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 Oxidation Catalysis Using Thin Film Model Pt Catalysts. A Research

 Proposal Submitted in partial Fulfillment of The Preliminary Examination

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APPENDICES

Appendix A Assumptions, definitions, and calculations.

In this work, the following assumptions were made:

- 1. All the gaseous behaviors obey the ideal gas law
- 2. The change in the system, pressure is very small and negligible.
- 3. The pressure in the system equals the atmospheric pressure (1 atm)
- 4. The vapor pressure of liquid benzene is based on the Antoine equation.

The Antoine equation, which is more satisfactory for general use, has the form (PERRY'S CHEMICAL ENGINEERS' HANDBOOK)

$$\log P^{sat} = A - \frac{B}{T + C} \tag{B.1}$$

where

P^{sat} = saturated vapor pressure (torr)

A, B, and C = antoine vapor-pressure constants for each pure substances. In case of benzene, A = 6.87987, B = 1196.760 and C = 219.161

T = temperature (
$$^{\circ}$$
C)

The total molar flow rate of the gaseous stream can be determined from the following equation:

$$N = q \times (P/RT) \tag{B.2}$$

where

q = total volumetric flow rate

P = total pressure of the system

R = gas constant (82.051 atm·ml·mol⁻¹·min⁻¹·K)

T = absolute ambient temperature (K)

The molar flow rate of each component can be obtained by multiplying its fraction derived from the gas chromatography analysis by the total molar flow rate.

The conversion is defined as:

% Conversion =
$$\frac{Mole\ reac\ \tan t\ in - Mole\ reac\ \tan t\ out}{Mole\ reac\ \tan t\ in} * 100\% (B.3)$$

The first selectivity is defined as:

% Selectivity =
$$\frac{P \times \text{Mole of } C_p \text{ produced}}{R \times \text{Mole of } C_R \text{ converted}} \times 100$$
 (B.4)

where

P = number of carbon atom in product

R = number of carbon atom in reactant

 C_p = product that has carbon P atom

 C_R = reactant that has carbon R atom

The second selectivity is defined as:

% Selectivity =
$$\frac{\text{Mole of product}}{\text{Total mole of all products}} \times 100$$
 (B.5)

To determine the energy efficiency of corona discharge system, the specific energy consumption was calculated in a unit of electron-volt per molecule of converted carbon (eV/ m_c) from the following equation:

Specific energy consumption =
$$\frac{P \times 60^{\circ}}{(1.602 \times 10^{-19}) \times \widetilde{N} \times M_{C}} \quad \text{eV/ mol C}_{6}\text{H}_{6}$$

Where
$$P = Power(W)$$

 \tilde{N} = Avogadro's number = 6.02 X 10^{23} molecules.g-mole⁻¹

 M_C = Rate of carbon in feed gas converted (g-mole.min⁻¹)

 $1 \text{ eV} = 1.602 \times 10^{-19} \text{ Ws}$

To determine the UV light intensity of corona discharge system, the intensity was calculated in a unit of μW . In this work, the following assumption was that the UV light spread out in all direction.

Intensity (μ W) = Intensity measured from UV meter (μ W/cm²)

Area of sphere (cm²)

Where Area of sphere = $4\P r^2$

r = 1.5 cm

Appendix B Experimental data.

Table B.1 Effect of total feed flow rate at 15,000, 500 Hz, a gap distance of 10 mm, and 1,500 ppm benzene in air

Feed flow rate	Stage (s)	% Conversion	%	Selectiv	vity	
(ml/min)	Stage (5)	C_6H_6	СО	CO ₂	C_1	C_2
60	1	81.02	10.39	71.69	u	u
	2	88.61	6.44	75.65	u	u
	3	85.93	5.91	75.32	u	u
	4	90.43	6.90	78.54	u	u
158	1	47.30	23.49	63.52	u	u
	2	65.73	21.34	72.41	u	u
	3	75.71	16.20	76.88	u	u
	4	83.75	15.63	74.17	u	u
235	1	41.72	29.29	64.49	u	u
	2	58.21	28.05	61.21	u	u
	3	69.67	21.68	69.33	u	u
	4	76.56	22.32	67.62	u	u
380	1	22.83	24.16	55.65	u	u
	2	44.96	28.18	48.51	u	u
	3	59.06	32.97	53.88	u	u
	4	70.56	32.47	55.84	u	u

u = below the GC detecting limit

Table B.2 Effect of frequency at 21,000, feed flow rate 500 ml/min, a gap distance of 10 mm, and 1,500 ppm benzene in air

