Institute of Paper Science and Technology

ANNUAL RESEARCH REVIEW

SLIDE MATERIAL

PROCESS SIMULATION AND CONTROL

March 23-24, 1992

Atlanta, Georgia

SLIDE MATERIAL

To The

PROCESS SIMULATION AND CONTROL

PROJECT ADVISORY COMMITTEE

March 23-24, 1992
Institute of Paper Science and Technology
Atlanta, GA

WATER REUSE
PROJECT 3725

March 23-24, 1992
Institute of Paper Science and Technology
Atlanta, GA

Project Advisory Committee Meeting

March 23, 1992

Project 3725: Water Reuse

Topics:

- Justification
- Equilibrium Calculations
- Components
- Methodology
- Applications

APPLICATIONS

- Water Reuse
- Mill Closure Effects
- Corrosion Effects
- Environmental - Waste Water Modeling

Equilibrium Calculations

Liquid-Solid-Gas(CO2)-Pulp

- Equilibrium Constants
- Adsorption Isotherms
- Solids Precipitation
- CO2 Partial Pressure Effect
- Redox Reactions

Unusual Features

Components Include:

- Surface Charge
- Carboxylate Concentration
- Electron
- 40 Other Components

Results of Calculations

Report:

- Components
- Dissolved Complexes
- Precipitates
- Adsorption Onto Pulp
- Component Distribution Percentage

Chemical Equilibrium Data Bases

- Thermodynamics
  - Equilibrium Constants
  - Stoichiometries
  - 500 Reactions
- MAPPS-To-MINEQL Relational Data
- Ionic Charge Data

CHEMICAL EQUILIBRIUM

$$C_i = K_i \prod_{j=1}^{n} X_j^{a_{ij}} \tag{1}$$

$$Y_j = \prod_{i=1}^{m} a_{ij} C_i - T_j \tag{2}$$

Logarithmic form,

$$C_i^* \quad = \quad K_i^* + \sum_{j=1}^{m} a_{ij} X_j^* \qquad (3)$$

$$\begin{aligned} C_i^* &= \log C_i \\ K_i^* &= \log K_j \\ X_j^* &= \log X_j \end{aligned} \qquad (4)$$

Matrix form

$$\overline{\overline{C}} = \overline{K} + \overline{\overline{A}}\ \overline{X} \qquad (5)$$

CO2 Partial Pressure

$$\log K' = \log K - \log P_{CO_2} \qquad (6)$$

JACOBIAN MATRIX Z_{JK}

$$Z_{jk} = \sum_{i=1}^{m} a_{ij} a_{ik} \frac{C_i}{X_k} \tag{7}$$

Solids Precipitation

One or more solid (non-fibrous) phases

Activity of solid I, $C_{II} = 1.$

$$X_{jj} = \left[K_{ii} \prod_{\substack{j=1 \\ j \neq jj}}^{n} X_j^{a_{ii,j}} \right]^{\frac{-1}{a_{ii,j}}} \tag{8}$$

$$Y_j = \sum_{\substack{i=1 \\ i \neq ii}}^{m} a_{i,j} C_i + a_{ii,j} S_{ii} - T_j \tag{9}$$

For component JJ, $Y_{JJ} = 0$

$$S_{ii} = \frac{-\left(\sum_{\substack{i=1 \\ i \neq ii}}^{m} a_{i,ii} C_i - T_{jj} \right)}{a_{ii,jj}} \tag{10}$$

Equilibrium Between Trace Cations and Fiber Solids

Protonation/Deprotonation Reactions at Amphoteric Surfaces

$$SOH + H^+ = SOH_2^+$$
$$SOH - H^+ = SO^- \qquad (11)$$

SOH = SURFACE HYDROXYL GROUP

$$[SOH]\,[H^+]\,[e^{\frac{-F\Psi}{RT}}]\,K_+ = [SOH_2^+]$$
$$[SOH]\,[H^+]^{-1}\,[e^{\frac{-F\Psi}{RT}}]\,K_- = [SO^-] \qquad (12)$$

POSITIVE SURFACE CHARGE = EXCESS OF POSITIVE GROUPS OVER NEGATIVE GROUPS

$$T_\sigma = [SOH_2^+] - [SO^-] \quad [\frac{mol}{L}] \qquad (13)$$

ADSORPTION ONTO A CHARGED SURFACES

"TOTAL CONCENTRATION" OF SURFACE CHARGE

$$T_\sigma = C\Psi\left(\frac{sa}{F}\right) \tag{14}$$

MASS ACTION EQUATIONS SOH, H^+, OH^-, AND ELECTROSTATIC POTENTIAL

$$[H^+]$$

$$[OH^-] \quad [H^+]^{-1} \quad K_1 = [OH^-]$$

$$[SOH^{2+}] \quad [SOH]\left(e^{\frac{-F\Psi}{RT}}\right)[H^+] \quad K_2 = [SOH_2^+] \tag{15}$$

$$[SOH]$$

$$[SO^-] \quad [SOH]\left(e^{\frac{-F\Psi}{RT}}\right)[H^+]^{-1} \quad K_3 = [SO^-]$$

REDOX REACTIONS

P ϵ = LOG(ELECTRON CONCENTRATION)

$$p\epsilon = -\log_{10}\epsilon \qquad E_H = 0.59\log_{10}\epsilon \tag{17}$$

Ionic Strength

Davies approximation for activity coefficient f

Ionic strength μ

$$\log f = -AZ^2\left(\frac{\mu^{1/2}}{1+\mu^{1/2}} - 0.2\mu\right) \tag{18}$$

Ionic strength:

$$\mu = \frac{1}{2}\sum_i Z_i^2 C_i \tag{19}$$

C_I = concentration of species I
Z_I = ionic charge of species I.

$$\log K^* = \left[\sum_j a_j Z_j^2 - \left(\sum_j a_j Z_j\right)^2\right] A\left(\frac{\mu^{1/2}}{1+\mu^{1/2}} - 0.2\mu\right) + \log K \tag{20}$$

SOLUTION TECHNIQUE

NEWTON RAPHSON METHOD - ITERATIVE FORMULA

$$y(x) = 0 \tag{21}$$

FOR X GIVEN THE VALUE OF X AND DY/DX AT THE NTH ITERATION

$$x^{n+1} = x^{n} - \frac{y^{n}}{\left.\frac{dy}{dx}\right|_{x^{n}}} \tag{22}$$

MATRIX EQUATION

$$\overline{Y}^{n} = \overline{\overline{Z}}^{n} \left(\overline{X}^{n} - \overline{X}^{n+1}\right) \tag{23}$$

Convergence

$$\frac{|Y_j|}{\max(Y_j)} \leq \epsilon \qquad (24)$$

$\mathrm{MAX}(Y_j)$ IS THE MAXIMUM OF THE ABSOLUTE VALUES OF THE SET OF TERMS

$$(a_{i,j}C_i) \; i=1,m \; ; \quad T_j \qquad (25)$$

TABLE I. MAPPS EQUILIBRIUM COMPONENTS

SYMBOL	SYMBOL	SYMBOL
CA(2+)	ZN(2+)	TIO(2+)
MG(2+)	AL(3+)	NH3
K+	CS(+)	S(2-)
NA+	CU(+)	SIO2(OH)2 (2-)
FE(3+)	H+	S2O3(2-)
FE(2+)	E-	CN-
MN(2+)	CO3(2-)	AC-
CU(2+)	SO4(2-)	ACAC-
BA(2+)	CL-	CIT(4-)
OX-	ENO	GLU(2-)
SAL(2-)	DIPO	NTA(3-)
DCTA(-4)	SUSAL(3-)	EDTA(4-)
PHTH(2-)	PHE(-)	SCN-
NH2OH	NO3-	TRIS
SURFACE CHARGE	SOH	

SOME OF THE MORE UNUSUAL COMPONENTS ARE DEFINED IN TABLE II.

SYMBOL	NAME
AC-	ACETATE
ACAC-	ACETYLACETONE
CIT(4-)	CITRATE
OX-	OXYLATE
SAL(2-)	SALICYLATE
ENO	ETHYLENEDIAMINE
DIPO	DIPYRIDYL
GLU(2-)	GLUTAMATE
NTA(3-)	NITRILOTRIACETATE
EDTA(4-)	ETHYLENEDIAMINE-TETRAACETATE
DCTA(4-)	1,2 DIAMINOCYCLOHEXANE TETRAACETATE
PHTH(2-)	PHTHALATE
PHE-	PHENYLALANINE
SCN-	THIOCYANATE
TRIS	TRIS(HYDROXYMETHYL)-AMINOMETHANE
SUSAL(3-)	SULFOSALICYLATE

EXECUTING MODULE 101 EQUIL01

IONIC STRENGTH = 6.00E-01 LOG F(Z=1) =-0.158

INPUT DATA

ID	X	LOGX	T	COMPONENTS
50	9.24E-09	-8.03	3.24E-04	H
101	5.07E-08	-7.29	6.79E-04	CO3-
20	2.43E-09	-8.61	1.82E-04	AL
1	5.57E-08	-7.25	7.07E-04	CA
6	1.79E-10	-9.75	5.85E-05	FE3
157	5.73E-09	-8.24	2.63E-04	NO3
159	5.88E-14	-13.23	1.79E-06	SOH
160	5.88E-14	-13.23	1.79E-06	CHRG
5	1.38E-09	-8.86	1.42E-04	NA
4	4.55E-10	-9.34	8.76E-05	K
103	6.80E-09	-8.17	2.84E-04	CL
2	2.59E-10	-9.59	6.86E-05	MG

ID	LOGK	SPECIES:	TYPE I - COMPONENTS
50	0.00	H	1
101	0.00	CO3-	1
20	0.00	AL	1
1	0.00	CA	1
6	0.00	FE3	1
157	0.00	NO3	1
159	0.00	SOH	1
160	0.00	CHRG	1
5	0.00	NA	1
4	0.00	K	1
103	0.00	CL	1
2	0.00	MG	1

ID	LOGK	SPECIES:	TYPE II - COMPLEXES				
1000	1.73	CO3-	1	CA	1		
1010	10.33	H	1	CO3-	1	CA	1
1350	-12.52	H	-1	CA	1		
1355	-15.95	CA	1	CL	2		
1360	1.93	CO3-	1	MG	1		
1370	10.33	H	1	CO3-	1	MG	1
1740	-11.52	H	-1	MG	1		
1750	-15.95	CL	2	MG	1		
1991	-15.32	K	1	CL	1		
1993	-15.32	K	2	CL	1		
2000	0.57	CO3-	1	NA	1		
2062	-15.95	CO3-	1	NA	2		
2066	-15.32	NA	1	CL	1		
2090	0.45	FE3	1	CL	1		
2100	0.52	FE3	1	CL	2		
2110	-0.60	FE3	1	CL	3		
2670	-2.33	H	-1	FE3	1		
2680	-5.65	H	-2	FE3	1		
2690	-21.05	H	-3	FE3	1		
2700	-22.13	H	-4	FE3	1		
2710	-2.30	H	-2	FE3	2		
10340	-5.13	H	-1	AL	1		

10350	-23.73	H	-4	AL	1		
10355	-16.90	AL	1	CL	3		
12530	9.57	H	1	C03-	1		
12540	15.55	H	2	C03-	1		
13595	-13.68	H	-1				
23010	2.00	H	1	SOH	1	CHRG	1
23020	1.32	H	-1	SOH	1	CHRG	1
23030	7.00	CA	1	SOH	1	CHRG	1
23040	7.00	SOH	1	CHRG	1	MG	1
23050	2.00	SOH	1	CHRG	1	K	1
23060	2.00	SOH	1	CHRG	1	NA	1
23070	17.00	FE3	1	SOH	1	CHRG	1
23130	17.00	AL	1	SOH	1	CHRG	1

ID	LOGK	SPECIES:	TYPE V - DISSOLVED SOLIDS		
20000	7.03	C03-	1	CA	1
20130	-22.22	H	-2	CA	1
20140	4.13	C03-	1	MG	1
20200	-16.72	H	-2	MG	1
20310	-3.95	H	-3	FE3	1
21180	-8.35	H	-3	AL	1

