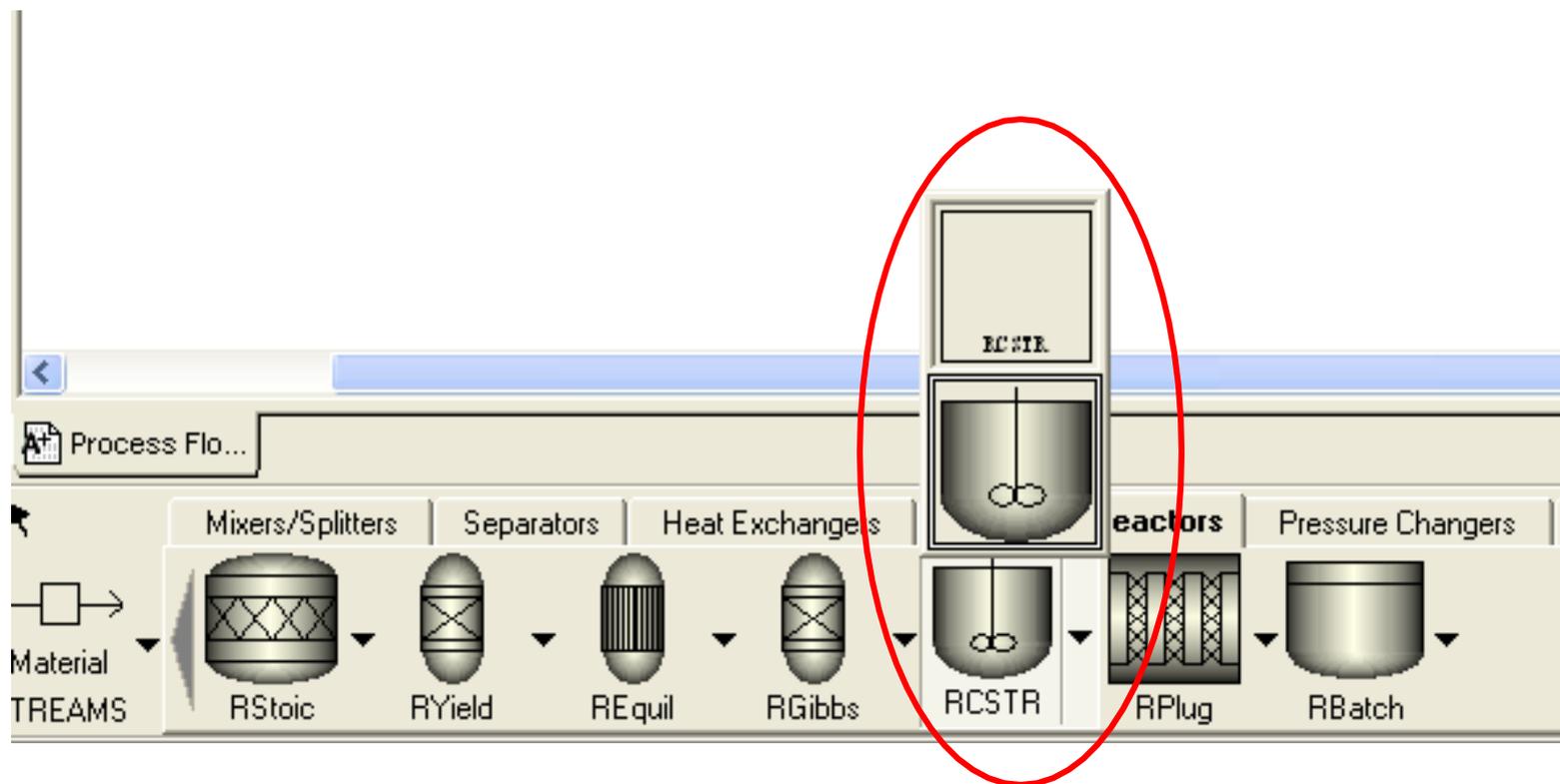
RCSTR 的流程连接

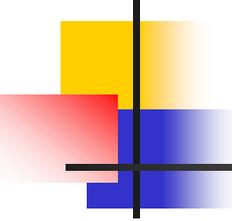


物料流

入口 至少一个物料流
出口 一个物料流

一、*RCSTR*—全混釜反应器





一、RCSTR—全混釜反应器

RCSTR有两组模型参数：

- 1、操作条件 (Operation Conditions)
 - 1) 压力 (Pressure)
 - 2) 温度/热负荷 (Temperature/Heat Duty)
- 2、持料状态 (Holdup)
 - 1) 有效相态 (Valid Phases)
 - 2) 设定方式 (Specification Type)

