

## **Process Development for Production of 900 TPD of Phthalic Anhydride (PAN) by oxidation of O-Xylene**

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### **Background:**

Phthalic anhydride (PAN), an anhydride of phthalic acid, is in a lustrous white colour solid state and is in the form of needles with a mild distinctive odour. Its molecular formula is  $C_8H_4O_3$  and its IUPAC name is 2-Benzofuran-1,3-dione. Its CAS No. is 85-44-9. PAN is used as a precursor to manufacture plasticizers, alkyd resins, polyester resins, dyes, and pigments.

### **Process Settings:**

System of units: C5

Special components used: Phthalic Anhydride, created using Component Creator using data from Chemeo

### **Process description:**

The raw reactants oxygen and o-xylene at 25 °C are mixed using a mixer and are preheated and introduced to a conversion reaction which is operated at 80% conversion at 350 °C, since the reaction is exothermic, the produced heat is used to preheat the reactants. The reactor outlet consists of PAN, water, oxygen and o-xylene at 350 °C are cooled to 154°C to condense PAN and a vapor-liquid separator is used to separate PAN and the exit stream pressure is reduced to 0.2 bar to evaporate the excess water at reduced pressure and separate using vapor-liquid separator and the stream is compressed to atmospheric pressure followed by distillation to eliminate excess o-xylene. The bottom product of the distillation column contains PAN with 99.99% purity at 225 °C is cooled to 25 °C and 1 atm at stream 21.

### **Result:**

The final product Phthalic Anhydride is produced in the stream 21 with a purity of 99.99% in liquid state at 25 °C at a rate of 900 TPD. The key stream details are mentioned in Table 1.

**Table 1:** Stream results for key streams involved in the process from the flowsheet developed using DWSIM

	S01	S02	S05	S07	S09	S10	S16	S20	S21
<b>Temperature (°C)</b>	25	25	350	154.814	154.814	136.547	185.035	225.348	25
<b>Pressure (bar)</b>	1.01325	1.01325	1.01325	1.01325	1.01325	0.2	1.01325	0.5	1.01325
<b>Mass Flow (kg/h)</b>	38590.6	42678.3	81268.9	81268.9	43690.9	43690.9	40020.6	39871.3	39871.3
<b>Molar Flow (kmol/h)</b>	1206	402	1608	1608	337.711	337.711	271.322	269.198	269.198
<b>Molar Fraction (Mixture) / O-xylene</b>	0	1	0.05	0.05	0.0197716	0.01977	0.004745	0.0001	0.0001
<b>Molar Fraction (Mixture) / Oxygen</b>	1	0	0.15	0.15	9.83E-07	9.83E-07	2.15E-12	0	0
<b>Molar Fraction (Mixture) / Phthalic anhydride</b>	0	0	0.2	0.2	0.842546	0.84255	0.992072	0.9999	0.9999
<b>Molar Fraction (Mixture) / Water</b>	0	0	0.6	0.6	0.137681	0.13768	0.003183	0	0

### Further Works:

Recycling of unreacted streams can be implemented, P&ID can be included, comparing with packed distillation column can be done using custom model designing, Phthalic Anhydride can be crystallized and separated to get in the solid state.

### Reference:

- Lorz PM., Ullmann's Encyclopedia of Industrial Chemistry, volume 27, 2007, 132-180.
- Jara, J. A. and A. Garea, 2005. Simulation of O-Xylene Oxidation into Phthalic Anhydride: Rigorous Multitubular Catalytic Reactor Modelling and Exportation into the Process Flowsheet.
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