REB, The Book
Example 2.6.2 Solution

A new reactor is being developed with the hope of generating ethylene by the oxidative dehydrogenation of ethane, reaction (1). Reactions (2) and (3) also take place at the operating conditions of 1 atm and 150 °C. The process starts with 90% ethane and 10% air (you may take air to contain 79% N_2 and 21% O_2) and ends with a 50% conversion of O_2 and a selectivity of 3 C_2H_4/CO_2. Calculate the final mole fraction of CO_2.

$$2\ C_2H_6 + O_2 \rightarrow 2\ C_2H_4 + 2\ H_2O \tag{1}$$

$$C_2H_4 + 3\ O_2 \rightarrow 2\ CO_2 + 2\ H_2O \tag{2}$$

$$2\ C_2H_6 + 7\ O_2 \rightarrow 4\ CO_2 + 6\ H_2O \tag{3}$$

Given Constants: $y_{C_2H_6,0}$ = 0.9, $y_{air,0}$ = 0.1, f_{O_2} = 0.5, and $S_{C_2H_4/CO_2}$ = 3

Basis: $n_{total,0}$ = 1 mol

Computational strategy: The initial molar amounts can be calculated directly using the given values and basis. The given conversion and selectivity can be used to calculate the apparent extents of the reactions, from which the final molar amounts can be calculated. Once the final molar amounts are known, the final mole fraction of CO_2 can be calculated.

The initial amounts of C_2H_6 and air are equal to their mole fractions times the total moles, equations (4) and (5). The initial amounts of O_2 and N_2 then can be calculated using the known composition of air, equations (6) and (7)

$$n_{C_2H_6,0} = y_{C_2H_6,0} n_{total,0} \tag{4}$$

$$n_{air,0} = y_{air,0} n_{total,0} \tag{5}$$

$$n_{O_2,0} = 0.21 n_{air,0} \tag{6}$$

$$n_{N_2,0} = 0.79 n_{air,0} \tag{7}$$

Before the apparent extents of reaction can be used, a complete mathematically independent subset of the reactions must be identified. I can see that reactions (1) and (2) must be independent because reaction (2) contains CO_2 and reaction (1) does not. I can also see that if reaction (1) occurs once and reaction (2) occurs twice, the result is reaction (3), so reaction (3) is not independent. Therefore reactions (1) and (2) are a complete, mathematically independent set of reactions and their apparent extents can be used to generate Table 1.

Table 1

Species	**Initial Amont**	**Later Amount**
C_2H_6	$n_{C_2H_6,0}$	$n_{C_2H_6,0} - 2\xi_1$
O_2	$n_{O_2,0}$	$n_{O_2,0} - \xi_1 - 3\xi_2$
C_2H_4	0	$2\xi_1 - \xi_2$
H_2O	0	$2\xi_1 + 2\xi_2$
CO_2	0	$2\xi_2$
N_2	$n_{N_2,0}$	$n_{N_2,0}$
Total	$n_{total,0}$	$n_{total,0} + \xi_1$

Writing the defining equations for the conversion and selectivity and substituting for the molar amounts in Table 1 yields equations (8) and (9).

$$f_{O_2} = \frac{n_{O_2,0} - n_{O_2}}{n_{O_2,0}} = \frac{\xi_1 + 3\xi_2}{n_{O_2,0}} \tag{8}$$

$$S_{C_2H_4/CO_2} = \frac{n_{C_2H_4}}{n_{CO_2}} = \frac{2\xi_1 - \xi_2}{2\xi_2} \tag{9}$$

Equations (8) and (9) can be solved to find ξ_1 and ξ_2. The results can then be used to calculate the final CO_2 mole fraction as shown in equation (10).

$$y_{CO_2} = \frac{n_{CO_2}}{n_{total}} = \frac{2\xi_2}{n_{total,0} + \xi_1} \qquad (10)$$

The calculations were performed as described above. Solving equations (8) and (9) gives ξ_1 = 5.65 x 10^{-3} mol and ξ_2 = 1.62 x 10^{-3} mol, but these values only apply for the chosen basis. The final CO_2 mole fractions is 0.00321, which is valid irrespective of the basis.