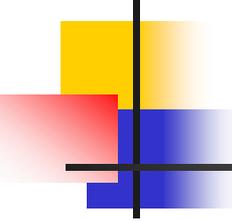
一、RCSTR—全混釜反应器

The screenshot displays the Aspen Plus software interface for configuring a Reactor (RCSTR). The left sidebar shows a tree view with 'Setup' and 'Blocks' expanded. The 'Setup' folder contains 'Setup', 'Components', 'Properties', 'Flowsheet', 'Streams', and 'Utilities'. The 'Blocks' folder contains 'B1', which is further expanded to show 'Setup', 'Convergence', 'User Subroutine', 'Dynamic', 'Block Options', 'Results', 'EO Variables', 'EO Input', 'Spec Groups', and 'Ports'. The main window shows the 'Specifications' tab for the reactor. The 'Operating conditions' section is highlighted with a red circle and labeled '操作条件' (Operating Conditions). It includes 'Pressure' set to 1 bar and 'Temperature' set to 35 C. The 'Holdup' section is also highlighted with a red circle and labeled '持料状态' (Holdup State). It includes 'Valid phases' set to Vapor-Liquid, 'Specification type' set to Reactor volume & Phase volume fraction, 'Reactor Volume' set to 5 cum, 'Reactor Residence time' set to hr, 'Phase' set to Condensed phase, 'Phase Volume' set to 3 cum, and 'Phase Volume fraction' set to 0.6.

操作条件

持料状态

Parameter	Value	Unit
Pressure	1	bar
Temperature	35	C
Valid phases	Vapor-Liquid	
Specification type	Reactor volume & Phase volume fraction	
Reactor Volume	5	cum
Reactor Residence time		hr
Phase	Condensed phase	
Phase Volume	3	cum
Phase Volume fraction	0.6	
Residence time		hr



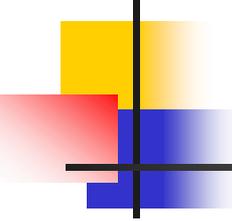
一、*RCSTR*—全混釜反应器

持料状态中的设定方式有7种：

1) 反应器体积 (Reactor Volume)

2) 停留时间 (Residence Time)

只需输入物料在反应器中的平均停留时间。

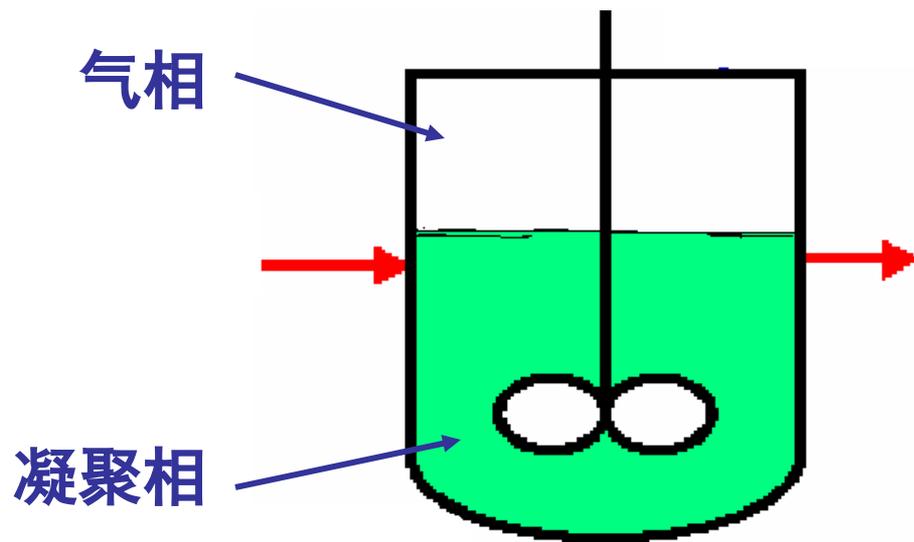


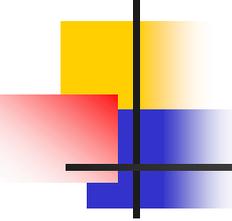
一、*RCSTR*—全混釜反应器

3) 反应器体积和相体积 (Reactor Volume & Phase Volume)

必须输入反应器体积、气相 (Vapor phase) 或凝聚相 (Condensed phase) 所占的体积。

一、*RCSTR*—全混釜反应器



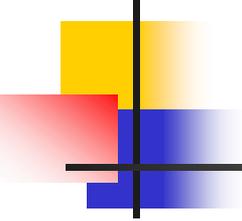


一、*RCSTR*—全混釜反应器

4) 反应器体积和相体积分率

(Reactor Volume & Phase Volume Fraction)

必须输入反应器体积和气相/凝聚相所占的体积分率 (Volume frac)。

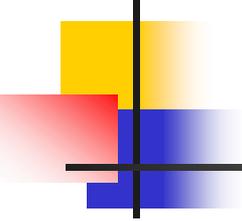


一、*RCSTR*—全混釜反应器

5) 反应器体积和相停留时间

(Reactor Volume & Phase Residence Time)

必须输入反应器体积和气相/凝聚相在反应器中的停留时间。

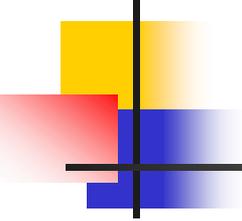


一、*RCSTR*—全混釜反应器

6) 停留时间和相体积分率

(Residence Time & Phase Volume Fraction)

必须输入物料在反应器中的总平均停留时间和气相/凝聚相所占的体积分率。



一、*RCSTR*—全混釜反应器

7) 相停留时间和体积分率

(Phase Residence Time & Volume Fraction)

必须输入气相/凝聚相在反应器中的停留时间和所占的体积分率。

一、RCSTR—全混釜反应器

The screenshot displays the Aspen Plus software interface for configuring a reactor. The left sidebar shows a tree view with 'Setup' selected. The main window is divided into tabs: 'Specifications', 'Streams', 'Reactions', 'PSD', 'Component Attr.', 'Utility', and 'Ca'. The 'Specifications' tab is active, showing 'Operating conditions' (Pressure: 1 bar, Temperature: 35 C) and 'Holdup' settings (Valid phases: Vapor-Liquid, Specification type: Reactor volume). A red circle highlights the 'Specification type' dropdown menu, which lists seven options: Reactor volume, Residence time, Reactor volume & Phase volume, Reactor volume & Phase volume fraction, Reactor volume & Phase residence time, Residence time & Phase volume fraction, and Phase residence time & volume fraction. A red arrow points from the text '7种设定方式' (7 setting methods) at the bottom to the dropdown menu.