ITERATIONS= 21: SOLID 21180 PRECIPITATES

ITERATIONS= 28: SOLID 20310 PRECIPITATES

OUTPUT DATA: ITERATIONS = 31

ID	X	LOGX	T	Y	SPECIES
50	1.19E-06	-5.92	3.24E-04	4.92E-08	H
101	7.20E-08	-7.14	6.79E-04	2.41E-08	C03-
2	6.85E-05	-4.16	6.86E-05	-4.21E-11	MG
1	7.06E-04	-3.15	7.07E-04	-4.59E-11	CA
103	2.84E-04	-3.55	2.84E-04	-5.82E-11	CL
157	2.63E-04	-3.58	2.63E-04	5.82E-11	N03
159	1.72E-07	-6.77	1.79E-06	1.33E-11	SOH
160	1.72E-07	-6.77	1.79E-06	1.33E-11	CHRG
5	1.42E-04	-3.85	1.42E-04	-5.90E-12	NA
4	8.76E-05	-4.06	8.76E-05	-7.28E-12	K
20	3.76E-10	-9.43	1.82E-04	0.00E+00	AL
6	1.50E-14	-13.83	5.85E-05	0.00E+00	FE3
2	6.85E-05	-4.16	0.00	MG 1	
1000	2.76E-09	-8.56	1.73	C03- 1	
1000	2.76E-09	-8.56	1.73	CA 1	
1010	1.30E-06	-5.88	10.33	H 1	
1010	1.30E-06	-5.88	10.33	C03- 1	
1010	1.30E-06	-5.88	10.33	CA 1	
1350	1.81E-10	-9.74	-12.52	H -1	
1350	1.81E-10	-9.74	-12.52	CA 1	
1355	6.38E-27	-26.19	-15.95	CA 1	
1355	6.38E-27	-26.19	-15.95	CL 2	
1360	4.24E-10	-9.37	1.93	C03- 1	
1360	4.24E-10	-9.37	1.93	MG 1	
1370	1.27E-07	-6.90	10.33	H 1	
1370	1.27E-07	-6.90	10.33	C03- 1	
1370	1.27E-07	-6.90	10.33	MG 1	
1740	1.75E-10	-9.76	-11.52	H -1	
1740	1.75E-10	-9.76	-11.52	MG 1	

1750	6.19E-28	-27.21	-15.95	MG	1
1750	6.19E-28	-27.21	-15.95	CL	2
1991	1.20E-23	-22.92	-15.32	CL	1
1991	1.20E-23	-22.92	-15.32	K	1
1993	1.05E-27	-26.98	-15.32	CL	1
1993	1.05E-27	-26.98	-15.32	K	2
2000	3.78E-11	-10.42	0.57	CO3-	1
2000	3.78E-11	-10.42	0.57	NA	1
2062	1.63E-31	-30.79	-15.95	CO3-	1
2062	1.63E-31	-30.79	-15.95	NA	2
2066	1.95E-23	-22.71	-15.32	CL	1
2066	1.95E-23	-22.71	-15.32	NA	1
2090	1.20E-17	-16.92	0.45	CL	1
2090	1.20E-17	-16.92	0.45	FE3	1
2100	3.97E-21	-20.40	0.52	CL	2
2100	3.97E-21	-20.40	0.52	FE3	1
2110	8.61E-26	-25.07	-0.60	CL	3
2110	8.61E-26	-25.07	-0.60	FE3	1
2670	5.84E-11	-10.23	-2.33	H	-1
2670	5.84E-11	-10.23	-2.33	FE3	1
2680	2.37E-08	-7.62	-5.65	H	-2
2680	2.37E-08	-7.62	-5.65	FE3	1
2690	7.94E-18	-17.10	-21.05	H	-3
2690	7.94E-18	-17.10	-21.05	FE3	1
2700	5.51E-13	-12.26	-22.13	H	-4
2700	5.51E-13	-12.26	-22.13	FE3	1
2710	7.93E-19	-18.10	-2.30	H	-2
2710	7.93E-19	-18.10	-2.30	FE3	2
10340	2.33E-09	-8.63	-5.13	H	-1
10340	2.33E-09	-8.63	-5.13	AL	1
10350	3.48E-10	-9.46	-23.73	H	-4
10350	3.48E-10	-9.46	-23.73	AL	1
10355	1.08E-37	-36.97	-16.90	CL	3
10355	1.08E-37	-36.97	-16.90	AL	1
12530	3.16E-04	-3.50	9.57	H	1
12530	3.16E-04	-3.50	9.57	CO3-	1
12540	3.62E-04	-3.44	15.55	H	2
12540	3.62E-04	-3.44	15.55	CO3-	1
13595	1.74E-08	-7.76	-13.68	H	-1
23010	3.51E-18	-17.46	2.00	H	1
23010	3.51E-18	-17.46	2.00	SOH	1
23010	3.51E-18	-17.46	2.00	CHRG	1
23020	5.14E-07	-6.29	1.32	H	-1
23020	5.14E-07	-6.29	1.32	SOH	1
23010	3.51E-18	-17.46	2.00	CHRG	1
23020	5.14E-07	-6.29	1.32	H	-1
23020	5.14E-07	-6.29	1.32	SOH	1
23020	5.14E-07	-6.29	1.32	CHRG	1
23030	2.08E-10	-9.68	7.00	CA	1
23030	2.08E-10	-9.68	7.00	SOH	1
23030	2.08E-10	-9.68	7.00	CHRG	1
23040	2.02E-11	-10.69	7.00	MG	1
23040	2.02E-11	-10.69	7.00	SOH	1
23040	2.02E-11	-10.69	7.00	CHRG	1
23050	2.59E-16	-15.59	2.00	SOH	1
23050	2.59E-16	-15.59	2.00	CHRG	1
23050	2.59E-16	-15.59	2.00	K	1
23060	4.19E-16	-15.38	2.00	SOH	1
23060	4.19E-16	-15.38	2.00	CHRG	1
23060	4.19E-16	-15.38	2.00	NA	1

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23070  4.41E-11  -10.36   17.00     SOH    1
23070  4.41E-11  -10.36   17.00     CHRG   1
23070  4.41E-11  -10.36   17.00     FE3    1
23130  1.11E-06   -5.96   17.00     SOH    1
23130  1.11E-06   -5.96   17.00     CHRG   1
23130  1.11E-06   -5.96   17.00     AL     1
21180  1.81E-04   -3.74   -8.35     H     -3
21180  1.81E-04   -3.74   -8.35     AL     1
20310  5.85E-05   -4.23   -3.95     H     -3
20310  5.85E-05   -4.23   -3.95     FE3    1
20140  6.72E-08   -7.17    4.13     CO3-   1
20140  6.72E-08   -7.17    4.13     MG     1
20200  9.31E-10   -9.03  -16.72     H     -2
20200  9.31E-10   -9.03  -16.72     MG     1
20130  3.03E-14  -13.52  -22.22     H     -2
20130  3.03E-14  -13.52  -22.22     CA     1
20000  5.50E-04   -3.26    7.03     CO3-   1
20000  5.50E-04   -3.26    7.03     CA     1
 OUTPCX ROUTINE

  PERCENTAGE DISTRIBUTION OF COMPONENTS


H
          97.5     PERCENT BOUND IN SPECIES #12530   H      1     CO3-   1
         223.1     PERCENT BOUND IN SPECIES #12540   H      2     CO3-   1


CO3-
          46.5     PERCENT BOUND IN SPECIES #12530   H      1     CO3-   1
          53.3     PERCENT BOUND IN SPECIES #12540   H      2     CO3-   1


MG
          99.8     PERCENT BOUND IN SPECIES #    2   MG     1


CA
          99.8     PERCENT BOUND IN SPECIES #    1   CA     1


CL
         100.0     PERCENT BOUND IN SPECIES #  103   CL     1


NO3
         100.0     PERCENT BOUND IN SPECIES #  157   NO3    1


SOH
           9.6     PERCENT BOUND IN SPECIES #  159   SOH    1
          28.7     PERCENT BOUND IN SPECIES #23020   H     -1     SOH    1
CHRG
```

```
   1
        61.8     PERCENT BOUND IN SPECIES #23130   SOH    1    CHRG   1    AL
   1



CHRG
         9.6     PERCENT BOUND IN SPECIES #  160   CHRG   1
        28.7     PERCENT BOUND IN SPECIES #23020   H     -1    SOH    1
CHRG
   1
        61.8     PERCENT BOUND IN SPECIES #23130   SOH    1    CHRG   1    AL
   1



NA
       100.0     PERCENT BOUND IN SPECIES #    5   NA     1



K
       100.0     PERCENT BOUND IN SPECIES #    4   K      1



AL
        99.4     PERCENT BOUND IN SPECIES #21180   H     -3    AL     1



FE3
       100.0     PERCENT BOUND IN SPECIES #20310   H     -3    FE3    1
?

DIS STR 113
STREAM    TYPE PULP     NUMBER =  113
     LAB = "STR 113 - PULP       "
     FLOW =  0.4967E+05 CU FT/HR    %DS =    0.21    %CONSIS =    1.20

      1 = NUMBER      113.000            2 = TYPE       3.00000
      3 = TEMP        110.694            4 = PRESS      14.7000
      5 = *HT CAP   0.989910             6 = *PH        5.92485
      7 =           0.000000E+00         8 = *ENTHALP  0.470202E+09
      9 = *GIBBS    0.368312E+09        10 = *FLOW     0.305499E+07
     11 = WATER     0.301182E+07        12 = FINES      10208.9
     13 = FIBER1      3289.73           14 = FIBER2     2130.12
     15 = FIBER3      4908.64           16 = FIBER4     4421.91
     17 = FIBER5      2009.25           18 = FIBER6     1795.00
     19 = FIBER7      729.292           20 = FIBER8     4274.01
     21 = FIBER9      2814.89           22 = SHIVE1    0.796530E-10
     23 = SHIVE2    0.233332E-10        24 = SHIVE3    0.000000E+00
     25 = CHIPS     0.000000E+00        26 = DIS CARB  0.000000E+00
     27 = DIS LIGN  0.000000E+00        28 = INERT     0.000000E+00
     29 = TALL OIL  0.000000E+00        30 = TURPENTN   2036.70
     31 = CH3OH(L)    145.425           32 = CH3SH      118.917
     33 = H2S         3817.58           34 = SULFUR    0.000000E+00
     35 = BND NAOH  0.000000E+00        36 = NEUT OH-  0.000000E+00
     37 = OH-       0.257463E-04        38 = SH-       0.000000E+00
     39 = S-2       0.000000E+00        40 = S2O3-2    0.000000E+00
```

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41 = S04-2      0.000000E+00
42 = C03-2      124.720
43 = NA+        10.0000
44 = K+         10.4894
45 = CL-        30.7930
46 = AL+3       5.66744
47 = SILICA     0.000000E+00
48 = CA+2       86.7657
49 = FE+3       0.255693E-08
50 = CAC03      0.000000E+00
51 = CA(OH)2    0.000000E+00
52 = CAO        0.000000E+00
53 = CAO BRNT   0.000000E+00
54 = CAS04      0.000000E+00
55 = NA2C03     0.000000E+00
56 = NA2S       0.000000E+00
57 = NA2S04     0.000000E+00
58 = NACL       0.000000E+00
59 = K2C03      0.000000E+00
60 = CARBON     0.000000E+00
61 = CL2        0.000000E+00
62 = CL02       110.000
63 = 02         0.000000E+00
64 = OX CELL    0.000000E+00
65 = CL LIGN    0.000000E+00
66 = CL BND     0.000000E+00
67 = H+         0.000000E+00
68 = CLO-       0.000000E+00
69 = CL02-      0.000000E+00
70 = CL03-      0.000000E+00
71 = H202       0.000000E+00
72 = SI02(OH)   0.000000E+00
73 = CS BND     0.000000E+00
74 = ZN BND     0.000000E+00
75 = AL BND     0.915428E-01
76 = MG BND     0.150349E-05
77 = MN BND     0.000000E+00
78 = FE BND     0.754210E-05
79 = CS++       0.000000E+00
80 = BA++       0.000000E+00
81 = MG+2       5.09890
82 = N2         0.000000E+00
83 = KNOTS      0.000000E+00
84 = NH3        0.000000E+00
85 = TIO+2      0.000000E+00
86 = S03-2      0.000000E+00
87 = N03-       50.0000
88 = ZN++       0.000000E+00
89 = CHCL3      0.000000E+00
90 = P          0.000000E+00
91 = MN+2       0.000000E+00
92 = DISSOL1    0.000000E+00
93 = BA BND     0.000000E+00
94 = K BND      0.000000E+00
95 = SUSSOL1    0.000000E+00
96 = CU+2       0.000000E+00
97 = CU BND     0.000000E+00
98 = AL BND     0.000000E+00
99 = CA BND     0.255458E-04
100 = NA BND    0.000000E+00
101 = TI02 ANA  0.000000E+00
102 = TI02 B    0.000000E+00
103 = CLAY FIL  0.000000E+00
104 = CLAY CAL  3.00000
105 = TALC      3.00000
106 = PLASTIC   10.0000
107 = KCL       0.000000E+00
108 = MGCL2     0.000000E+00
109 = CACL2     0.000000E+00
110 = K2S04     0.000000E+00
111 = MGS04     0.000000E+00
112 = NAAL02    0.000000E+00
113 = ALCL3     0.000000E+00
114 = AC-1      0.000000E+00
115 = CN-1      0.000000E+00
116 = ACAC-1    0.000000E+00
117 = CIT-4     0.000000E+00
118 = OX-1      0.000000E+00
119 = SAL-2     0.000000E+00
120 = TRIS      0.000000E+00
121 = EDTA-4    0.000000E+00
122 = DCTA-4    0.000000E+00
123 = E-1       0.000000E+00
124 = EN0       0.000000E+00
125 = GLU-2     0.000000E+00
126 = DIP       0.000000E+00
127 = SCN-1     0.000000E+00
128 = NH2OH     0.000000E+00
129 = PHE-1     0.000000E+00
130 = NTA-3     0.000000E+00
131 = SUSAL-3   0.000000E+00
132 = PHTH-2    0.000000E+00
133 = FE+2      0.000000E+00
134 = CASI02    0.000000E+00
135 = CAOX+     0.000000E+00
136 = MGC03     0.000000E+00
137 = MGOX      0.000000E+00
138 = MG(OH)2   0.000000E+00
139 = FE(OH)3   19.1292
?
```

