

SHELL EO/EG PROCESS MEMORANDUM 104

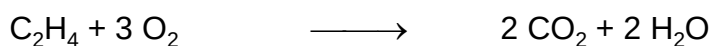
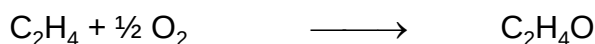
SUBJECT : REACTOR SELECTIVITY AND CONVERSION
CALCULATIONS

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ANALYSER BASED CALCULATIONS

- 1.1** In order to properly assess the performance of the EO reactors, it is important to periodically determine the reactor selectivity and oxygen conversion.

The reactions occurring in the EO reactor are as follows:



It is assumed that all other reactions are insignificant.

Selectivity and the oxygen conversion can be defined as follows:

$$\text{Selectivity} = s = \frac{\text{moles of EO formed}}{\text{moles of C}_2\text{H}_4 \text{ reacted}}$$

$$\text{Oxygen conversion} = c = \frac{\text{moles of oxygen reacted}}{\text{moles of oxygen in feed}}$$

- 1.2** To determine the reactor selectivity and the oxygen conversion, it is possible to use algebraic equations based on the stoichiometry of the above reactions. To apply the resulting equations it is necessary to know accurately at least two of the three component compositions viz. EO (total basis), carbon dioxide (dry basis), oxygen (dry basis). To ensure



accuracy of measurement and thereby improve the level of confidence in the final results, it is normal to measure all three component compositions in the common reactor feed and common reactor product gases.

- 1.3** Based on the above parameters, the mole balance around the EO reactor is as follows (r = moles of Ethylene reacted):

	moles in (mole %)	moles reacted	moles out
Oxygen (O ₂)	d	-(3r-2.5rs)	d-3r+2.5rs
Carbon dioxide (CO ₂)	b	+(2r-2rs)	b+2r-2rs
Ethylene (C ₂ H ₄)	a	-r	a-r
EO (C ₂ H ₄ O)	e	+rs	e+rs
Water (H ₂ O)	W	+(2r-2rs)	W+2r-2rs
Inerts (CH ₄ , N ₂ , Ar, C ₂ H ₆ , etc..)	n	-----	n
Total	100	-0.5rs	100-0.5rs

- 1.4** Assuming equal molar volumes for all components

volume shrinkage on total basis (including water) can be expressed as

$$t = \frac{100 - 0.5rs}{100} = \frac{MW_{in}}{MW_{out}}$$

and volume shrinkage on a dry basis (water free) can be expressed as

$$p = \frac{100 - W + 1.5rs - 2r}{100}$$

- 1.5** As EO is measured on a total basis (including water, hot sample line), while carbon dioxide and oxygen are measured on a dry basis, the measured reactor inlet and outlet compositions can be expressed as a function of the parameters used above as follows:



$$\text{Inlet EO concentration (\%mole)} = \varepsilon = e \quad (1)$$

$$\text{Inlet CO}_2 \text{ concentration (\%mole)} = \beta = \frac{100b}{(100-W)} = \frac{b}{(1-\frac{W}{100})} \quad (2)$$

$$\text{Inlet O}_2 \text{ concentration (\%mole)} = \delta = \frac{100d}{(100-W)} = \frac{d}{(1-\frac{W}{100})} \quad (3)$$

$$\text{Outlet EO concentration (\%mole)} = E = \frac{100(e+rs)}{(100-0.5rs)} \quad (4)$$

$$\text{Outlet CO}_2 \text{ concentration (\%mole)} = B = \frac{100(b+2r-2rs)}{(100-W+1.5rs-2r)} \quad (5)$$

$$\text{Outlet O}_2 \text{ concentration (\%mole)} = D = \frac{100(d-3r+2.5rs)}{(100-W+1.5rs-2r)} \quad (6)$$

1.6 Equations 1-6 can be solved simultaneously to arrive at the selectivity if the compositions of any two components, both in the common feed and common product, and the water concentration are known.

Based on EO (total) and Oxygen (dry) we have

$$s = \frac{300 - 2D}{250 - 1.5D + (1 - \frac{W}{100})(\delta - D)(100 + 0.5E) / (E - \varepsilon)}$$

Based on EO (total) and carbon dioxide (dry) we have

$$s = \frac{200 + 2B}{200 + 1.5B + (1 - \frac{W}{100})(B - \beta)(100 + 0.5E) / (E - \varepsilon)}$$

Based on oxygen and carbon dioxide (both on dry basis) we have

$$s = \frac{(\delta - D)(200 + 2B) - (B - \beta)(300 - 2D)}{(\delta - D)(200 + 1.5B) - (B - \beta)(250 - 1.5D)}$$

1.7 The oxygen conversion can be calculated using the following equations.

$$c = \frac{(\text{moles in} - \text{moles out})}{\text{moles in}} = \frac{(d - pD)}{d} = \frac{(1 - \frac{W}{100})\delta - pD}{(1 - \frac{W}{100})\delta}$$



where

$$p = \frac{100 - W + (1 - \frac{W}{100})\beta + 0.5\varepsilon - 0.005WE + 0.005(1 - \frac{W}{100})\beta E}{100 + B + 0.5E + 0.005BE}$$

- 1.8** The accuracy of the selectivity calculated can be checked by calculating the oxygen closure around the reactors. When the oxygen closure around the EO reactors is within $\pm 1\%$, the selectivity data is normally satisfactory. The Shell oxygen closure is:

$$\frac{pD + 0.5tE + 1.5pB - 1.5(1 - \frac{W}{100})\beta - 0.5\varepsilon}{(1 - \frac{W}{100})\delta} \times 100\%$$

with

$$p = \frac{100 - W + (1 - \frac{W}{100})\beta + 0.5\varepsilon - 0.005WE + 0.005(1 - \frac{W}{100})\beta E}{100 + B + 0.5E + 0.005BE}$$

and

$$t = \frac{100 + 0.5\varepsilon}{100 + 0.5E}$$



FEED METER BASED CALCULATIONS

In order to check the selectivity values derived from analytical data, selectivity calculations can also be performed from the battery limit oxygen and ethylene feed flows. This equation is as follows:

$$s = 1.2 - 0.35 \frac{\text{tons of oxygen reacted}}{\text{tons of ethylene reacted}}$$

Note that the above equation is based on oxygen and ethylene reacted. This data can be obtained by subtracting the known plant losses (mainly process vent) and can be approximated to actual feed rates when high purity feed stock is used. It should also be realised that the accuracy of this method of calculation is highly dependent on the accuracy of flow measurement in the feed stock supply lines.