7种设定方式

一、RCSTR—全混釜反应器

- Setup
- Components
- Properties
- Flowsheet
- Streams
- Utilities
- Blocks
 - B1
 - Setup
 - Convergence
 - User Subroutine
 - Dynamic
 - Block Options
 - Results
 - EO Variables
 - EO Input

Specifications

Operating conditions

Pressure: 1 bar

Temperature: 35 C

Holdup

Valid phases: Vapor-Liquid

Specification type: Reactor volume & Phase volume

Reactor

Volume: 5 cum

Resi. time: hr

Phase

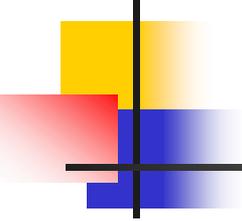
Phase: Condensed phase

Volume: 3 cum

Volume frac: 0.6

Residence time: hr

凝聚相

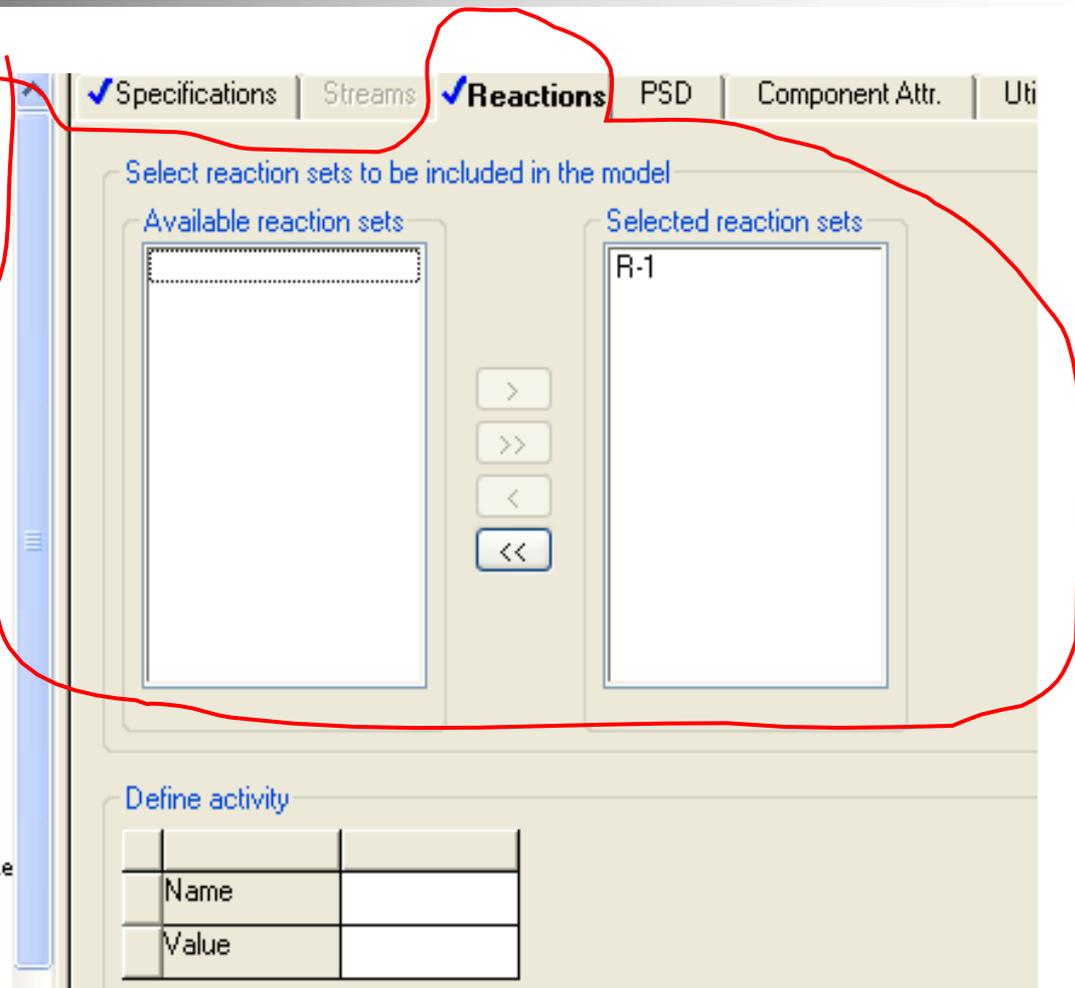
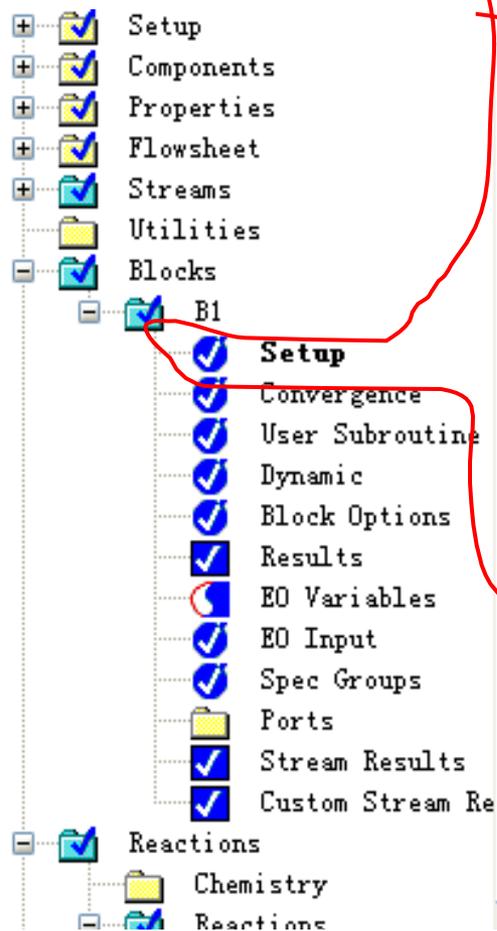


