

SHELL INTERNATIONAL CHEMICALS B.V.
AMSTERDAM - THE NETHERLANDS

SHELL EO/EG PROCESS MEMORANDUM 103

SUBJECT : REACTOR LOOP GAS FLAMMABLE LIMIT CALCULATIONS

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INTRODUCTION

The flammable limits of gaseous mixtures under conditions similar to those which occur in the feed and product streams of the EO reactor have been studied in an extensive experimental program.

The flammable limit calculation must be automatically and continually calculated and evaluated based on actual plant conditions in order to ensure the safe operating conditions of the process with respect to the oxygen concentrations in the gas loop.

The following equation was developed for the flammable limits of plant gases and may be used to determine the maximum safe oxygen concentration as required for plant operation:

$$L_f(\text{O}_2, \text{\%mole}) = 17.10 - 0.16936 \cdot P - 0.03191 \cdot T - 0.05185 \cdot [\text{C}_2\text{H}_4] + 0.02585 \cdot [\text{CH}_4] \\ - 0.018 \cdot [\text{Ar}] + 0.071 \cdot [\text{C}_2\text{H}_6] - 0.03 \cdot [\text{EO}]^2$$

where $L_f(\text{O}_2, \text{\%mole})$ is the oxygen concentration at the flammable limit in %mole (dry basis); T is the gas temperature in °C; P is the pressure in kg/cm²g; [] refer to concentrations in %mole (dry, O₂ - free).

The range of conditions tested in the experimental program is:

Pressure, kg/cm ² g		12.7 - 28.0
Temperature, °C		153 - 260
Methane	concentration, %mole	13 - 66
Ethane	concentration, %mole	0.6 - 1.8
Ethylene	concentration, %mole	17 - 45
Argon	concentration, %mole	0 - 40
Ethylene Oxide	concentration, %mole	0 - 7.1

Temperature was found to have the most significant effect.

In general the data indicate that the flammable limit oxygen concentration increases with decreasing temperature, despite variations in the other variables. The carbon dioxide concentration was varied over the range of 2.5 - 11.7 %mole and was found to have no effect.

Acetaldehyde at a concentration of 0.1 %mole also was found to have no significant effect. Most experiments were carried out with 1 %mole water in the gas mixture. Water concentration was varied over the range of 0 to 2.7 % and found to have no effect. Figure 1 shows flammability limits of oxygen, ethylene and nitrogen with parameters of temperature and pressure.

The application of the above equation to a typical reactor feed gas for both start-up and normal compositions is shown in table 1. The licensee can substitute his



particular design or start-up conditions in the above equation for his specific limit values.

An alternative form of the above equation in English units is:

$$L_f(O_2, \% \text{mole}) = 17.67 - 0.01191 \cdot P - 0.01773 \cdot T - 0.05185 \cdot [C_2H_4] + 0.02585 \cdot [CH_4] \\ - 0.018 \cdot [Ar] + 0.071 \cdot [C_2H_6] - 0.03 \cdot [EO]^2$$

where $L_f(O_2, \% \text{mole})$ is the oxygen concentration at the flammable limit in %mole (dry basis); T is the gas temperature in °F; P is the pressure in psig; [] refer to concentrations in %mole, on a water- and oxygen-free basis.



FIGURE 1:

