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APPENDICES

APPENDIX A Fenton process and Fenton/Air process.

Table A.1 %TOC remaining when the simulated wastewater was treated with Air with different air flow rates at any time

Time (hr)	Air flow rate					
	1/min		2 l/min		3 l/min	
	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining
0	5846.5	100.00	5687.0	100.00	6152.3	100.00
0.5	5637.5	96.43	5464.8	96.09	5742.0	93.33
1.0	5461.5	93.41	5299.8	93.19	5452.7	88.63
1.5	5395.5	92.29	5249.2	92.30	5144.7	77.95
2.0	5329.5	91.16	5128.2	90.17	4796.0	75.95
2.5	5314.1	90.89	5033.6	88.51	4660.7	75.76
3.0	5313.0	90.87	4950.0	87.04	4562.8	74.15
3.5	5308.6	90.80	4868.6	85.61	4530.9	73.65
4.0	5306.4	90.76	4747.6	83..48	4446.2	72.27
4.5	5305.3	90.74	4745.4	83.44	4434.2	72.07
5.0	5305.0	90.69	4744.3	83.42	4424.2	71.91

Table A.2 Composition of contaminant when the simulated wastewater was treated with Air with different air flow rates at any time

Time (hr)	% wt ethanol			% wt isopropanol		
	Air 1 l/min	Air 2 l/min	Air 3 l/min	Air 1 l/min	Air 2 l/min	Air 3 l/min
0	1.0011	0.912	1.1094	0.2050	0.2017	0.2080
0.5	0.9668	0.9431	0.9579	0.1959	0.1930	0.1930
1.0	0.9439	0.9233	0.9065	0.1936	0.1891	0.1829
1.5	0.9285	0.9156	0.8422	0.1896	0.1866	0.1741
2.0	0.9153	0.8996	0.7828	0.1878	0.1822	0.1621
2.5	0.9139	0.8887	0.7607	0.1868	0.1784	0.1574
3.0	0.9131	0.8694	0.7551	0.1848	0.1756	0.1542
3.5	0.9120	0.8517	0.7456	0.1846	0.1725	0.1522
4.0	0.9117	0.8315	0.7228	0.1836	0.1690	0.1492
4.5	0.9101	0.8263	0.7144	0.1834	0.1680	0.1476
5.0	0.9089	0.8193	0.7138	0.1833	0.1679	0.1464

Table A.3 %TOC remaining when the simulated wastewater was treated with H_2O_2 /Air with different hydrogen peroxide flow rates at any time

Time (hr)	Air 1 l/min		Air 2 l/min		Air 3 l/min	
	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining
0	5930.1	100.00	5677.1	100.00	5710.1	100.00
0.75	5584.7	94.18	5154.6	90.80	5192.6	89.89
1.50	5243.7	88.43	4819.1	84.89	4760.3	83.37
2.25	4921.4	82.99	4507.8	79.40	4389.7	76.84
3.00	4833.4	81.51	4235.0	74.60	4030.4	70.58
4.00	4433.0	74.75	3985.3	70.20	3608.4	63.19
5.00	4284.5	72.25	3753.2	66.11	3417.2	59.84
6.00	4044.7	68.21	3531.0	62.20	3226.3	56.50
7.00	3940.5	66.44	3278.0	57.74	2754.4	48.24
8.00	3605.8	60.81	3080.0	54.25	2686.2	47.04

Table A.4 %TOC remaining when the simulated wastewater was treated with Fenton (batch) with different ferrous sulfate amounts at any time

Time (hr)	No $FeSO_4$		$FeSO_4$ 0.0075 g		$FeSO_4$ 0.015 g	
	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining
0	7797.9	100.00	7691.2	100.00	7607.6	100.00
0.3	6965.2	89.32	6913.5	89.89	6861.8	90.20
0.7	6963.0	89.29	6882.7	89.49	6910.2	90.83
1.0	6947.6	89.10	6821.1	88.69	6793.6	89.30
1.5	6982.8	89.55	6803.5	88.46	6782.6	89.16
2.0	6989.4	89.63	6740.8	87.64	6782.6	89.16
2.5	7004.8	89.83	6726.5	87.46	6781.5	89.14
3.0	6966.3	89.34	6721.0	87.39	6619.8	87.02
3.5	6967.4	89.35	6719.9	87.37	6619.8	87.02
4.0	6964.1	89.31	6681.4	86.87	6653.9	87.46
5.0	6965.2	89.32	6663.8	86.64	6633.0	87.19