一、*RCSTR*—全混釜反应器

化学反应式的设定：

*RCSTR*中的化学反应通过选用预定义的化学反应对象来设定。

一、RCSTR—全混釜反应器



一、RCSTR—全混釜反应器

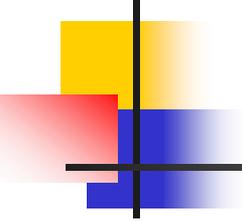
设置化学反应对象：

The screenshot shows a software interface for configuring a reactor model. On the left is a tree view with the following structure:

- Utilities
 - Blocks
 - B1
 - Setup
 - Convergence
 - User Subroutine
 - Dynamic
 - Block Options
 - Results
 - EO Variables
 - EO Input
 - Spec Groups
 - Ports
 - Stream Results
 - Custom Stream Re
- Reactions
 - Chemistry
 - Reactions
 - R-1
 - Input
 - Results

A red circle highlights the 'Reactions' folder and its sub-items in the tree view. A red line connects this circle to a table in the main window. The main window has tabs for 'Stoichiometry', 'Kinetic', 'Equilibrium', and 'Activity'. The 'Stoichiometry' tab is active, and it contains the following table:

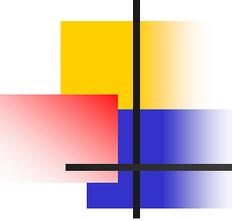
Rxn No.	Reaction type	Stoichiometry
1	Kinetic	$4 \text{ NH}_3 + 6 \text{ CH}_2\text{O} \rightarrow \text{C}_6\text{H}_{12}\text{N}_4 + 6 \text{ H}_2\text{O}$



一、*RCSTR*—全混釜反应器

设置化学反应对象目的：

为三类动力学反应器模块和 *RadFrac* 模块提供反应的计量关系、平衡关系和动力学关系。



一、RCSTR—全混釜反应器

创建化学反应对象时，需赋予对象 *ID* 和选择对象类型。对于小分子反应，常用的类型有三种：

1、LHHW 型

(Langmuir-Hinshelwood-Hougen-Watson)

2、幂律型 (Power Law)

3、反应精馏型 (Reac-Dist)

一、RCSTR—全混釜反应器

The screenshot displays a software interface for configuring a reactor. On the left, a tree view shows the 'Reactions' folder selected. In the center, the 'Object manager' table lists the reactor configuration:

Name	Type	Status
R-1	POWERLAW	Results Available

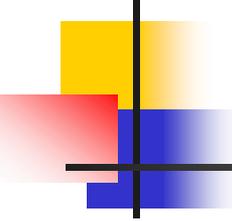
A 'Create new ID' dialog box is open, showing the following fields:

- Enter ID: R-2
- Select type: POWERLAW (selected from a dropdown menu)

The dropdown menu lists the following reaction types: EMULSION, FREE-RAD, GENERAL, IONIC, LHHW, POWERLAW, REAC-DIST, SEGMENT-BAS, STEP-GROWTH, USER, USERACM, and ZIEGLER-NAT. The 'POWERLAW' type is circled in red.

Red annotations include:

- An arrow pointing to the 'POWERLAW' type in the 'Object manager' table with the text '选择动力学类型' (Select kinetic type).
- An arrow pointing to the 'POWERLAW' type in the dropdown menu with the text '常用的动力学类型' (Common kinetic type).
- A red circle around the 'Reactions' folder in the tree view.



