



PuriSim CATOX Reactor Design

Client: CLIENT NAME

PROJECT:

EXAMPLE Catalytic H2 Deoxo

DATE:

10/3/2023

Design Basis, Criteria, and/or Comments
5000 Nm³/hr of H₂ @ 100°C
and 40 barg w/ 0.3 mol % O₂,
Needing Removal to < 1 ppmv

400mm ID x 3180mm Bed Ht.
with 300 kg of Catalyst

Catalyst:

Type	RCI OxiGone 125		Wt%
Constituents	Pd on Al ₂ O ₃	Palladium	0.250
Form / size	2 - 4 mm Beads	Platinum	--
Sock-loading Density	750 kg/m ³	Rhodium	--
		Ruthenium	--

Process Conditions:

Primary Feed Gas Rate	5,000 Nm ³ /h	Inlet Temp.:	212 °F / 100 °C
Secondary Feed Gas	None	Outlet Temp.:	301.8 °F / 149.9 °C
Secondary Gas Rate	--	Effluent Split to Recycle	0.000
Avg Gas MW in Reactor	2.33	Recycle Rate	0 Nm ³ /h
Gas Viscosity	0.0117 cp	Total Gas Into Rx	5,000 Nm ³ /h
Inlet Pressure	40 bar-g	Ergun Pressure Drop	0.154 bar

Bed Dimensions & Catalyst Quantity:

Bed Diameter	400 mm	Bed Volume	0.400 m ³
Bed Height	3183 mm	Bed Mass	300 kg
L/D Ratio	7.96		
Contact Time	7.52 sec		
Space Velocity	12500 hr ⁻¹		
Superficial Velocity	0.423 m/s		

Fluid Dynamics

*** FDI = 21.4

See our paper Fluid Dynamics in Packed Beds for more on the FDI - how it's calculated and how it's used in deciding best bed dimensions.

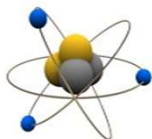
SEE P. 2 FOR STREAM COMPOSITIONS, MATERIAL BALANCE AND ANY SPECIAL NOTES.

Run No. 1302

Run ID: Design Case - 5000 Nm³/hr

*** The Fluid Dynamics Index or FDI is a metric for the degree of turbulence in the catalyst bed. Designing for FDI > 1 at minimum flow will minimize the possibility of channeling in the bed.

Page 1 of 2



PuriSim CATOX Reactor Design

Material Balance for CLIENT NAME

PROJECT:

EXAMPLE Catalytic H2 Deoxo

DATE:

10/3/2023

STREAM RATES:

	Main <u>Feed</u>	2nd Feed <u>(None)</u>	Recycle <u>(None)</u>	Combined <u>Feeds</u>	Forward <u>Product</u>
Nm3/hr	5,000	--	--	5,000	4,985
Kmols/hr	223.2	--	--	223.2	222.5
Kg/hr	520.0	--	--	520.0	520.0
MW	2.33	--	--	2.33	2.34

STREAM COMPOSITIONS:

<u>Comp.</u>	<u>Component Name</u>	<u>(mol%)</u>	<u>(mol%)</u>	<u>(mol%)</u>	<u>Rx In (mol%)</u>	<u>Rx Out (mol%)</u>
1	HYDROGEN	98.3000	--	--	98.3000	97.9940
2	OXYGEN	0.3000	--	--	0.3000	< 1 ppmv
3	WATER	1.4000	--	--	1.4000	2.0060
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						

Notes:

(1) This is an EXAMPLE of a reactor design/simulation for the Hydrogen Deoxo Application.

Run No. 1302

Run ID: Design Case - 5000 Nm3/hr

CONFIDENTIAL! FOR CLIENT INTERNAL USE ONLY.

Page 2 of 2