Table A.5 %TOC remaining when the simulated wastewater was treated with Fenton (semi-batch) with different ferrous sulfate amounts at any time

Time (hr)	No $FeSO_4$		$FeSO_4$ 0.003 g		$FeSO_4$ 0.0075 g	
	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining
0	7884.8	100.00	6998.2	100.00	7833.1	100.00
0.75	7505.3	95.19	6770.5	96.75	7489.9	95.62
1.50	7315.0	92.77	6733.1	96.21	7439.3	94.97
2.25	7064.2	89.59	6336.0	90.54	7257.3	92.66
3.00	6838.7	86.73	6136.96	87.69	7119.2	90.89
3.75	6515.3	82.63	65743.1	86.17	6713.3	85.70
4.50	6271.1	79.53	5743.1	82.07	6465.8	82.54
5.25	6084.1	77.16	5481.3	78.32	6073.1	77.53
6.00	5924.6	75.14	5181.0	74.03	5700.2	72.77
7.00	5718.9	72.53	5077.6	72.56	5305.3	67.73
8.00	5467.0	69.34	4637.6	66.27	4786.1	61.10

Table A.5 continued

Time (hr)	No $FeSO_4$		$FeSO_4$ 0.0113 g		$FeSO_4$ 0.015 g	
	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining	TOC (ppm)	% TOC remaining
0	7884.8	100.00	7889.3	100.0	9194.9	100.00
0.75	7505.3	95.19	7588.9	94.99	8906.7	96.87
1.50	7315.0	92.77	7629.6	95.50	8526.1	92.73
2.25	7064.2	89.59	7224.8	90.43	8143.3	88.56
3.00	6838.7	86.73	6865.1	85.93	7832.0	85.18
3.75	6515.3	82.63	6697.9	83.84	7614.2	82.81
4.50	6271.1	79.53	6371.2	79.75	7393.1	80.40
5.25	6084.1	77.16	5991.7	75.00	7242.4	78.77
6.00	5924.6	75.14	5787.1	72.44	6857.4	74.58
7.00	5718.9	72.53	5473.6	68.51	6619.8	71.99
8.00	5467.0	69.34	5145.8	64.41	6362.4	69.19

Table A.6 Composition of contaminants when the simulated wastewater was treated with Fenton (semi-batch) with different ferrous sulfate amounts at any time

Time (hr)	% wt ethanol				% wt isopropanol			
	$FeSO_4$ 0.003g	$FeSO_4$ 0.0075g	$FeSO_4$ 0.0113g	$FeSO_4$ 0.015g	$FeSO_4$ 0.003g	$FeSO_4$ 0.0075g	$FeSO_4$ 0.0113g	$FeSO_4$ 0.015g
0	1.0080	1.0594	1.0979	1.0793	0.2260	0.2166	0.2312	0.2329
0.75	1.0026	1.0100	1.0016	1.0496	0.2230	0.2043	0.2210	0.2262
1.50	0.9609	0.9789	0.9425	0.9720	0.2157	0.1938	0.2116	0.2209
2.25	0.9362	0.9043	0.9207	0.9622	0.2114	0.1876	0.2036	0.2180
3.00	0.9183	0.8854	0.8827	0.9117	0.2084	0.1752	0.1967	0.2075
3.75	0.8456	0.8327	0.8545	0.8654	0.1954	0.1714	0.1882	0.2052
4.50	0.7664	0.7802	0.8200	0.8348	0.1837	0.1594	0.1841	0.2017
5.25	0.7200	0.7463	0.7769	0.8078	0.1773	0.1526	0.1780	0.1965
6.00	0.6925	0.7172	0.7404	0.7973	0.1711	0.1461	0.1682	0.1891
7.00	0.6660	0.6625	0.7191	0.7782	0.1644	0.1383	0.1580	0.1822
8.00	0.6800	0.6383	0.6927	0.7266	0.1507	0.1362	0.1497	0.1678

Table A.7 %TOC remaining when the simulated wastewater was treated with Fenton/Air (semi-batch) with different ferrous sulfate amounts at any time