一、*RCSTR*—全混釜反应器

每个化学反应对象可以包含多个化学反应，每个化学反应都要设置计量学参数和动力学参数

一、RCSTR—全混釜反应器

Convergence
User Subroutine
Dynamic
Block Options
Results
EO Variables
EO Input
Spec Groups
Ports
Stream Results
Custom Stream Result
Model Summary

Utilities
Reactions
Chemistry
Reactions
R-1
Input
Results
EO Variables

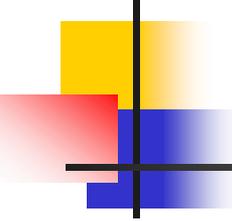
METCBAR

Stoichiometry Kinetic Equilibrium Activity

Rxn No.	Reaction type	Stoichiometry
1	Kinetic	$4 \text{ NH}_3 + 6 \text{ CH}_2\text{O} \rightarrow 6 \text{ H}_2\text{O} + \text{C}_6\text{H}_{12}\text{N}_4$
2	Kinetic	$4 \text{ NH}_3 + 6 \text{ CH}_2\text{O} \rightarrow \text{C}_6\text{H}_{12}\text{N}_4$

每个化学反应
都需输入及联
系数和动力学
参数

一个反应对象
下可有多
个化学反
应



一、*RCSTR*—全混釜反应器

在化学反应计量表单中，为每一个化学反应创建一个对象，并选择对象为动力学（**kinetic**）或平衡（**Equilibrium**）型。输入化学反应计量系数(**Coefficient**)，对于幂律型反应对象，还要输入方程式中浓度因子的级数。

一、RCSTR—全混釜反应器

Reaction configuration details:

Rxn No.	Reaction type	Stoichiometry
1	Equilibrium	4 NH ₃ + 6 CH ₂ O <-> 6 H ₂ O + C ₆ H ₁₂ N ₄

Edit Reaction dialog box details:

Reaction No.: 1

Reaction type: Equilibrium

Reactants:

Component	Coefficient	Exponent
NH ₃	-4	
CH ₂ O	-6	
*		

Products:

Component	Coefficient	Exponent
H ₂ O	6	
C ₆ H ₁₂ N ₄	1	
*		

一、RCSTR—全混釜反应器

输入动力学参数：活化能和频率因子

Stoichiometry Kinetic Equilibrium Activity

1) 4 NH₃ + 6 CH₂O -> 6 H₂O + C₆H₁₂N₄

Reacting phase: Liquid Rate basis: Reac (vol)

Power Law kinetic expression

If To is specified: Kinetic factor= $k(T/T_o)^n e^{-E/R}[1/T-1/T_o]$

If To is not specified: Kinetic factor= $kT^n e^{-E/RT}$

k: 1420

n: 0

E: 25700000 J/kmol

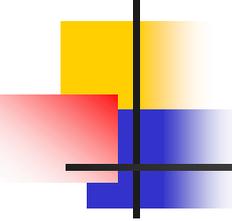
To: C

[C_i] basis: Molarity

Edit reactions

Solids

浓度基准



一、*RCSTR*—全混釜反应器

反应物浓度基准:

摩尔浓度

质量摩尔浓度

分压

质量浓度

活度（摩尔）

逸度

一、RCSTR—全混釜反应器

✓ Stoichiometry ✓ **Kinetic** Equilibrium Activity

1) 4 NH₃ + 6 CH₂O → 6 H₂O + C₆H₁₂N₄

Reacting phase: Liquid Rate basis: Reac (vol)

Power Law kinetic expression

If T₀ is specified: Kinetic factor = $k(T/T_0)^n e^{-(E/R)(1/T-1/T_0)}$

If T₀ is not specified: Kinetic factor = $kT^n e^{-E/RT}$

k: 1420

n: 0

E: 25700000 J/kmol

T₀: C

[C_i] basis: Molarity

- Molarity
- Molality
- Mole fraction
- Mass fraction
- Partial pressure
- Mass concentration
- Mole gamma
- Fugacity

Edit reactions

Solids

一、RCSTR—全混釜反应器

LHHW型的反应速率方程：

$$-r_A = \frac{[\text{动力学因子}] \cdot [\text{推动力表达式}]}{[\text{吸附表达式}]}$$

动力学因子仍用修正的Arrhenius方程表

示：

$$[\text{动力学因子}] = k \left(\frac{T}{T_0} \right)^n \exp \left[- \left(\frac{E}{R} \right) \left(\frac{1}{T} - \frac{1}{T_0} \right) \right]$$

一、RCSTR—全混釜反应器

LHHW型动力学方程:

Stoichiometry **Kinetic** Equilibrium Activity

1)

Reacting phase: Liquid Rate basis: Reac (vol)

LHHW kinetic expression

$$r = \frac{[\text{Kinetic factor}][\text{Driving force expression}]}{[\text{Adsorption expression}]}$$

Kinetic factor

If T_0 is specified: Kinetic factor = $k(T/T_0)^n e^{-(E/R)(1/T-1/T_0)}$

If T_0 is not specified: Kinetic factor = $kT^n e^{-E/RT}$

k:

n:

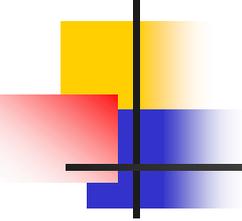
E: kcal/mol

T_0 : C

Solids

Driving Force

Adsorption



一、*RCSTR*—全混釜反应器

$$[\text{推动力表达式}] = K_1 \prod_i C_i^{p_i} - K_2 \prod_j C_j^{q_j}$$

$$\text{其中: } \ln K_1 = A_1 + \frac{B_1}{T} + C_1 \ln T + D_1 T$$

点击Driving force 弹出浓度推动力表单

一、RCSTR—全混釜反应器

Driving Force Expression

Reacting phase: Liquid

[Ci] basis: Molarity

Enter term: Term 1

Term 1

Concentration exponents for reactants:

Component	Exponent
NH3	
CH2O	

Concentration exponents for products:

Component	Exponent
C6H12N4	
H2O	

Coefficients for driving force constant:

A: B: C: D:

Let's you select the phase in which reaction occurs.