FLAMMABILITY LIMITS OXYGEN-ETHYLENE-NITROGEN

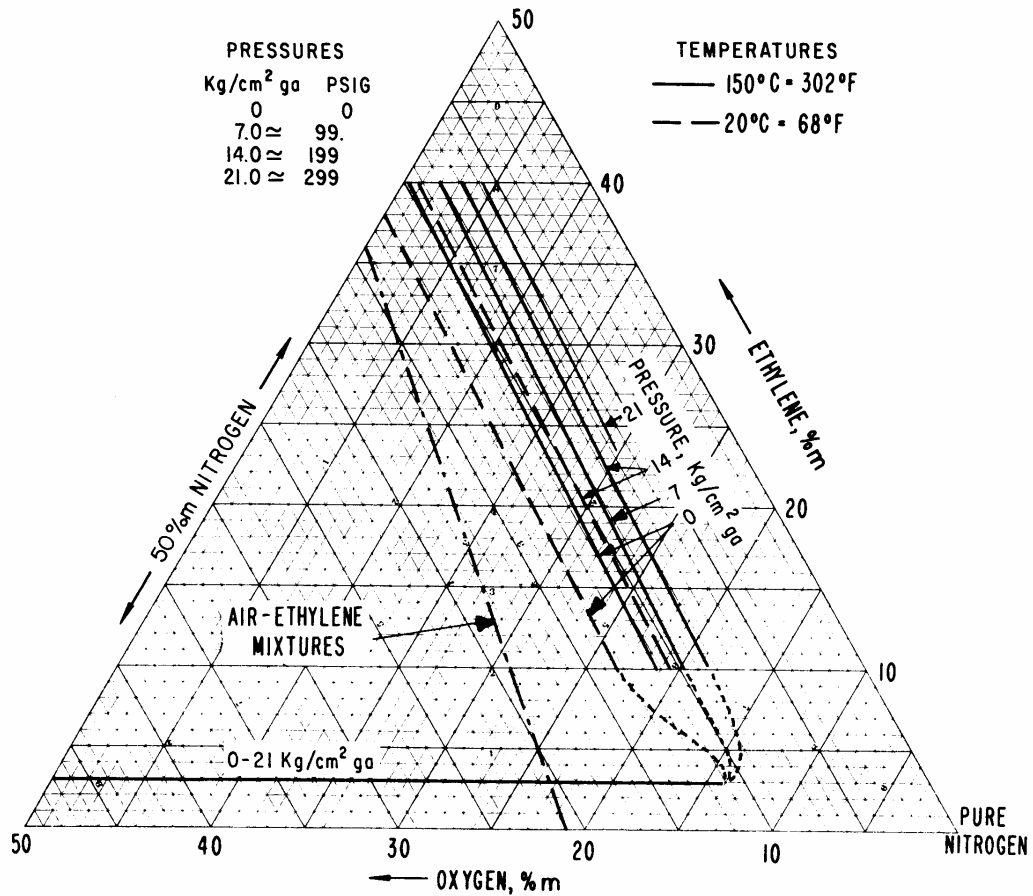


Figure C-1. Flammability Limits: Oxygen-Ethylene-Nitrogen



TABLE 1
ESTIMATED OXYGEN CONTENTS AT FLAMMABLE LIMIT
AN EXAMPLE

$$L_f(\text{O}_2, \text{\%mole}) = 17.10 - 0.16936 \cdot P - 0.03191 \cdot T - 0.05185 \cdot [\text{C}_2\text{H}_4] + 0.02585 \cdot [\text{CH}_4] \\ - 0.018 \cdot [\text{Ar}] + 0.071 \cdot [\text{C}_2\text{H}_6] - 0.03 \cdot [\text{EO}]^2$$

	Normal		Start-up	
	Inlet	Outlet	Inlet	Outlet
Pressure, kg/cm ² g	16.86	14.94	16.86	14.94
Temperature, °C	138	249	138	249
Composition, %				
N ₂	1.13	1.14	61.40	61.40
Ar	10.04	10.17		
O ₂	8.13	4.43	3.0	3.0
CH ₄	37.55	38.03		
C ₂ H ₄	35.00	32.07	35.0	35.0
C ₂ H ₆	1.04	1.05		
CO ₂	6.50	8.27		
EO	0.01	2.53		
H ₂ O	0.60	2.30	0.60	0.60
	Inlet	Outlet	Inlet	Outlet
Composition, H ₂ O and O ₂ Free Basis, % m				
N ₂	1.24	1.22	63.69	63.69
Ar	11.00	10.90		
CH ₄	41.14	40.78		
C ₂ H ₄	38.35	34.39	36.31	36.31
C ₂ H ₆	1.14	1.13		
CO ₂	7.12	8.87		
EO	0.01	2.71		
Flammable Limit, %mole				
Constant	17.10	17.10	17.10	17.10
-0.16936 (kg/cm ² g)	-2.86	-2.53	-2.86	-2.53
-0.03191 T (°C)	-4.40	-7.95	-4.40	-7.95
-0.05185 [C ₂ H ₄]	-1.99	-1.78	-1.88	-1.88
+0.02585 [CH ₄]	1.06	1.05		
-0.018 [Ar]	-0.20	-0.20		
+0.071 [C ₂ H ₆]	0.08	0.08		
-0.03 [EO] ²		-0.22		
L _f (O ₂ , %mole) dry basis	8.79	5.55	7.96	4.74

