# Process Development for the Production of Propylene Oxide by Direct Oxidation Method 

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## A. Background

Propylene Oxide (PO) is an industrially important chemical widely used in manufacture of unsaturated propylene glycols, polyol foam, polyester resin, food, drug, cosmetics and personal care products. PO has a huge demand globally, especially in the field of petrochemicals, pharmaceuticals and food industry. The worldwide consumption of PO was about 2.8 million tonnes in 2013. Dow, Lyondell Chemical Company and Shell Eastern Petroleum are the major players in the market. The present work is focused on production of PO by direct oxidation of Propylene. The other conventional methods of production of PO involves chlorohydrin process which produces a bi-product Calcium Hydroxide and it is difficult to dispose to the environment.

## B. Description of Flow Sheet

Propylene and Oxygen from storage are pumped into a buffer drum. The mixture is fed to the conversion reactor at 313.5 K , in which the vapor phase oxidation of Propylene to Propylene oxide takes place. The reaction is highly exothermic. The water supplied in the cooling jacket is heated by the exothermicity of reaction and low pressure steam is produced. The exit stream from the reactor is fed to separator, where Propylene and PO, and traces of Oxygen are recovered at the bottom stream and the rest of Oxygen is obtained as top. Thus the mixture of Propylene and PO are separated in a series of Flash-Distillation columns. The product streams are cooled to room temperature and sent to storage. Production capacity of the plant is 94 tons per day

## C. Stream Results

| Stream No. | Temperature | Pressure | Molar Flow | Mole fraction |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  |  | P | O | PO |
| 1 | 313.15 | $1+\mathrm{E} 05$ | 27.78 | 1 | 0 | 0 |
| 2 | 313.15 | $1+\mathrm{E} 05$ | 13.89 | 1 | 1 | 0 |
| 3 | 313.15 | $1+\mathrm{E} 05$ | 41.67 | 0.66 | 0.34 | 0 |
| 4 | 313.15 | $1+\mathrm{E} 05$ | 30.55 | 0.18 | 0.09 | 0.73 |
| 5 | 313.15 | $1+\mathrm{E} 05$ | 2.78 | 0.01 | 0.99 | 0 |
| 6 | 313.15 | $1+\mathrm{E} 05$ | 27.78 | 0.20 | 0 | 0.80 |
| 7 | 313.15 | $1.7+\mathrm{E} 05$ | 18.29 | 0.29 | 0 | 0.71 |
| 8 | 313.15 | $1.7+\mathrm{E} 05$ | 9.48 | 0.03 | 0 | 0.97 |
| 9 | 302 | $1.75+\mathrm{E} 05$ | 8.03 | 0.55 | 0 | 0.45 |
| 10 | 302 | $1.75+\mathrm{E} 05$ | 10.26 | 0.07 | 0 | 0.93 |

* P - Propylene, O - Oxygen, PO - Propylene Oxide


## D. Conclusion and Recommendation

The results obtained in OpenModelica (v1.13) are validated using DWSIM. This work illustrates that open source simulator serves as a good platform for carrying out process development flowsheeting with ease.

Unit System: (SI)
Molar flow rate -mol/s
Mass flow rate - kg/s
Volumetric flow rate $-\mathrm{m}^{3} / \mathrm{s}$
Density - $\mathrm{kg} / \mathrm{m}^{3}$
Temperature - K
Pressure - Pa