Activity

H2O

Rate basis: Reac (vol)

Solids

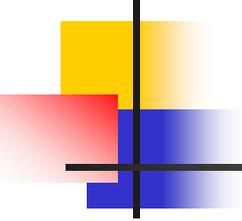
Driving Force

Adsorption

浓度推动力

浓度推动力常数K

第一项幂的乘积
(正反应浓度推动力)



一、RCSTR—全混釜反应器

$$[\text{吸附表达式}] = \left[\sum_i K_i \left(\prod_j C_j^{v_j} \right) \right]^m$$

$$\text{其中：} \quad \ln K_i = A_i + \frac{B_i}{T} + C_i \ln T + D_i T$$

点击Adsorption项，弹出吸附项
(Adsorption) 输入表单

一、RCSTR—全混釜反应器

Stoichiometry **Kinetic** Equilibrium Activity

1) 4 NH₃ + 6 CH₂O → C₆H₁₂N₄ + 6 H₂O

Reacting phase: Liquid Rate basis: Reac (vol)

LHHW kinetic expression
$$r = \frac{[\text{Kinetic factor}][\text{Driving force expression}]}{[\text{Adsorption expression}]}$$

Kinetic factor
If T₀ is specified: Kinetic factor = $k(T/T_0)^n e^{-(E/R)(1/T-1/T_0)}$
If T₀ is not specified: Kinetic factor = $kT^n e^{-E/RT}$

k:
n:
E: kcal/mol
T₀: C

Solids
Driving Force
Adsorption

Adsorption Expression

Reacting phase: Liquid
[C_i] basis: Molarity
Adsorption expression exponent:

Concentration exponents

	Component	Term no. 1
*		

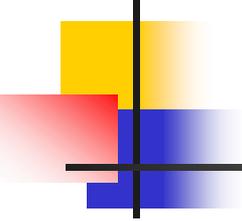
Adsorption constants

	Coefficient	Term no.
A:		
B:		
C:		
D:		

吸附项表单

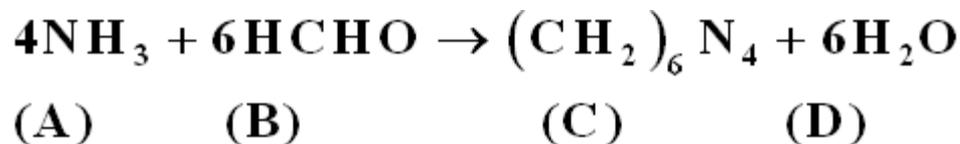
吸附项常数K

吸附项组分



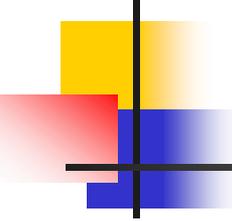
一、RCSTR—示例1

甲醛与氨反应生成乌洛托品反应式如下：



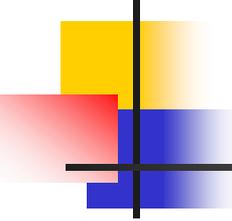
$$-r_A = kC_A C_B^2 \quad \text{kmol} / \text{m}^3 \cdot \text{s}$$

$$k = 1420 \exp\left[-\frac{2.57 \times 10^7}{RT}\right] \quad \text{m}^6 / \text{kmol}^2 \cdot \text{s}$$



***RCSTR*—示例1**

反应器容积为 5m^3 ，装填系数为0.6，为保证釜内惰性环境，输入氮气并使出釜物料的气相分率为0.001，加料氨水的浓度为 $4.1\text{Kmol}/\text{m}^3$ ，流量为 $32.5\text{m}^3/\text{hr}$ ，甲醛水溶液浓度为 $6.3\text{Kmol}/\text{m}^3$ ，流量为 $32.5\text{m}^3/\text{hr}$ ，求 35°C 下乌洛托品的产量和输入的氮气量，并分析 $20\text{--}60^\circ\text{C}$ 范围内，温度对甲醛转化率的影响。