SYSTEMS ANALYSIS
PROJECT 3741

March 23-24, 1992
Institute of Paper Science and Technology
Atlanta, GA

Project Advisory Committee Meeting

March 23, 1992

Project 3741: Systems Analysis

Topics:

- New Stream Structure
- Solids Separation
- Dynamic Modules
- Systems Integration
- Applications
- Windows

Goals

- Develop And Test The PI-MAPPS Interface And The Continuous Digester Application
- Develop And Test New Dynamic Blocks
- Add To MAPPS Stream Components For Improved Papermaking Simulation

New Databases For MAPPS Stream Structures

- Suspended Solids Data
- Equilibrium Data
- Added Components To Stream Database
- Dye Reflectance Added To PAT Stream Database

New Stream Structure

- Combined Pulping, Bleaching, Paper, Waste, And Recovery Streams Into A Single Stream
- Approximately 160 Components
- Includes All Previous Components From Pulp, Bleach, Paper, And Recovery Except Lignin And Cellulose

- Plus - 30 New Suspended Solids
  - New Trace Ions
  - Adsorbed Ions Onto Pulp
  - MAPPS Components Not Previously Used
- Streams Are Now Numbered
  - 1: Water
  - 2: Gaseous
  - 3: Pulp
  - 4: Fuel
  - 5: Energy And Heat
  - 6: Information
- All Modules Rewritten To Work With "Streamlined" Stream Structure

New PATS

- Carboxylate Concentration
- CD Stretch
- Suspended Solids Attributes
  - Specific Gravity
  - Adsorption Coefficient
  - Standard Deviation Of Diameter
- Saturated Dye Loadings
  - Red, Blue, And Yellow

Validation

New Stream Structure Tested On CEDED, Power, And Linerboard Papermachine

Solids Separation

- 43 Solids Components
  - 10 Fibrous
  - 33 Nonfibrous
- New HYFRAC Cyclone Calculations
- FOUR01 And MPFORM Separations

SOLIDS SEPARATION

PRESSURE DROP

$$\Delta P = \rho\left(\frac{V_i^2}{2g_c}\right)\frac{\alpha^2}{N}\left[\left(\frac{D_c}{D_o}\right)^{2n} - 1\right] \tag{1}$$

REJECT SEPARATION EFFICIENCY

$$\epsilon_r = 1 - e^{-\left(\frac{D_p}{D_{50}} - 0.115\right)^2} \tag{2}$$

D_p = PARTICLE DIAMETER

D_{50} = DIAMETER FOR 50% SEPARATION EFFICIENCY

$$D_{50} = 2.7\,\xi_2\sqrt{\xi_1} \tag{3}$$

$$\xi_1 = \frac{\xi_0}{\rho_p - \rho_l} \tag{4}$$

$$\xi_0 = \tan\left(\frac{\Theta}{2}\right)\frac{\mu_l(1-RF)}{D_c Q} \tag{5}$$

RF = TOTAL REJECT FLOW SPLIT
θ = ANGLE OF THE CYCLONE
Q = VOLUMETRIC FLOW RATE
μ_L = LIQUID PHASE VISCOSITY

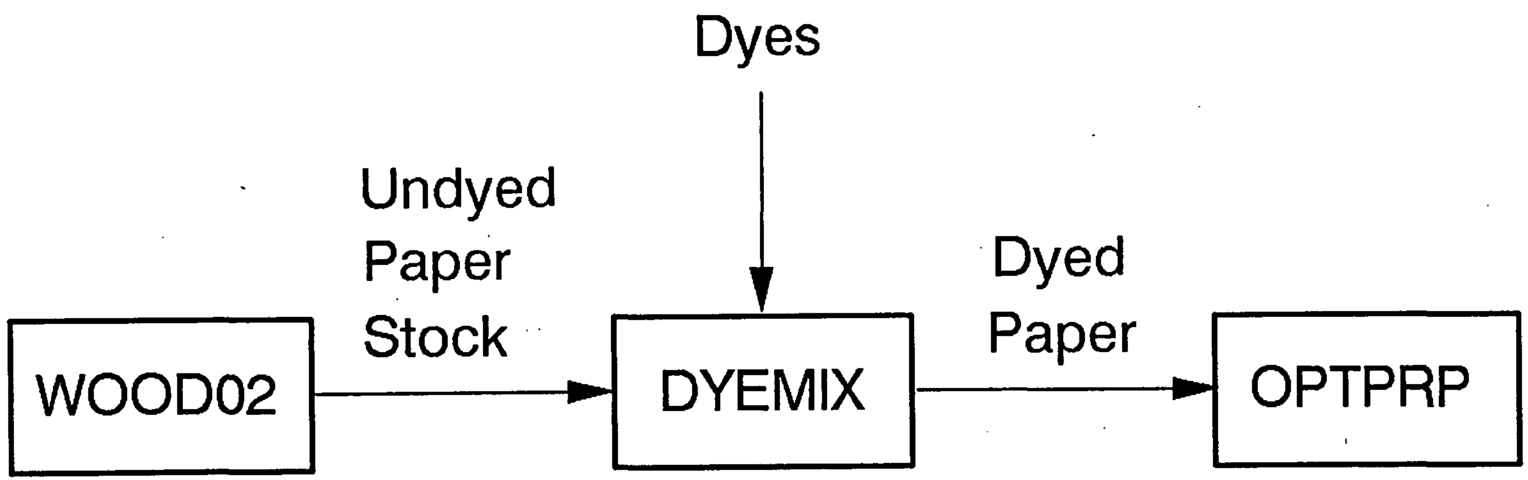
SCREEN REJECT FRACTION

$$\epsilon_r = RF + \frac{1}{2}(1-RF)\left(1-\frac{1}{e}\right)\left(1+\tanh\left(p_1\left(D_s - p_2 + 15D_s(RFD_s)^{1/2}\right)\right)\right) \tag{6}$$

Saturated Color & Optical Properties

- L * a * b
- R
  - Two Illuminants
  - Two Angles
- Tappi Opacity 457 And 572 nm
- Brightness 457 nm

The MAPPS Dyeing Process Model



COLOR MATCHING

$$\bar{x}(\lambda), \bar{y}(\lambda), \bar{z}(\lambda)$$

TRISTIMULUS VALUES, X, Y, Z

$$\begin{aligned} X &= k\sum R(\lambda)S(\lambda)\bar{x}(\lambda) \\ Y &= k\sum R(\lambda)S(\lambda)\bar{y}(\lambda) \\ Z &= k\sum R(\lambda)S(\lambda)\bar{z}(\lambda) \end{aligned}$$

SPECTRAL POWER DISTRIBUTION S
WAVELENGTH INTERVAL R
SCALING FACTOR K

$$k = \frac{100}{\sum S(\lambda)\bar{y}(\lambda)}$$

ILLUMINANT C AND D65
2 AND 10 DEGREE FIELD OF VIEW

NEED FUNCTIONS CORRELATED WITH HUE, SATURATION, DEPTH, VIVIDNESS, REDNESS-GREENESS AND YELLOWNESS-BLUENESS

CIE 1976 L* A* B* SPACE

$$L* = 116\left[\frac{Y}{Y_n}\right]^{\frac{1}{3}} - 16 \qquad \mathit{for}\ \frac{Y}{Y_n} > 0.008856$$

$$L* = 903.3\frac{Y}{Y_n} \qquad \mathit{for}\ \frac{Y}{Y_n} \leq 0.008856$$

A* AND B* FUNCTIONS OF X/X_N, Y/Y_N AND Z/Z_N

VISUAL COLOR DIFFERENCE DEFINED BY

$$\Delta E = \sqrt{\Delta L*^2+\Delta a*^2+\Delta b*^2}$$

COLOR MATCHING - TOLERANCE IN COMMERCIAL

COLOR MATCHES < 2

BLACK VS. WHITE = 100

Prediction of Saturated Color in Paper

Kubelka-Monk

$$R_\infty = 1 + \frac{K}{S} - \sqrt{2\frac{K}{S} + \left(\frac{K}{S}\right)^2}$$

Assumptions:

Dyes don't contribute to scattering - only influence absorption

Dye Absorption Coefficient - K_I
Light scattering caused only by substrate

$$\left(\frac{K}{S}\right)_{dyed\ sheet} = \left(\frac{K}{S}\right)_{substrate} + \sum_{i=1}^{m} K_i C_i$$

Reflectance of Base Sheet:

$$\left(\frac{K}{S}\right)_{undyed\ pulp} = \beta_0 + \beta_1\lambda + \beta_2\left(\frac{K}{S}\right)_{\lambda=457} + \beta_3\lambda^2 + \beta_4\lambda^3 + \beta_4\lambda\left(\frac{K}{S}\right)_{\lambda=457}$$

Reflectance at 457 determined from Performance Attribute System

Delta E Values for IPST Handsheets
Dye Loadings in Oz./ton

Blue - Red Black	2 degrees Illum C	2 degrees Illum D65	10 deg Illum C	10 deg Illum D65
2.5/0/0	1.13	0.989	0.7788	0.733
0/2.5/0	1.33	1.27	0.988	0.988
0/2/0	0.65	0.60	0.448	0.62
1.35/0/.45 /0	1.49	1.36	1.07	0.95
1.35/0.75/ 0	1.55	1.50	1.07	1.00
1.8/0.45/0	1.39	1.28	1.04	0.99
1.8/0.75/0	1.42	1.30	1.02	0.93
1.5/0.6/ 1.2	1.42	1.30	1.04	0.95
1.5/0.6/ 1.8	1.38	1.28	1.06	0.99

