

## **The Phthalic Anhydride Process**

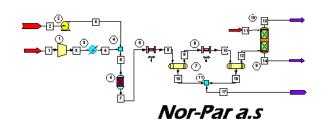
## **DESCRIPTION:**

One of the routes to make Phthalic Anhydride (PA) is to oxygenate o-Xylene with air in a catalytic process.

Extensive laboratory/computational work has been carried out to develop actual kinetic model for the reactor. Then the data were input to CHEMCAD's Kinetic Reactor model as the Extended Kinetic Equation. Heat transfer was also included into the model.

As we were not permitted by the technology owner to publish data, the Training Book example involves simpler model for a similar process.

Reactive absorption has been employed to model a scrubber converting anhydrides into respective carboxylic acids.



	Compressor Summary
Equip. No.	1
Name	
Type of Compressor:	2
Pressure out bar	1.6000
Efficiency	0.7500
Actual power kW	603.0629
Cp/Cv	1.3989
Ideal Cp/Cv	1.3975
Calc Pout bar	1.6000
Theoretical power kW	442.3389

		Scds Rigor	ous Distillatio	n Summary	
Gquip.	No.	1	.0		
	Name				
ło. of	stages		2		
Lst fee	d stage		1		
and fee	d stage		2		
'op pre	ssure bar	1.0	132		
Reactiv	e distillati	ion ?	Y		
eflux	mole kmol/h	r 1558.7	957		
leflux :	mass kg/hr	30063.6	094		
(eactio	n stolchlome	vrics and Par	ameters for uni	c no. 10	
No. of	liquid read	tions = 2			
	vapor react				
	-		Vol. unit : 2		
Time u	nit: 2 Pre	ss. unit : 0	Temp unit : 0		
			-		
Tray r	eaction volu		-		
Tray r	eaction volu		-		
-			Vapor rxn vol		
3	tg Liq	une s	-		
3	tg Liq 1 2.00	umes IXN Vol	Vapor rxn vol		
3	tg Liq 1 2.00 2 2.00	umes IXN Vol 000e+001 000e+001	Vapor rxn vol 0.0000e+000 0.0000e+000		
3 Reacti	tg Liq 1 2.00 2 2.00 on 1 Typ	umes IXN Vol 100e+001 100e+001 .e = 0 Pha	Vapor rxn vol 0.0000e+000 0.0000e+000 se = 0		
3 Reacti	tg Liq 1 2.00 2 2.00 on 1 Typ	umes IXN Vol 100e+001 100e+001 .e = 0 Pha	Vapor rxn vol 0.0000e+000 0.0000e+000	0.0000¢+000	
3 Reacti A =	tg Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001	umes IXN vol 000e+001 000e+001 ce = 0 Pha E = 0.0000	Uapor rxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 =		Advert For
B Reacti A = Comp	tg Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001 Stoich.	umes IKN vol 1000+001 1000+001 ve = 0 Pha E = 0.0000 Exp.factor	Vapor rxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac.	Adsorb E	Adsorb Emp.
3 Reacti A = Comp 2	tg Liq 1 2.00 2 2.00 0n 1 Typ 1.0000e+001 Stoich. -1.00e+000	umes rmn vol 1000+001 000+001 F = 0 Pha F = 0.0000 Exp.factor 0.0000+000	Uapor rxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000	Adsorb E 0.0000e+000	0.0000e+000
3 Reacti A = Comp 2 10	tg Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001 Stoich. -1.00e+000 -1.00e+000	<pre>xmes xmes xm, vol 000e+001 000e+001 xe = 0 Pha E = 0.0000 Exp.factor 0.0000e+000 0.0000e+000</pre>	Uapor xxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000	Adsorb E 0.0000e+000 0.0000e+000	0.0000e+000 0.0000e+000