Time (hr)	$FeSO_4$ 0.0015g		$FeSO_4$ 0.003g		$FeSO_4$ 0.0075g		$FeSO_4$ 0.01g	
	TOC (ppm)	%TOC remaining	TOC (ppm)	%TOC remaining	TOC (ppm)	%TOC remaining	TOC (ppm)	%TOC remaining
0	5176.6	100.00	6829.9	100.00	6486.8	100.00	5907.0	100.00
0.75	4860.4	93.90	6277.7	91.91	6155.6	94.90	5800.3	98.19
1.50	4603.5	88.93	5728.8	83.88	5658.9	87.56	5314.1	89.96
2.25	4349.4	84.02	5265.7	77.10	5376.4	82.86	5124.9	86.76
3.00	4142.6	80.03	4480.3	65.60	5003.9	77.14	4798.2	81.23
3.75	3950.1	76.31	4215.3	61.72	4681.9	72.17	4337.3	73.43
4.50	3603.6	69.61	3730.1	54.61	4463.3	69.39	4250.4	71.96
5.25	3331.9	64.36	3439.7	50.36	4473.4	64.34	3837.4	64.97
6.00	2954.2	57.03	3339.6	48.90	3896.3	60.06	3495.8	59.18
7.00	2732.4	52.78	3248.3	47.56	3680.6	56.74	3313.2	56.09
8.00	2541.6	48.58	3092.1	45.27	3468.3	53.47	3152.6	53.37

Table A.8 Composition of contaminant when the simulated wastewater was treated with Fenton/Air (semi-batch) with different ferrous sulfate amounts at any time

Time (hr)	% wt ethanol				% wt isopropanol			
	$FeSO_4$ 0.0015g	$FeSO_4$ 0.003g	$FeSO_4$ 0.0075g	$FeSO_4$ 0.01g	$FeSO_4$ 0.0015g	$FeSO_4$ 0.003g	$FeSO_4$ 0.0075g	$FeSO_4$ 0.01g
0	0.9748	0.9907	1.0020	0.9129	0.2123	0.2256	0.2132	0.1857
0.75	0.9447	0.8396	0.9392	0.8465	0.1830	0.1937	0.1995	0.1840
1.50	0.9475	0.7507	0.9239	0.8020	0.1707	0.1672	0.1953	0.1779
2.25	0.9465	0.7158	0.8991	0.7776	0.1568	0.1517	0.1826	0.1677
3.00	0.7963	0.6586	0.8667	0.7567	0.1417	0.1487	0.1637	0.1611
3.75	0.6773	0.6222	0.8496	0.7227	0.1158	0.1364	0.1587	0.1541
4.50	0.6176	0.6088	0.7435	0.7076	0.1102	0.1163	0.1471	0.1485
5.25	0.5641	0.5495	0.6937	0.6751	0.1022	0.1103	0.1409	0.1453
6.00	0.4853	0.5082	0.6369	0.6304	0.0903	0.1029	0.1294	0.1263
7.00	0.4558	0.4641	0.5637	0.5401	0.0893	0.0921	0.1187	0.1032
8.00	0.4436	0.4227	0.4829	0.4696	0.0831	0.0821	0.1040	0.0916