Delta E Values for Couch Handsheets
Dye Loadings in Lb/Ton

Blue/Red/ Yellow	2 Degree Illum C	2 Degree Illum D65	10 Degree Illum C	10 Degree Illum D65
0/0/0	3.65	3.88	3.62	3.73
1/1/3	2.77	2.92	2.87	3.08
3/1/1	4.9	5.1	4.9	5.1
1/3/1	3.45	3.72	3.41	3.65
10/10/5	0.41	0.407	0.500	0.679
5/10/10	1.57	1.36	1.27	1.14
10/5/10	1.66	1.77	1.92	2.08
5/15/5	2.76	2.68	2.51	2.48
15/5/5	2.51	2.41	2.38	2.31
5/5/15	1.64	1.65	1.65	1.75

Delta E Values for Machine Papers
Dye Loadings in Lb/Ton

Blue/Red/ Yellow	2 Degree Illum C	2 Degree Illum D65	10 Degree Illum C	10 Degree Illum D65
0/0/0	4.16	4.10	3.80	3.78
1/1/3	2.45	2.31	2.11	2.03
3/1/1	0.703	0.631	0.331	0.425
1/3/1	2.35	2.13	1.87	1.60
10/10/5	5.07	5.02	4.62	4.60
5/10/10	5.81	5.61	5.16	4.97
10/5/10	5.69	5.60	5.65	5.63
5/15/5	6.03	6.00	5.45	5.40
15/5/5	4.47	4.34	4.00	3.86
5/5/15	6.39	6.18	5.73	5.60

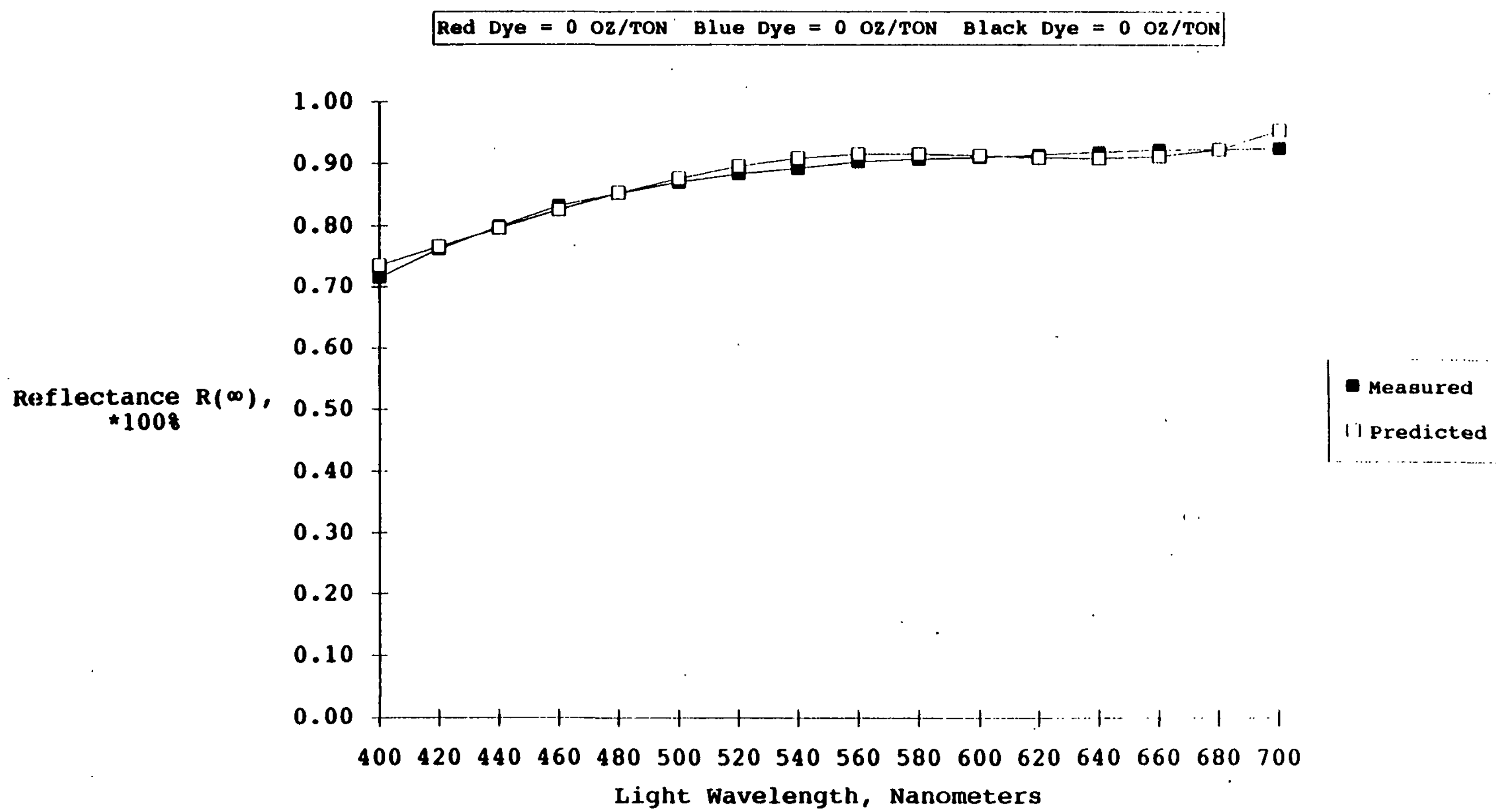


Figure 44. Measured and Predicted Reflectance of IPST Handsheets (No dye)

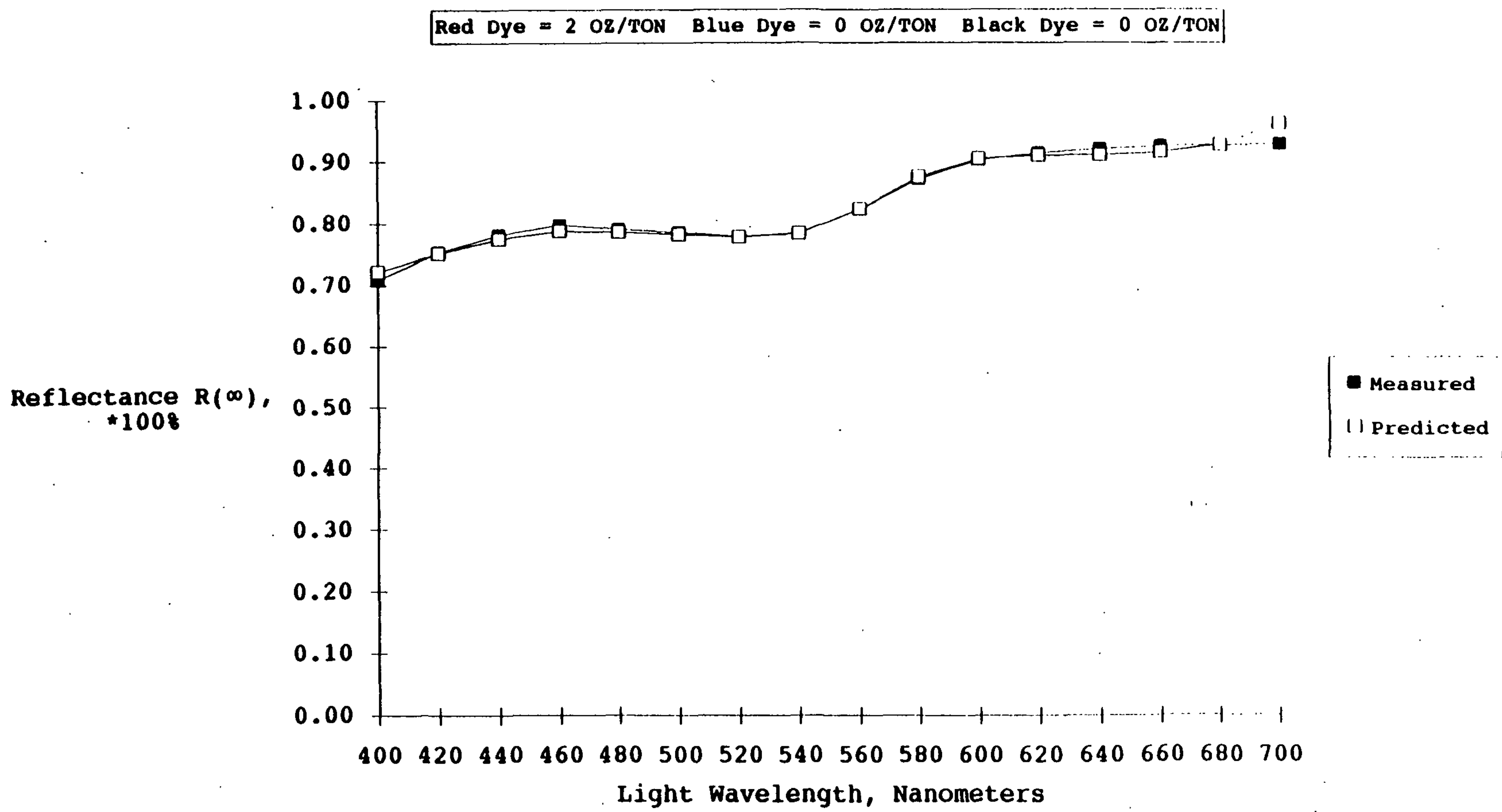


Figure 46. Measured and Predicted Reflectance of IPST Handsheets

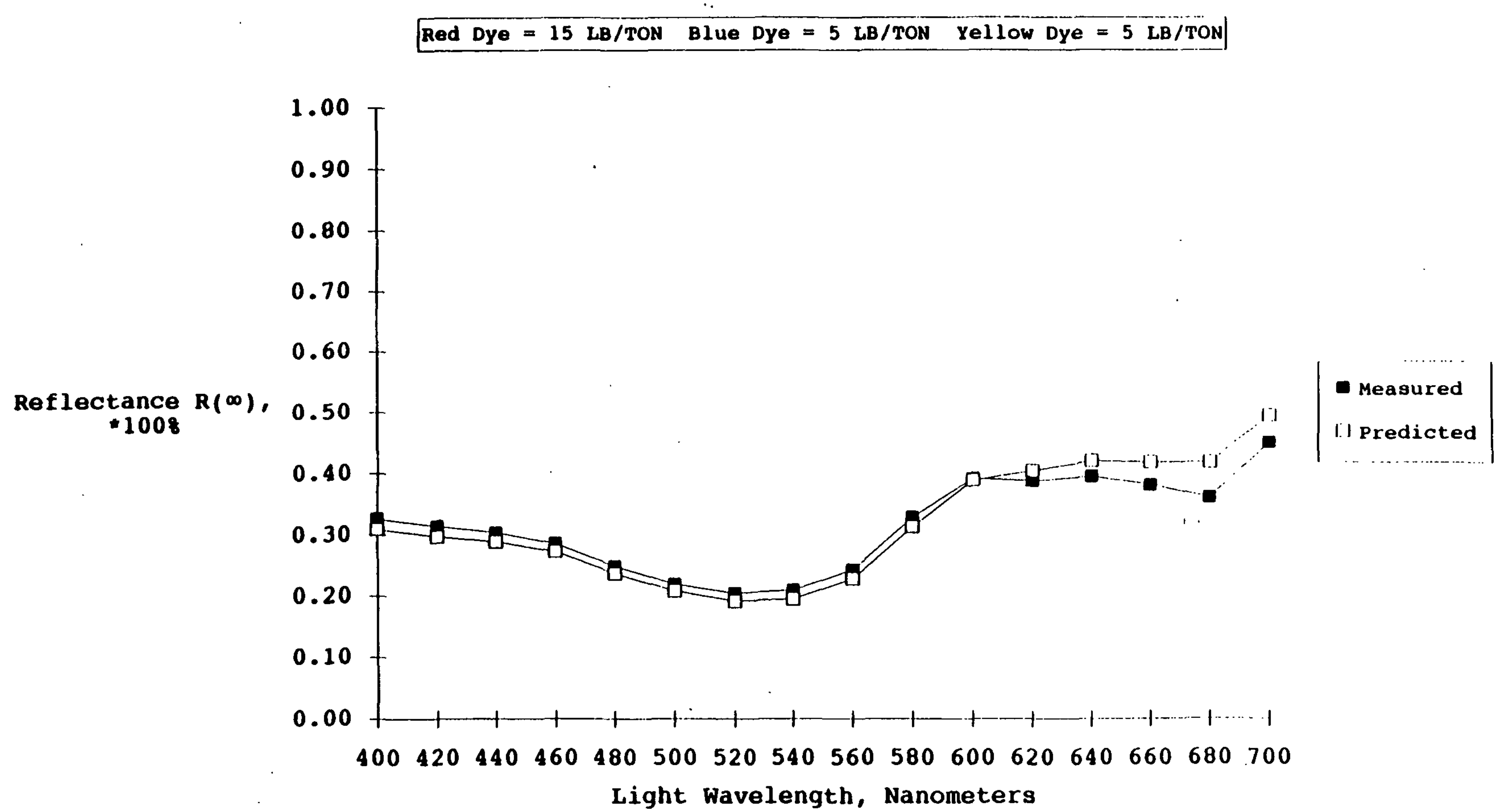


Figure 31. Measured and Predicted Reflectance of Couch Handsheets (Case 7)