3 Reacti A = Comp 2	tg Liq 1 2.00 2 2.00 0n 1 Typ 1.0000e+001 Stoich. -1.00e+000	umes rmn vol 1000+001 000+001 F = 0 Pha F = 0.0000 Exp.factor 0.0000+000	Uapor xxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000	Adsorb E 0.0000e+000 0.0000e+000	0.0000e+000
3 Reacti A = Comp 2 10	tg Liq 1 2.00 2 2.00 on 1 Typ 1.0000+001 Stoich. -1.00e+000 1.00e+000	<pre>unes ixn vol i00e+001 i00e+001 ive = 0 Pha E = 0.0000 Exp.factor 0.0000e+000 0.0000e+000 0.0000e+000</pre>	Uapor xxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000	Adsorb E 0.0000e+000 0.0000e+000	0.0000e+000 0.0000e+000
3 Reacti A = Comp 2 10 11 Reacti	ty Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001 Stoich. -1.00e+000 -1.00e+000 1.00e+000 on 2 Typ	<pre>xmes xmes xmes xmes xe = 0 Pha E = 0.0000 Exp.factor 0.0000e+000 0.0000e+000 0.0000e+000 xe = 0 Pha</pre>	Uapor xxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000 0.0000e+000 se = 0	Àdsorb E 0.0000e+000 0.0000e+000 0.0000e+000	0.0000e+000 0.0000e+000
3 Reacti A = Comp 2 10 11 Reacti	ty Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001 Stoich. -1.00e+000 -1.00e+000 1.00e+000 on 2 Typ	<pre>xmes xmes xmes xmes xe = 0 Pha E = 0.0000 Exp.factor 0.0000e+000 0.0000e+000 0.0000e+000 xe = 0 Pha</pre>	Uapor xxn vol 0.0000e+000 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000 0.0000e+000	Àdsorb E 0.0000e+000 0.0000e+000 0.0000e+000	0.0000e+000 0.0000e+000
3 Reacti A = Comp 2 10 11 Reacti	ty Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001 Stoich. -1.00e+000 -1.00e+000 1.00e+000 on 2 Typ	<pre>xmes xmes xmes xmes xe = 0 Pha E = 0.0000 Exp.factor 0.0000e+000 0.0000e+000 0.0000e+000 xe = 0 Pha</pre>	Uapor xxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000 0.0000e+000 se = 0	Àdsorb E 0.0000e+000 0.0000e+000 0.0000e+000	0.0000e+000 0.0000e+000
S Reacti A = Comp 2 10 11 Reacti A = Comp	ty Liq 1 2.00 2 2.00 on 1 Typ 1.0000e+001 Stoich. -1.00e+000 -1.00e+000 i.000e+001 000 2 Typ 1.0000e+001	<pre>umes Exn vol 000+001 000+001 E = 0 Pha E = 0.0000 Exp.factor 0.0000+000 0.00000+000 0.00000+000 c.e = 0 Pha E = 0.0000</pre>	Uapor rxn vol 0.0000e+000 0.0000e+000 se = 0 e+000 Fara3 = Adsorb Fac. 0.0000e+000 0.0000e+000 0.0000e+000 se = 0 e+000 Fara3 =	Adsorb E 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000	0.0000e+000 0.0000e+000 0.0000e+000
Reacti A = Comp 2 10 11 Reacti A = Comp 3	ty Liq 1 2.000 2 2.000 on 1 Typ 1.0000e+001 Stoich. -1.00e+000 1.00e+000 on 2 Typ 1.0000e+001 Stoich.	<pre>xmes xmes xmes xmes xe = 0 Pha E = 0.0000 Exp.factor 0.0000e+000 0.0000e+000 0.0000e+000 c.e = 0 Pha E = 0.0000 Exp.factor</pre>	Uapor rxn vol 0.0000e+000 ocouoe+000 e= 0 e+000 Para3 = Adsorb Fac. 0.0000e+000 0.0000e+000 0.0000e+000 se = 0 e+000 Para3 = Adsorb Fac. 0.0000e+000	Adsorb E 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 Adsorb E	0.0000e+000 0.0000e+000 0.0000e+000