APENDIX B FORTRAN program.

```
      PROGRAM FENTON_AIR

      IMPLICIT NONE
      DOUBLE PRECISION H,AL,BE,H2,FSO,Fe2,VV,V,T
      DOUBLE PRECISION Fe3,OHR,OH,ET,ISO,HH,OOH,X
      INTEGER I,J,M,N,Q
      PARAMETER (M=11)
      DOUBLE PRECISION K(M)

C *********** K-VALUE ***********

      K(1)=76.51
      K(2)=3.1E-3
      K(3)=2.7E-3
      K(4)=2E+3
      K(5)=2.7E+7
      K(6)=8.3E+5
      K(7)=3.
      K(8)=3.6E+9
      K(9)=5.5E+9
      K(11)=1.4E+11

C ***   GUESS K,ALPHA,BETA   ***

      K(10)=1E+9
      AL=1.
      BE=1.

      DO I=1,12
      K(I)=K(I)/60.
```

```
      END DO


C **** INTIAL CONCENTRATION ****  H2=H2O2        X=FeOOH2+
      C0=VV

      H=0.00001
      H2=30.
      V=H2/60.

      VV=((V*1.1*1000./(500.))/34.)
      FSO=0.0075
      FSO=FSO/278.02
      Fe2=FSO*1000./500.
      Fe3=0.
      OH=0.
      OHR=0.
      HH=0.
      OOH=0.
      ET=(1/46.)*(1000./500.)
      ISO=(0.2/60.)*(1000./500.)
      X=0.
      H2=0.
      T=0.

      J=50000000.
      Q=1.

      OPEN(1,FILE='data1.dat')
      WRITE(1,101)T,ET,ISO,H2,Fe2,Fe3,OHR,X,HH,OOH,OH

      DO I=1,J
```

```
      CALL E(T,H,AL,BE,H2,Fe2,VV,V,Fe3,OHR,OH,ET,ISO,HH,OOH,K,X)
      T=T+H
      N=I/100000.
      IF (N.EQ.Q) THEN
        WRITE(1,101)T,ET,ISO,H2,Fe2,Fe3,OHR,X,HH,OOH,OH
        Q=Q+1
    ELSE
      ENDIF
  ENDDO

101  FORMAT(E15.4,10E15.3)

      STOP
      END

C ***********************************************************
   SUBROUTINE
E(T,H,AL,BE,H2,Fe2,VV,V,Fe3,OHR,OH,ET,ISO,HH,OOH,K,X)

      IMPLICIT NONE
      DOUBLE PRECISION H,AL,BE,H2,Fe2,VV,V,T,A,AAA
      DOUBLE PRECISION Fe3,OHR,OH,ET,ISO,HH,OOH,X
      DOUBLE PRECISION Q,TEMP,MWA,P,MW
      INTEGER M
      PARAMETER (M=11)
      DOUBLE PRECISION K(M),R(M),AC(M),PVAP(M),AA(M),B(M),C(M)


   Q=2.
      AC(1)=0.
   AC(2)=0.
      MW=18.
```

```
      P=1.
      TEMP=273.15+25.
      MWA=494.+(V*T)

AA(1)=8.32109
      B(1)=1718.10
      C(1)=237.52
      AA(2)=8.11778
      B(2)=1580.92
      C(2)=219.61

      PVAP(1)=(EXP(AA(1)-(B(1)/(TEMP+C(1)))))/14.696
      PVAP(2)=(EXP(AA(2)-(B(2)/(TEMP+C(2)))))/14.696

R(1)=K(1)*Fe2*H2
      R(2)=K(2)*((-X*HH)+(Fe3*H2))
      R(3)=K(3)*X
      R(4)=K(4)*Fe3*OOH
      R(5)=K(5)*OHR*H2
      R(6)=K(6)*OOH*OOH
      R(7)=K(7)*OOH*H2
      R(8)=K(8)*OOH*OHR
      R(9)=K(9)*OHR*OHR
      R(10)=K(10)*(ET**AL)*(ISO**BE)*OHR
      R(11)=K(11)*HH*OH

Fe2=Fe2+(H*(-R(1)-R(2)-R(3)))
      Fe3=Fe3+(H*(R(1)-R(2)-R(3)))
      OHR=OHR+(H*(R(1)-R(5)+R(7)-R(9)-R(10)))
      X=X+(H*(R(2)-R(3)))
      HH=HH+(H*(R(2)+R(4)-R(11)))
      OOH=OOH+(H*(R(3)+R(5)-R(6)-R(7)-R(8)))
```

```
      OH=OH+(H*(R(1)-R(11)))

      AAA=((R(10)-(V*ET/(500.+(V*T)))))
      ET=ET+(H*(AAA-((Q*MW*PVAP(1)*ET*AC(1)/(22.4*MWA*P)))))

AAA=((R(10)-(V*ISO/(500.+(V*T)))))
      ISO=ISO+(H*(AAA-((Q*MW*PVAP(2)*ISO*AC(2)/(22.4*MWA*P)))))

A=(-R(1)-R(2)-R(5)+R(6)-R(7)-R(9)-R(10)+(V*(VV-H2)/(500.+(V*T))))
      H2=H2+(H*A)

RETURN

      END

C     ******************************************************
```

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