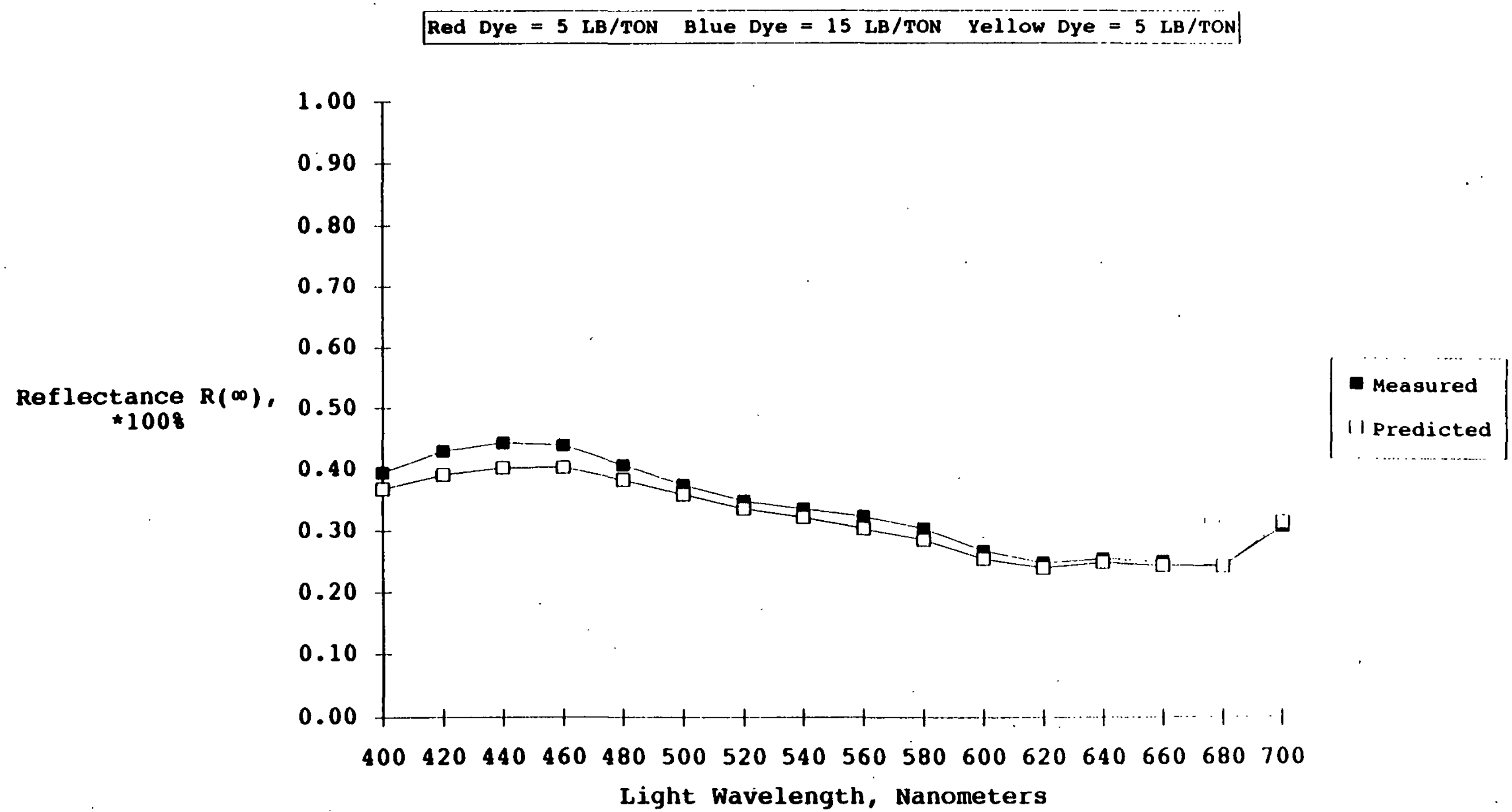


Figure 23. Measured and Predicted Reflectance of the Calibration Handsheets (Mix 8)

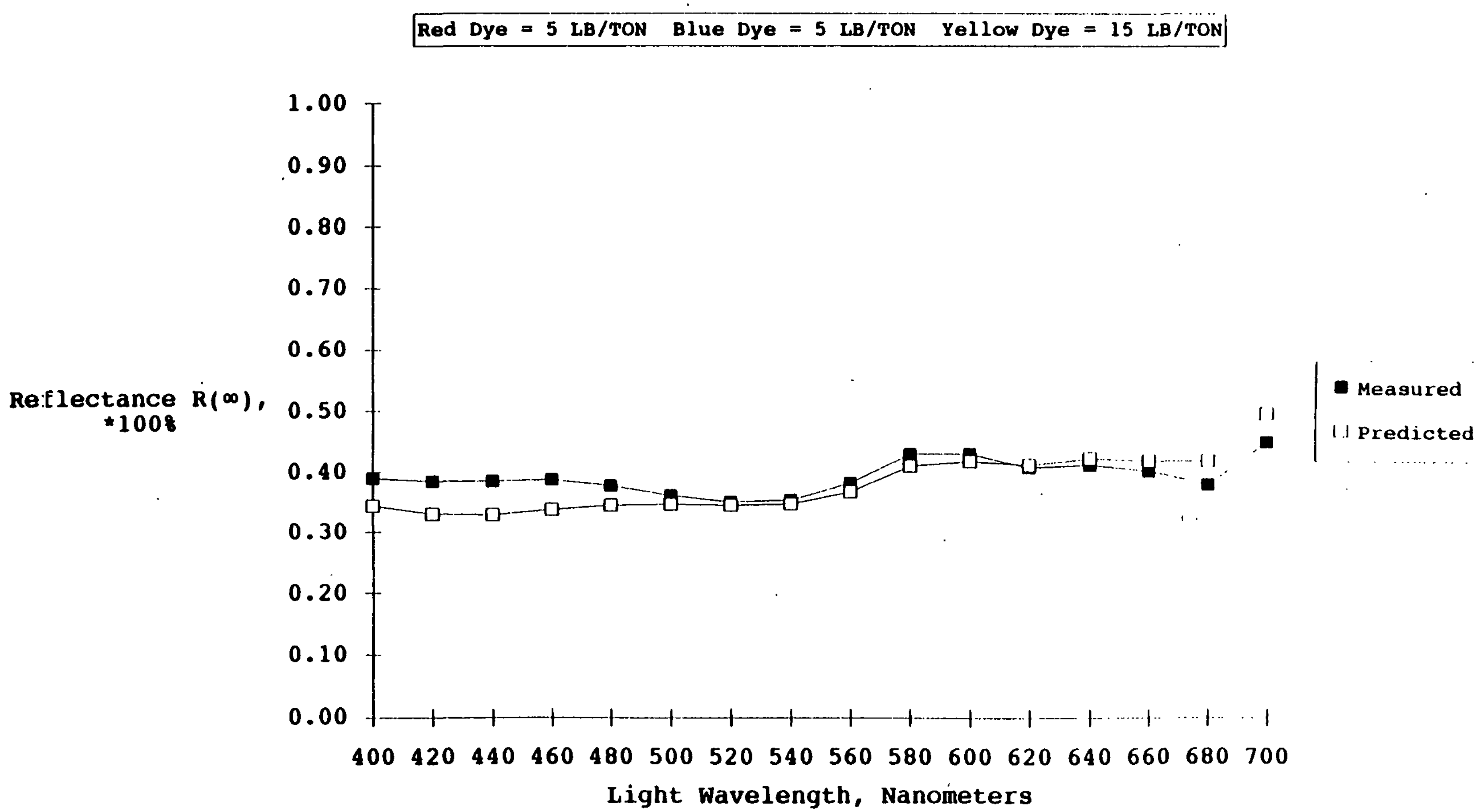


Figure 24. Measured and Predicted Reflectance of the Calibration Handsheets (Mix 9)