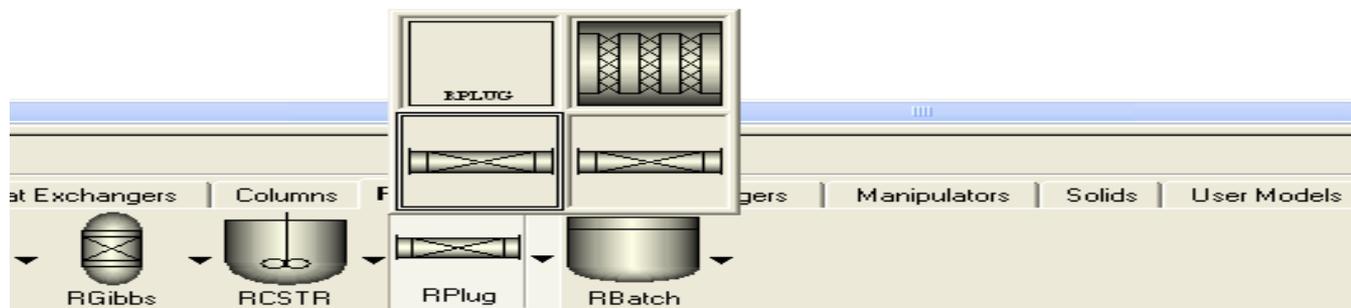
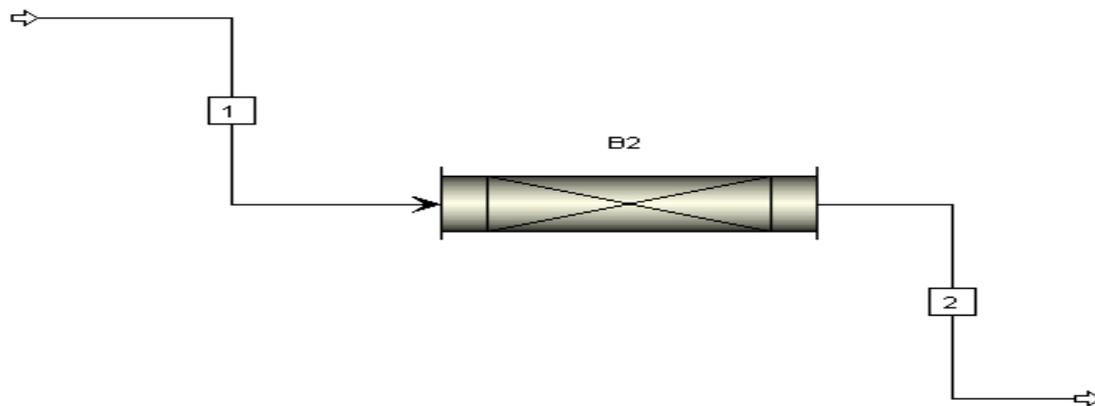


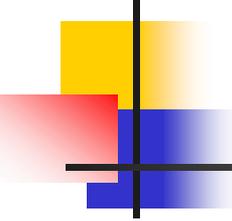
二、R-Plug 平推流反应器

性质：无返混的管式反应器，可有换热夹套，可模拟单、两、三相体系，必须有动力学方程。

应用：已知化学反应式和动力学方程，计算所能达到的转化率或反应器体积，以及相应的热负荷。

二、R-Plug 平推流反应器





二、R-Plug 平推流反应器

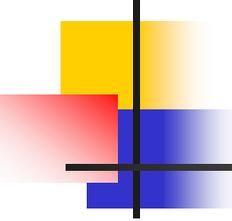
R-Plug有四组模型参数：

模型设定 (Specifications)

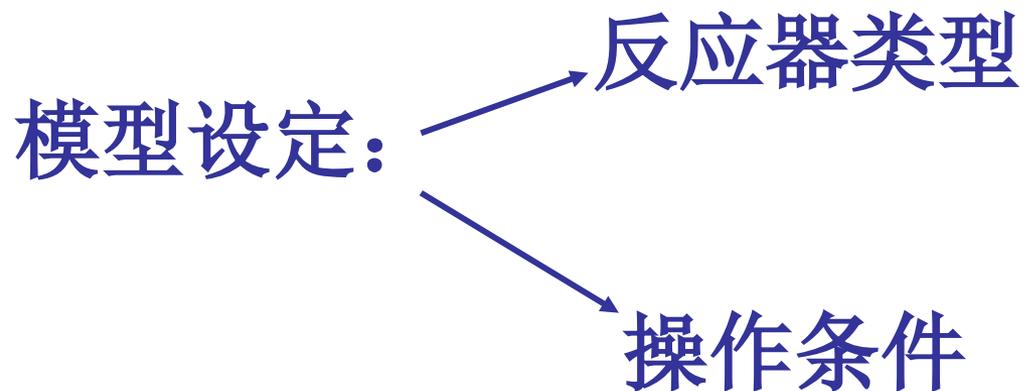
反应器构型 (Configuration)

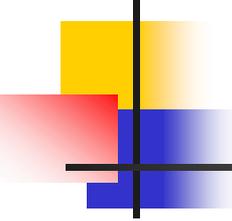
化学反应 (reaction)

压力 (Pressure)



二、R-Plug 平推流反应器





二、R-Plug 平推流反应器

反应器类型:

指定反应温度

绝热反应器

恒定冷却剂温度反应器

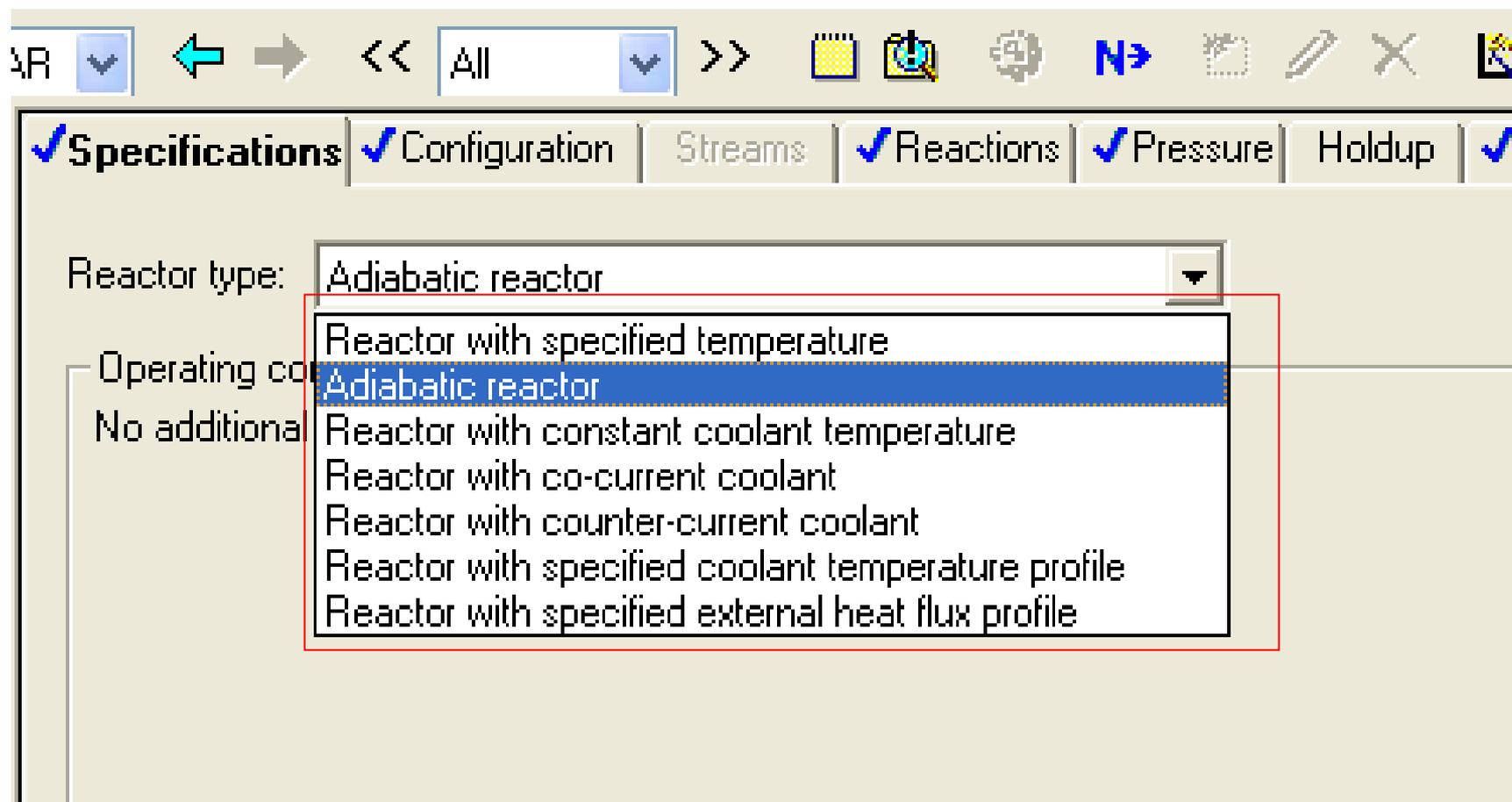
与冷却剂并流

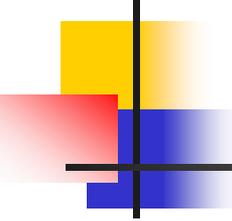
与冷却剂逆流

指定冷却剂温度变化曲线

指定外部热流变化曲线

二、R-Plug 平推流反应器





二、R-Plug 平推流反应器

指定反应器温度有三种操作状态

1) 进料温度下的恒温

2) 指定反应器等温度

3) 反应器内温度沿床层分布曲线

二、R-Plug 平推流反应器

Specifications Configuration Streams Reactions Pressure

Reactor type: Reactor with specified temperature

Operating condition

Constant at inlet temperature

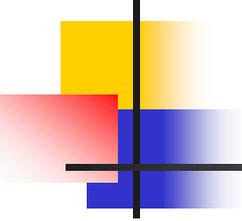
Constant at specified reactor temperature

Temperature profile

Temperature: [] C

	Location	Temperature
		C
*		

← 三种操作状态



对于有冷却剂的反应器类型：

（流程图中需连接冷却剂）

在操作条件中需输入传热系数**U**、冷却剂出口温度、或蒸汽分率

二、R-Plug 平推流反应器

Specifications | Configuration | Streams | Reactions | Pressure | Holdup

Reactor type:

Operating condition

Heat transfer specification

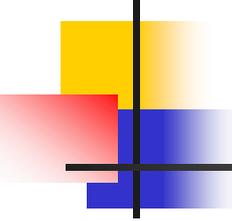
Specify heat transfer parameters

U (coolant-process stream): kcal/hr-sqm-K

Calculate in user subroutine

Coolant temperature: C





二、R-Plug 平推流反应器

反应器构型表单：

单管或多管反应器

反应管的根数

反应管的长度或直径

反应物料的有效相态

冷却剂的有效相态

以上内容仅为本文档的试下载部分，为可阅读页数的一半内容。如要下载或阅读全文，请访问：<https://d.book118.com/305202324142012003>