4.1 Lean NO_x Trap

Summary

This [Jupyter notebook] demonstrates the calculation of mass balances for a lean NOx trap used to meet air quality standards for nitrogen oxides in the exhaust of diesel powered trucks and automobiles.

Problem Statement

Some diesel car and truck manufacturers, including Volkswagen and others, have introduced Lean NO_x Traps (LNT) in exhaust systems to meet stringent air quality standards for nitrogen oxides.

An LNT includes a small amount of platinum (Pt) in a barium oxide (BaO) wash coat spread over a ceramic monolith. Under under lean fuel conditions, NO is converted to NO_2 by the reaction

$$NO\,(g) + \frac{1}{2}O_2\,(g) \longrightarrow NO_2\,(g)$$

catalyzed by Pt. Nitrogen dioxide is then adsorbed into the trap by the reaction

$$BaO\,(s) + 2\,NO_2\,(g) + \frac{1}{2}O_2\,(g) \longrightarrow Ba(NO_3)_2\,(s)$$

The washcoat has to be regenerated once it has been saturated with nitrogen oxides. To regenerate, a small amount of diesel fuel to release the NO_x which reacts with the hydrocarbons to form water and nitrogen.

Consider an LNT operating with a total inflow of 1 kg/min with 850ppm NO, 150ppm NO_2, and O_2 in substantial excess.

Needed data is in the following table.

Molecular Species	MW
$Ba(NO_3)_2$	261.3
BaO	153.3
NO	30.0
NO_2	46.0
O_2	32.0

The exhaust gas is to be reduced to 50ppm NO with no residual NO_2.

1. Identify the relevant stream and system variables. Perform a degree of freedom analysis.
2. Calculate the extents of reaction. Be sure to show units.
3. The washcoat is initially loaded with 100 grams of BaO. How long is it before the trap must be regenerated?

Solution

Part a. Degree of Freedom Analysis

The relevant stream and system variables are labeled on the following diagram. The inlet specifications have been translated to flow rates. The outlet flow of NO_2 is zero, and the flow of $\dot{m}_{NO,2}$ is 50 ppm of the total outlet mass flow.

Variables	
Stream Variables	6
Accumulation Variables	2
Extents of Reaction	2
TOTAL VARIABLES	10

Equations	
Mass Balances	5
Inlet Specifications	2
Outlet Specification	2
TOTAL EQUATIONS	8

$$DOF = Variables - Equations = 10 - 9 = \boxed{1}$$

Part b. Material Balances

$$\begin{aligned}
\dot{r}_{Ba(NO_3)_2} &= M_{Ba(NO_3)_2}\dot{\xi}_2 \\
\dot{r}_{BaO} &= -M_{BaO}\dot{\xi}_2 \\
0 &= \dot{m}_{NO,1} - \dot{m}_{NO,2} - M_{NO}\dot{\xi}_1 \\
0 &= \dot{m}_{NO_2,1} - \dot{m}_{NO_2,2} + M_{NO_2}\dot{\xi}_1 - 2M_{NO_2}\dot{\xi}_2 \\
0 &= \dot{m}_{O_2,1} - \dot{m}_{O_2,2} - \frac{1}{2}M_{O_2}\dot{\xi}_1 - \frac{1}{2}M_{O_2}\dot{\xi}_2
\end{aligned}$$

The flow of stream 2 is essentially 1 kg/min because only a small part is reactive. The material balances for NO and NO_2 are

$$0 = \underbrace{\dot{m}_{NO,1}}_{0.85\ g/min} - \underbrace{\dot{m}_{NO,2}}_{0.05\ g/min} - \underbrace{M_{NO}}_{30.0}\dot{\xi}_1$$

$$0 = \underbrace{\dot{m}_{NO_2,1}}_{0.15\ g/min} - \underbrace{\dot{m}_{NO_2,2}}_{0\ g/min} + \underbrace{M_{NO_2}}_{46.0}\dot{\xi}_1 - 2\underbrace{M_{NO_2}}_{46.0}\dot{\xi}_2$$

Solving the first equation

$$\dot{\xi}_1 = \frac{\dot{m}_{NO,1} - \dot{m}_{NO,2}}{M_{NO}} = \frac{0.85\ g/min - 0.05\ g/min}{30.0\ g/gmol} = \boxed{0.0267\ \mathrm{gmol/min}}$$

The solving for the second

$$\dot{\xi}_2 = \frac{0.15\ g/min + 46.0\ g/gmol \times 0.0267\ gmol/min}{2 \times 46.0 g/gmol} = \boxed{0.015\ \mathrm{gmol/min}}$$

Part c. The rate of consumption of BaO

$$\dot{r}_{Ba(NO_3)_2} = M_{Ba(NO_3)_2}\dot{\xi}_2 = 153.3 \times 0.015 \; gmol \qquad /$$

so the 100 grams of \ce{BaO} will need to be regenerated in

$$t = \frac{100 \; g}{2.3 \; g/min} = \boxed{43.6 \text{ min}}$$

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