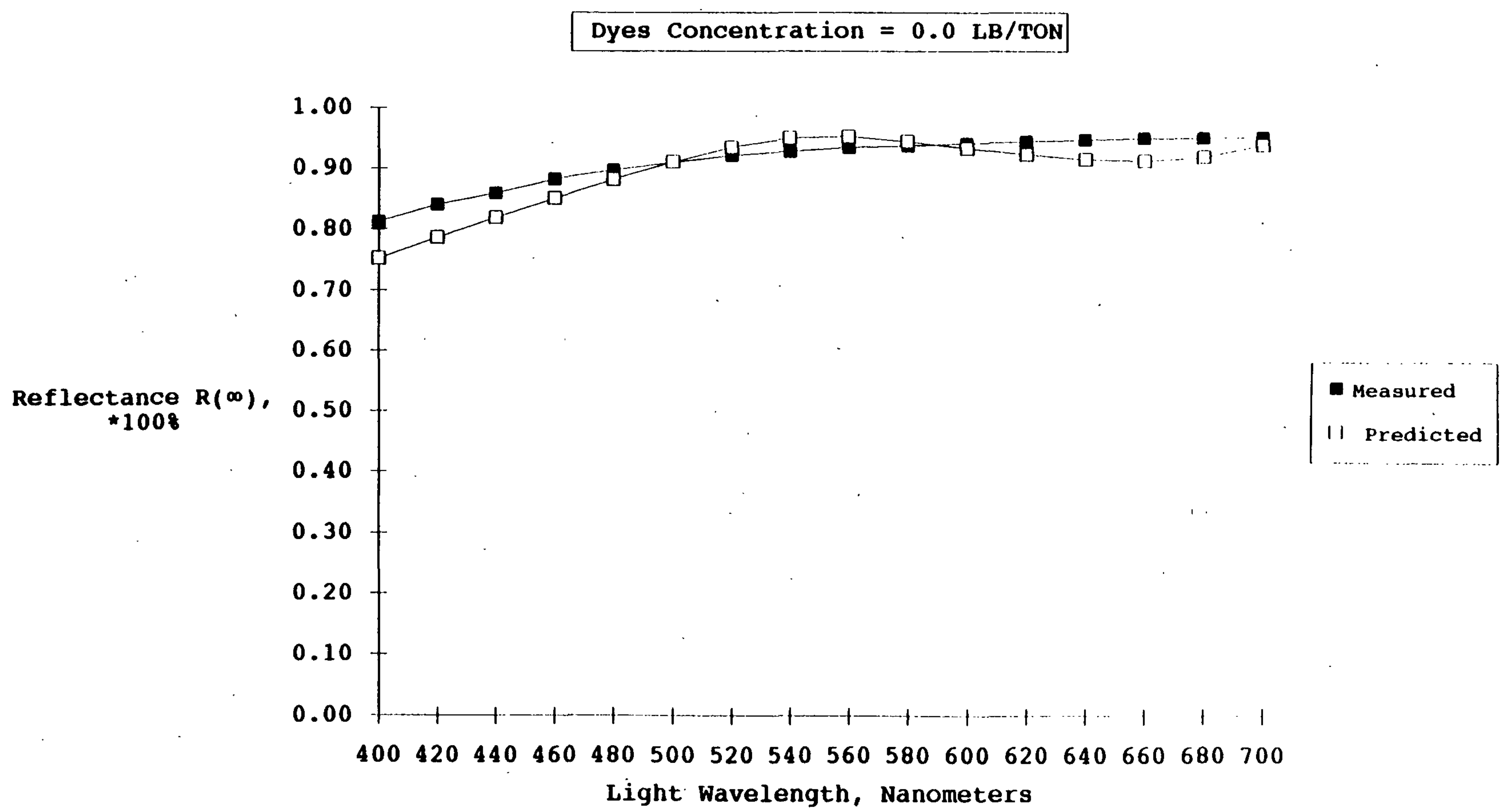


Figure 34. Measured and Predicted Reflectance of Machine Paper

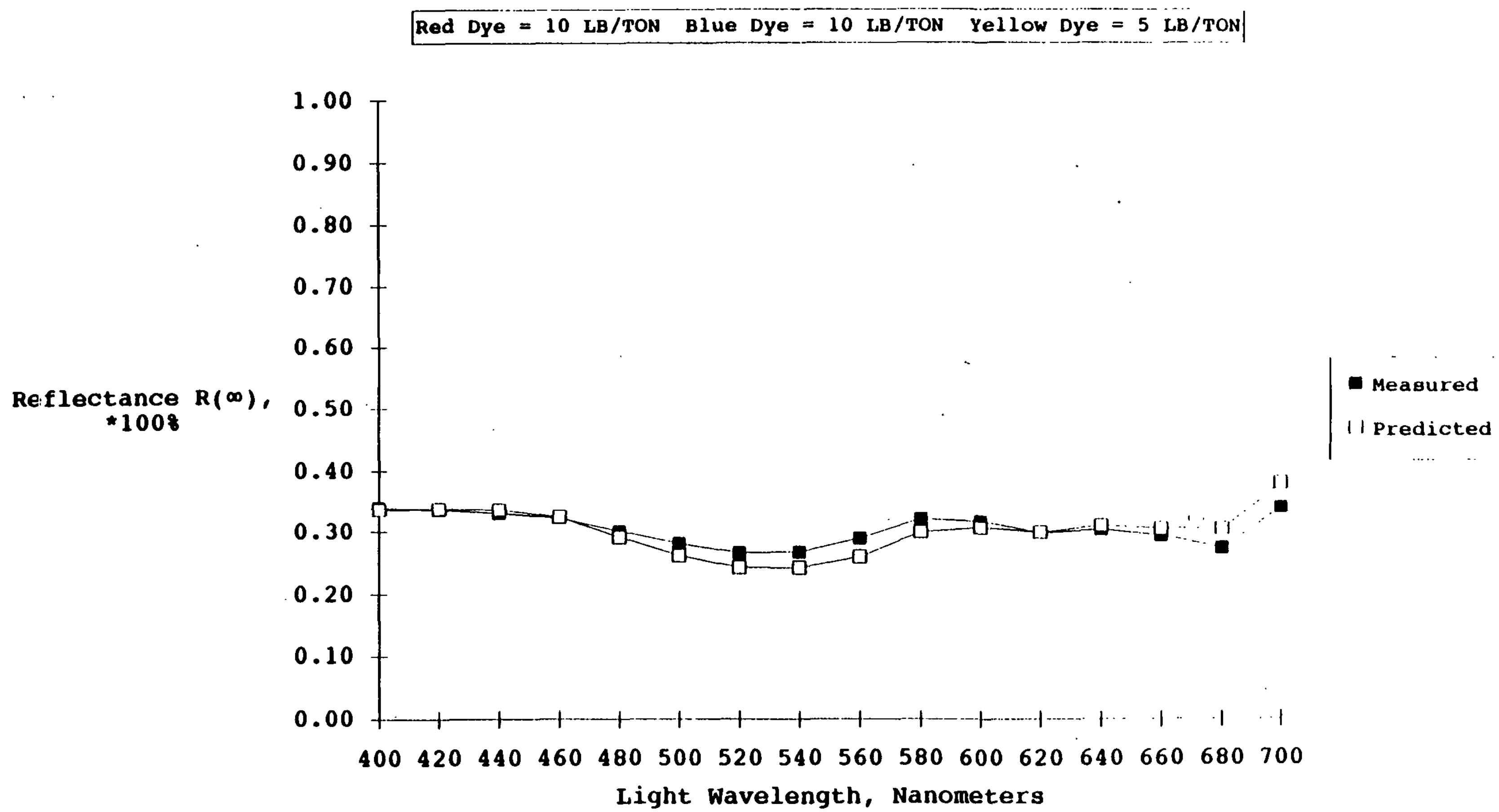


Figure 38. Measured and Predicted Reflectance of Machine Paper (Case 4)

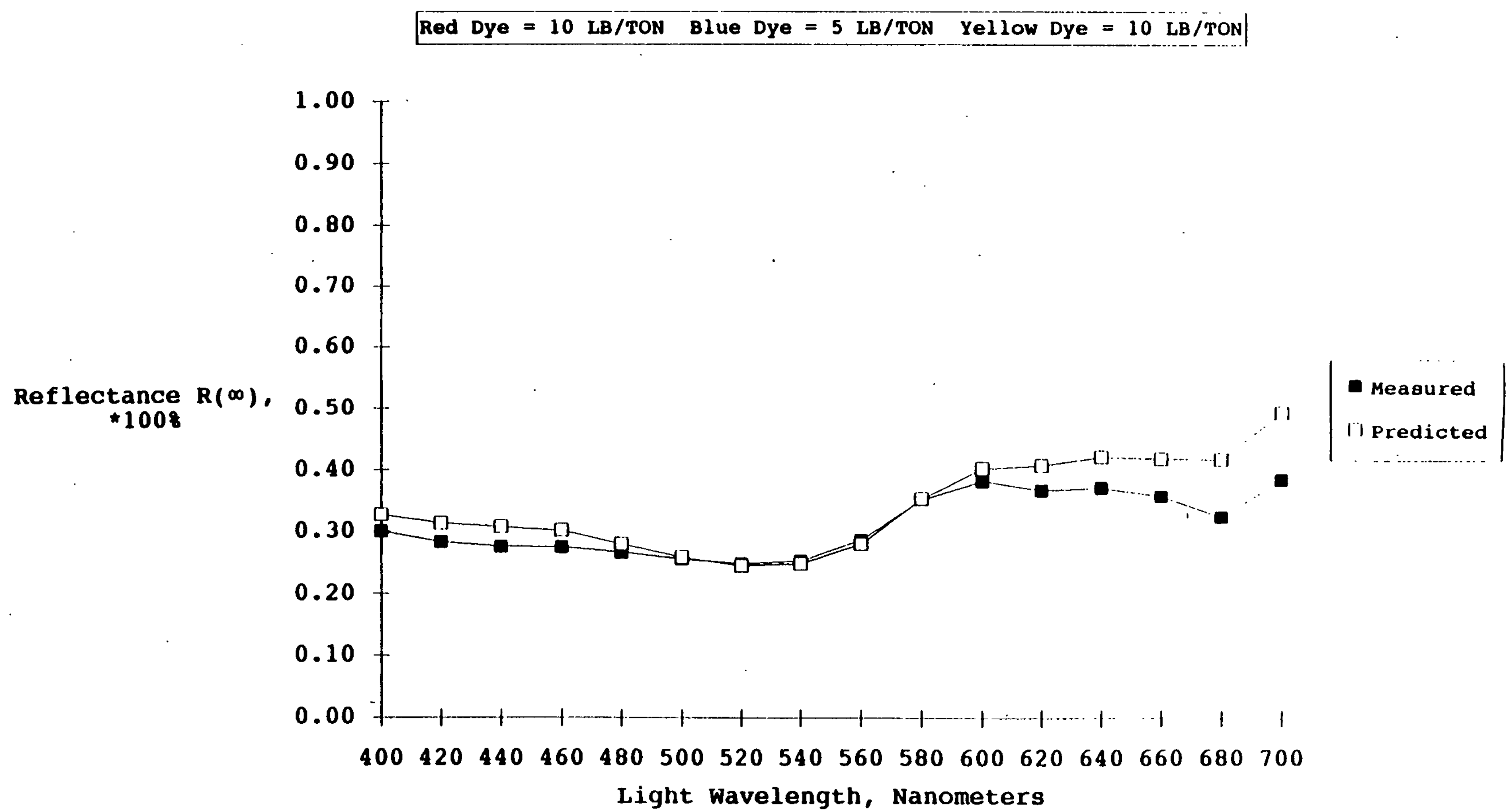


Figure 39. Measured and Predicted Reflectance of Machine Paper (Case 5)