Frequency	Stage (s)	% Conversion	% Selectivity		vity	
(Hz)	Blage (3)	C ₆ H ₆	CO	CO ₂	C_1	C_2
50	1	73.02	13.09	65.26	u	u
	2	80.54	8.02	69.39	u	u
	3	88.11	4.11	70.52	u	u
	4	90.24	3.30	74.90	u	u
100	1	55.21	14.96	57.79	u	u
	2	74.73	9.31	65.75	u	u
	3	81.49	5.79	65.55	u	u
	4	84.55	4.04	71.27	u	u
200	1	41.38	17.45	62.01	u	u
	2	54.59	14.78	62.58	u	u
:	3	70.21	11.31	68.36	u	u
	4	76.20	8.34	69.98	u	u
300	1	29.43	20.58	53.67	u	u
	2	51.99	21.41	58.96	u	u
	3	68.71	16.44	62.15	u	u
	4	71.97	15.21	67.01	u	u
400	1	27.30	27.38	58.13	u	u
	2	41.44	22.87	62.82	u	u
	3	53.81	17.77	65.29	u	u
	4	60.71	15.91	67.16	u	u
500	1	23.26	24.72	48.92	u	u
	2	43.83	33.84	54.53	u	u
	3	50.72	24.57	58.23	u	u
	4	59.44	22.84	59.06	u	u

Table B.2 Effect of frequency at 21,000, feed flow rate 500 ml/min, a gap distance of 10 mm, and 1,500 ppm benzene in air

Frequency	Stage (s)	% Conversion	% Selectivity			
(Hz)	Blage (3)	C_6H_6	CO	CO ₂	C_1	C_2
600	1	27.90	40.62	36.36	u	u
	2	44.34	41.37	42.82	u	u
	3	52.53	35.40	53.84	u	u
	4	63.04	32.52	48.65	u	u
700	1	22.52	48.90	33.30	u	u
	2	36.31	46.92	42.56	u	u
	3	49.41	45.72	42.23	u	u
	4	58.43	41.64	41.43	u	u

Table B.3 Effect of frequency on current and power consumption at 21,000, feed flow rate 500 ml/min, a gap distance of 10 mm, and 1,500 ppm benzene in air

	G ₄ ()	Current	De Come d'aday (N/CH Malanda)
Frequency (Hz)	Stage (s)	(A)	Power Consumption(eV/ C ₆ H ₆ Molecule)
50	1	2.280	113.20
	2	3.690	176.80
	3	5.850	251.67
	4	7.160	302.90
100	1	1.539	87.81
	2	2.260	103.19
	3	3.650	149.75
	4	4.440	179.19
200	1	1.083	84.10
	2	1.546	93.67
	3	2.460	118.05
	4	2.900	127.85
300	1	0.927	89.47
	2	1.256	75.89
	3	2.020	89.41
	4	2.300	100.75
400	1	0.821	85.94
	2	1.070	79.71
	3	1.834	101.15
	4	2.000	103.98
500	1	0.786	88.69
	2	0.979	67.21
	3	1.700	95.97
	4	1.870	93.11

Table B.3 Effect of frequency on current and power consumption at 21,000, feed flow rate 500 ml/min, a gap distance of 10 mm, and 1,500 ppm benzene in air

Frequency (Hz)	Stage (s)	Current (A)	Power Consumption(eV/ C ₆ H ₆ Molecule)
600	1	0.738	70.29
	2	0.886	59.92
	3	1.553	84.87
	4	1.728	82.15
700	1	0.733	88.82
	2	0.872	72.74
	3	1.537	92.89
	4	1.664	85.00

Table B.4 Effect of voltage at feed flow rate 500 ml/min, 300 Hz, a gap distance of 10 mm, and 1,500 ppm benzene in air

Voltage	Stage (s)	% Conversion	%	Selectiv	vity	
(V)	Stage (5)	C ₆ H ₆	CO	CO ₂	C_1	C_2
12,000	1	27.13	31.38	49.87	u	u
	2	39.33	24.74	58.49	u	u
	3	50.09	23.70	62.29	u	u
	4	56.87	20.30	64.01	u	u
15,000	1	28.40	23.76	55.44	u	u
	2	41.61	21.94	62.62	u	u
	3	54.76	19.50	70.21	u	u
	4	61.27	16.66	69.15	u	u
18,000	1	29.42	23.22	60.48	u	u
	2	41.16	20.14	68.69	u	u
	3	57.81	16.44	69.76	u	u
	4	63.49	13.07	71.34	u	u
24,000	1	32.40	20.95	66.53	u	u
	2	57.20	17.47	68.91	u	u
	3	69.24	14.07	68.54	u	u
	4	73.90	11.21	75.81	u	u

Table B.5 Effect of voltage on current at feed flow rate 500 ml/min, 300 Hz, a gap distance of 10 mm, and 1,500 ppm benzene in air

Voltage (V)	Stage (s)	Current
12,000	1	0.755
	2	1.443
	3	1.598
	4	1.755
15,000	1	0.806
	2	1.530
	3	1.750
	4	1.963
18,000	1	0.863
	2	1.642
	3	1.920
	4	2.140
24,000	1	0.960
	2	1.781
	3	2.100
	4	2.490

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