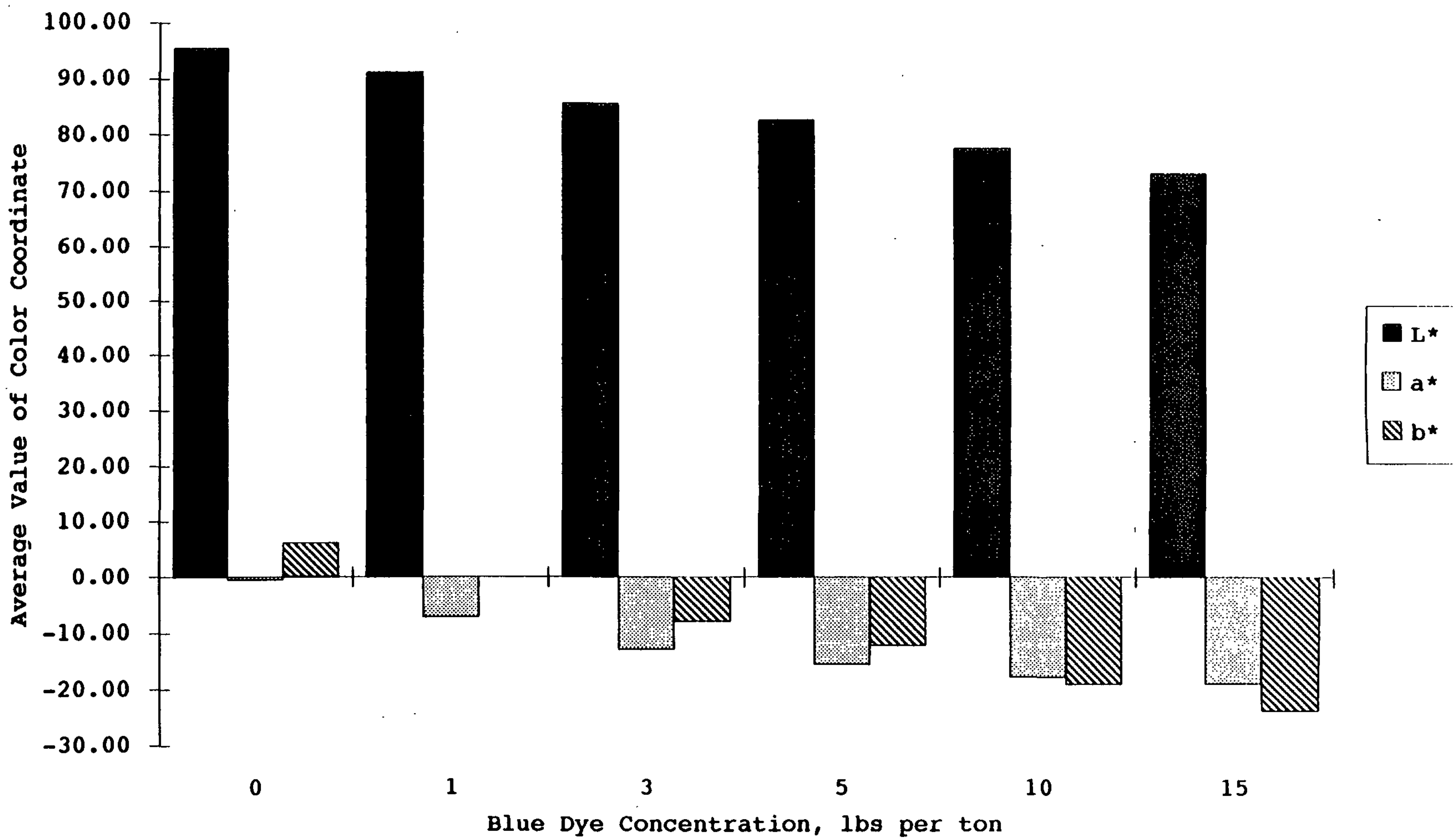


Figure 58. Effects of Blue Dye Concentration on the Color Coordinates

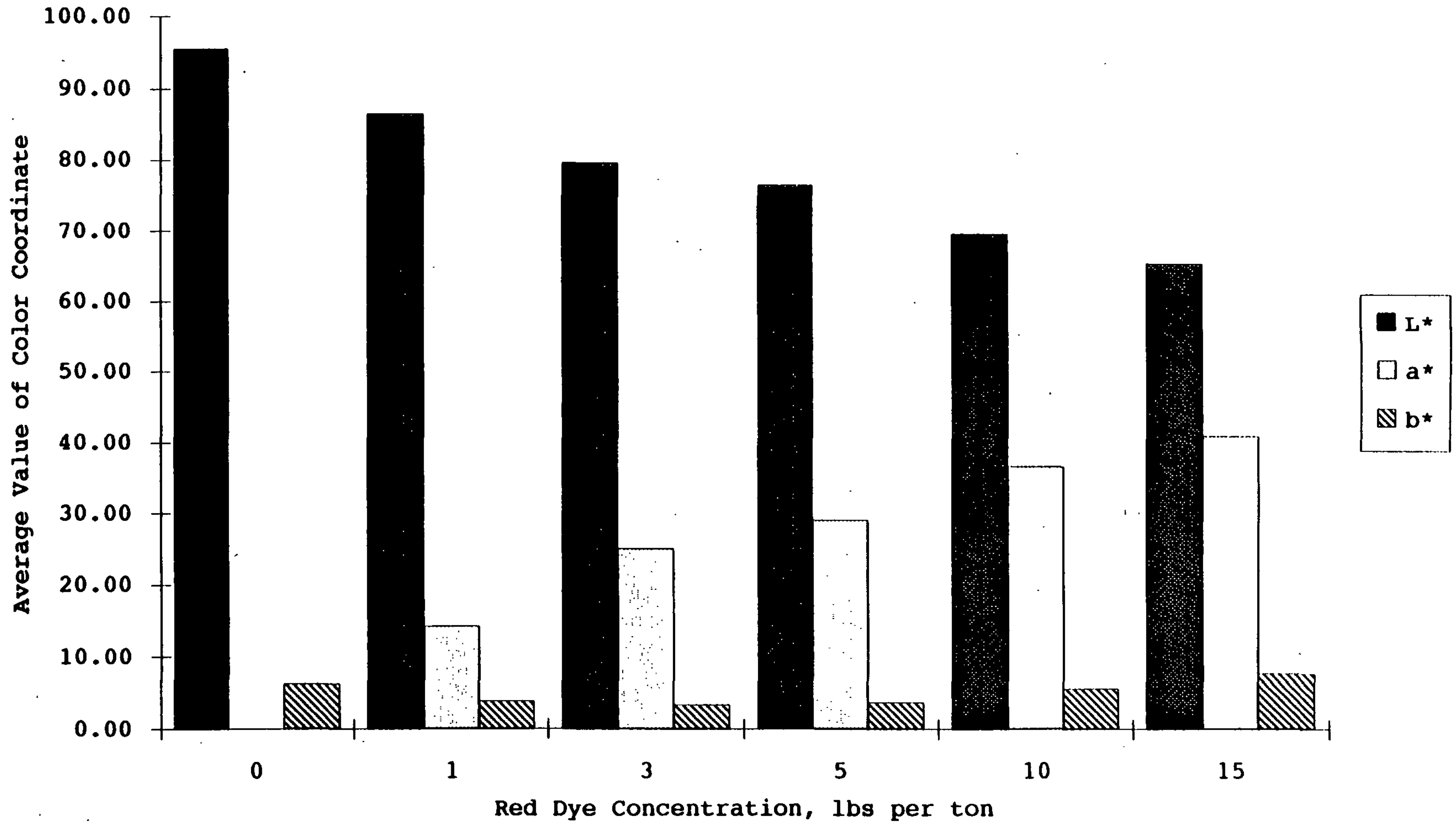


Figure 57. Effects of Red Dye Concentration on the Color Coordinates

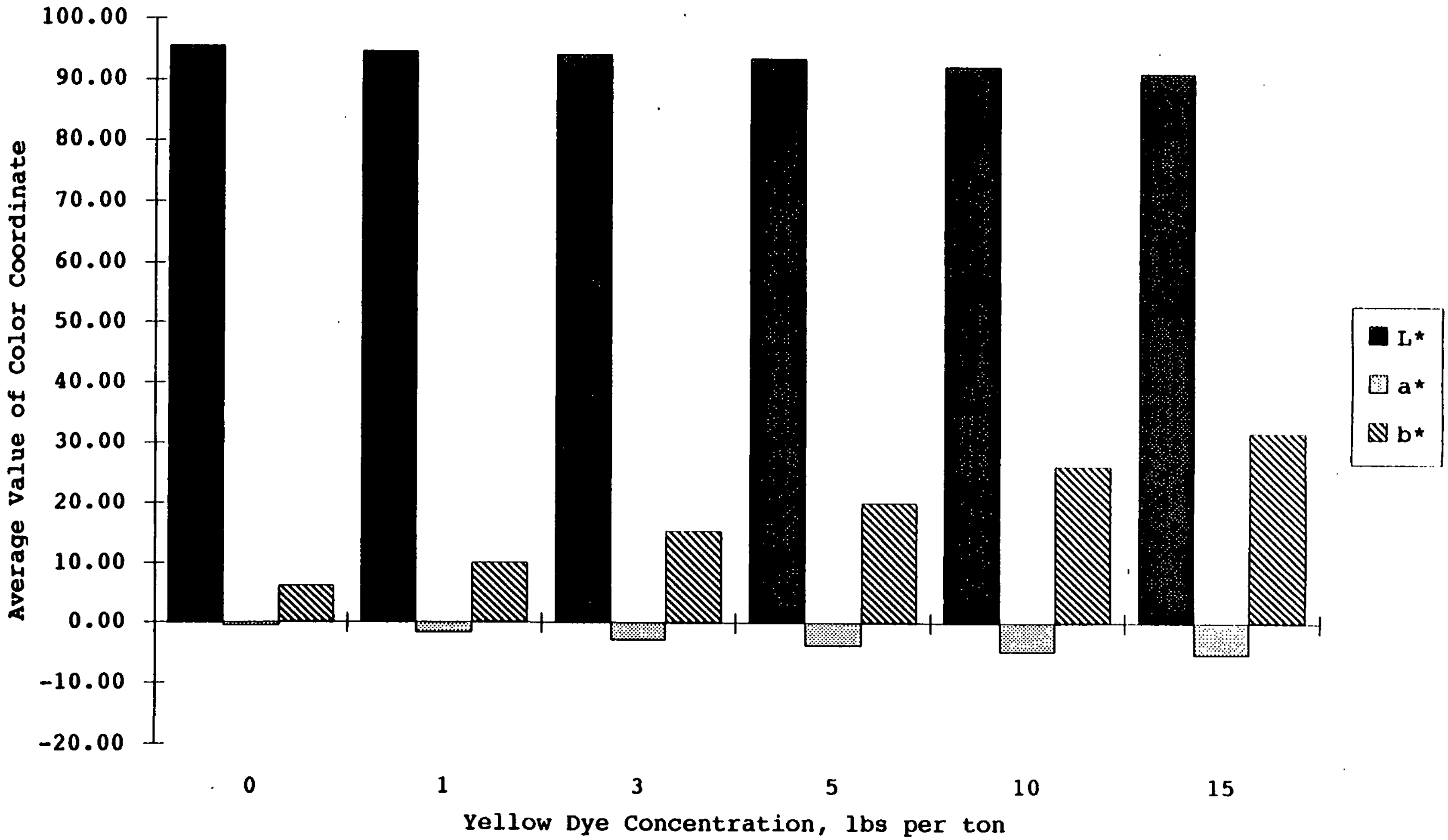
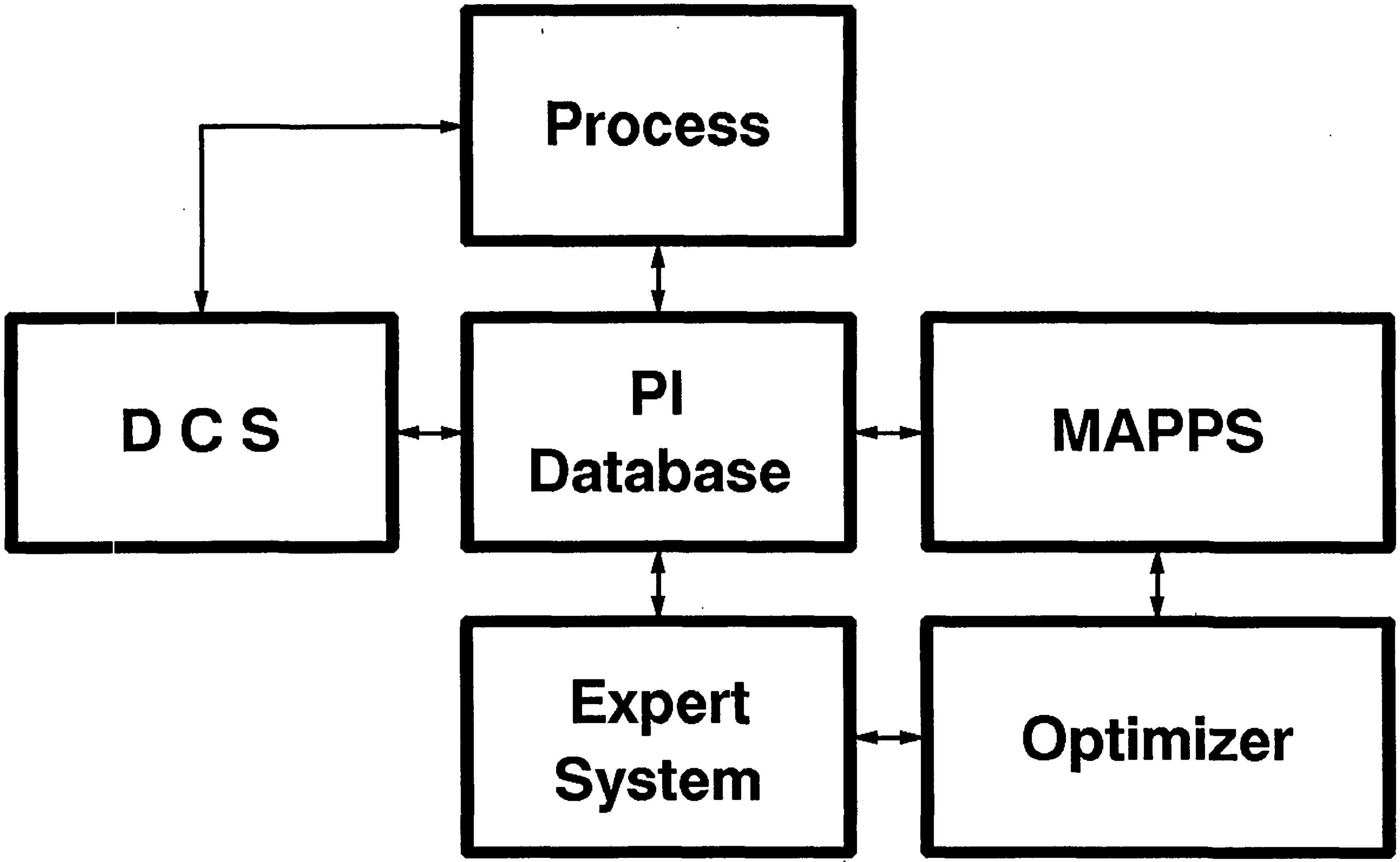


Figure 59. Effects of Yellow Dye Concentration on the Color Coordinates

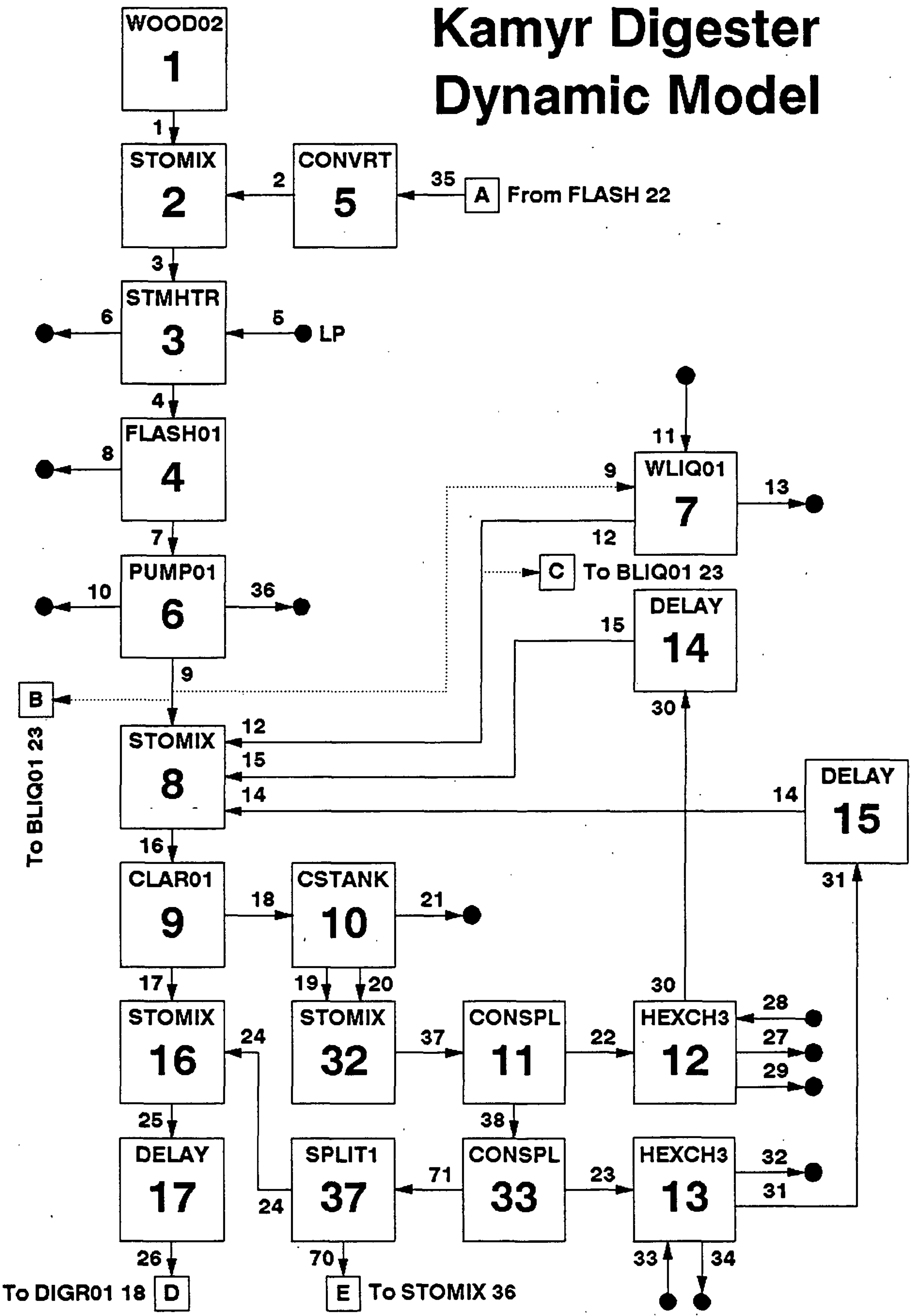
Continuous Digester Model

- Chip Impregnation, Transport, And Kinetics
- Screen Rejects

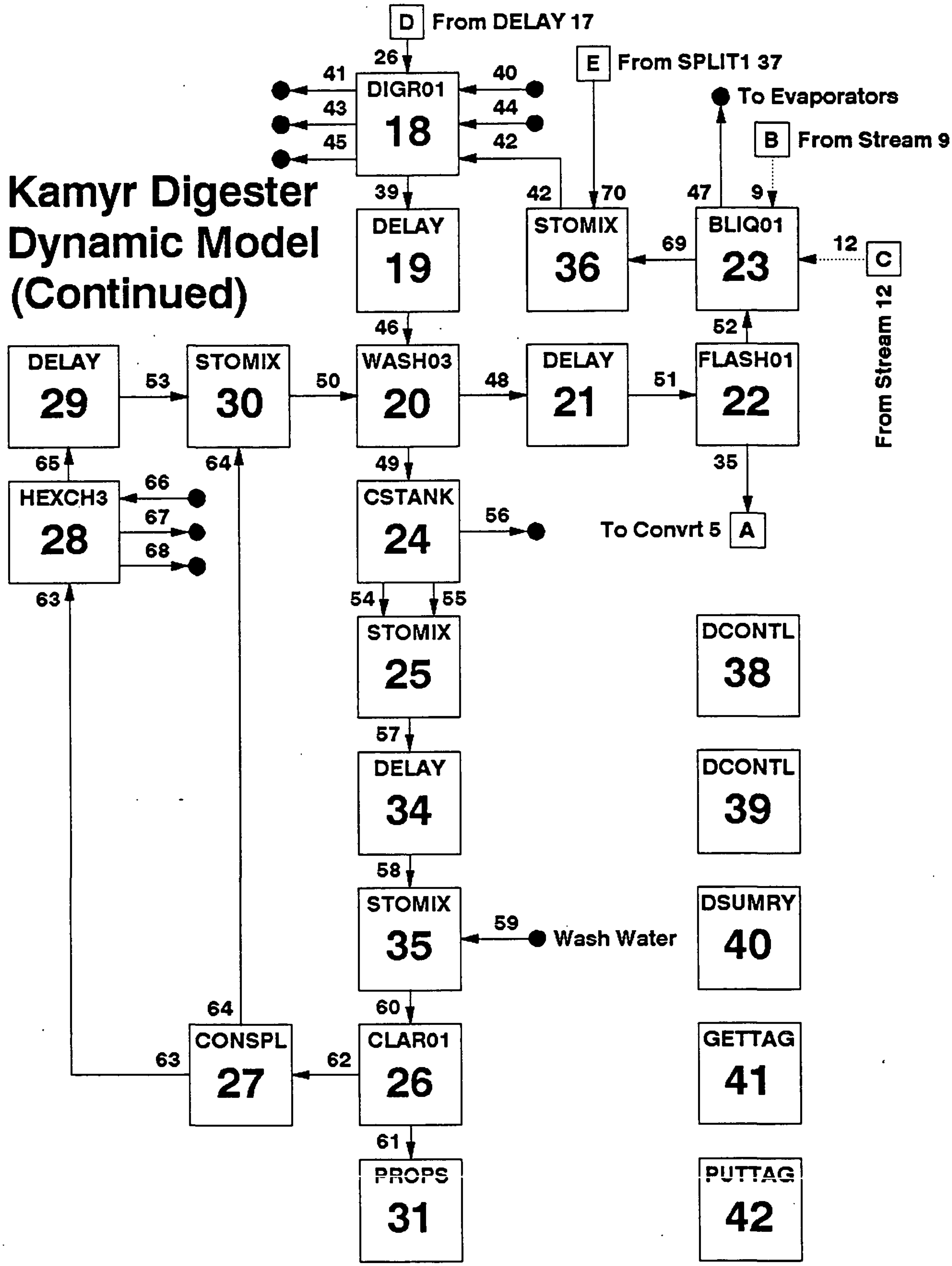
Millwide System Layout

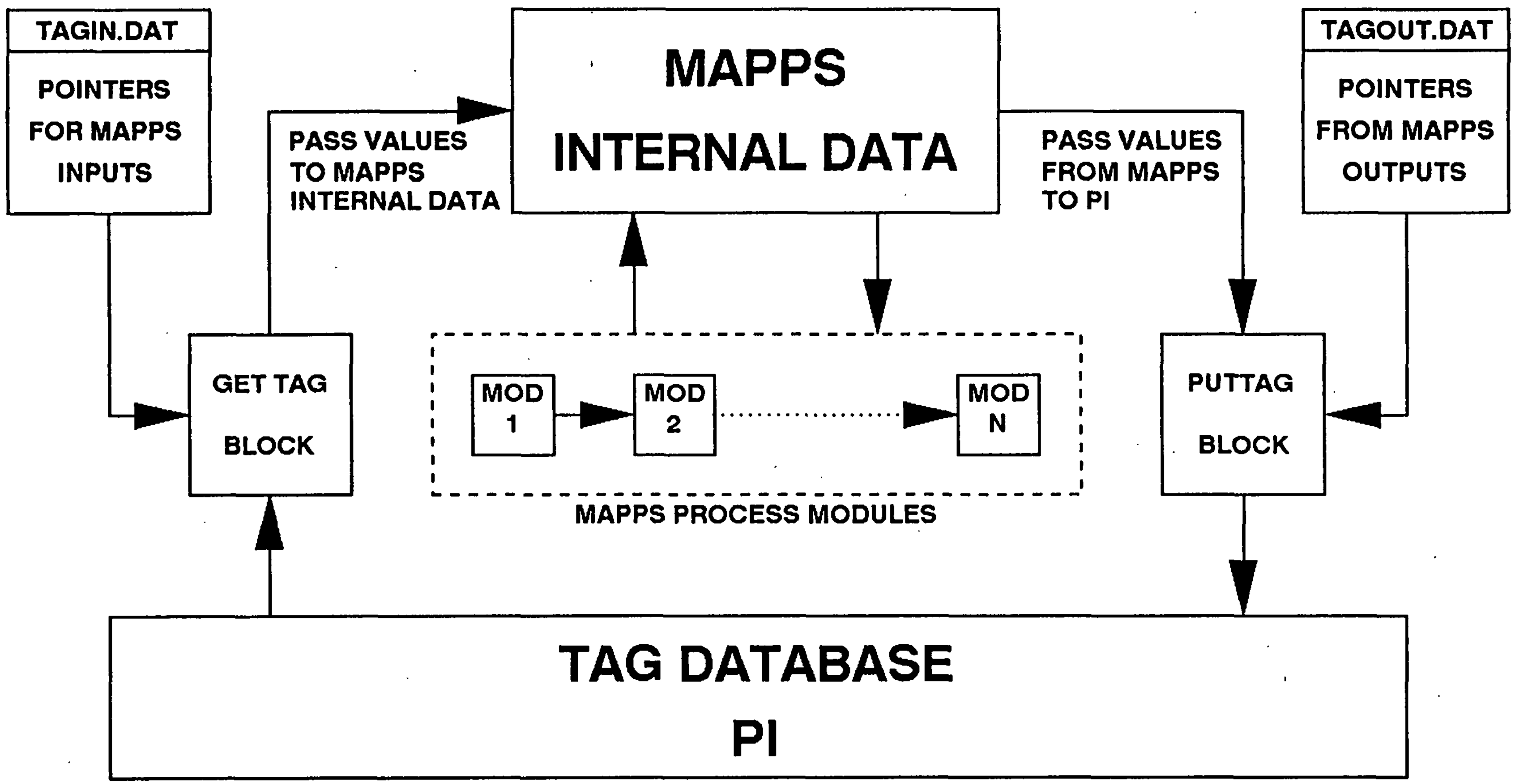


Kamyr Digester Dynamic Model



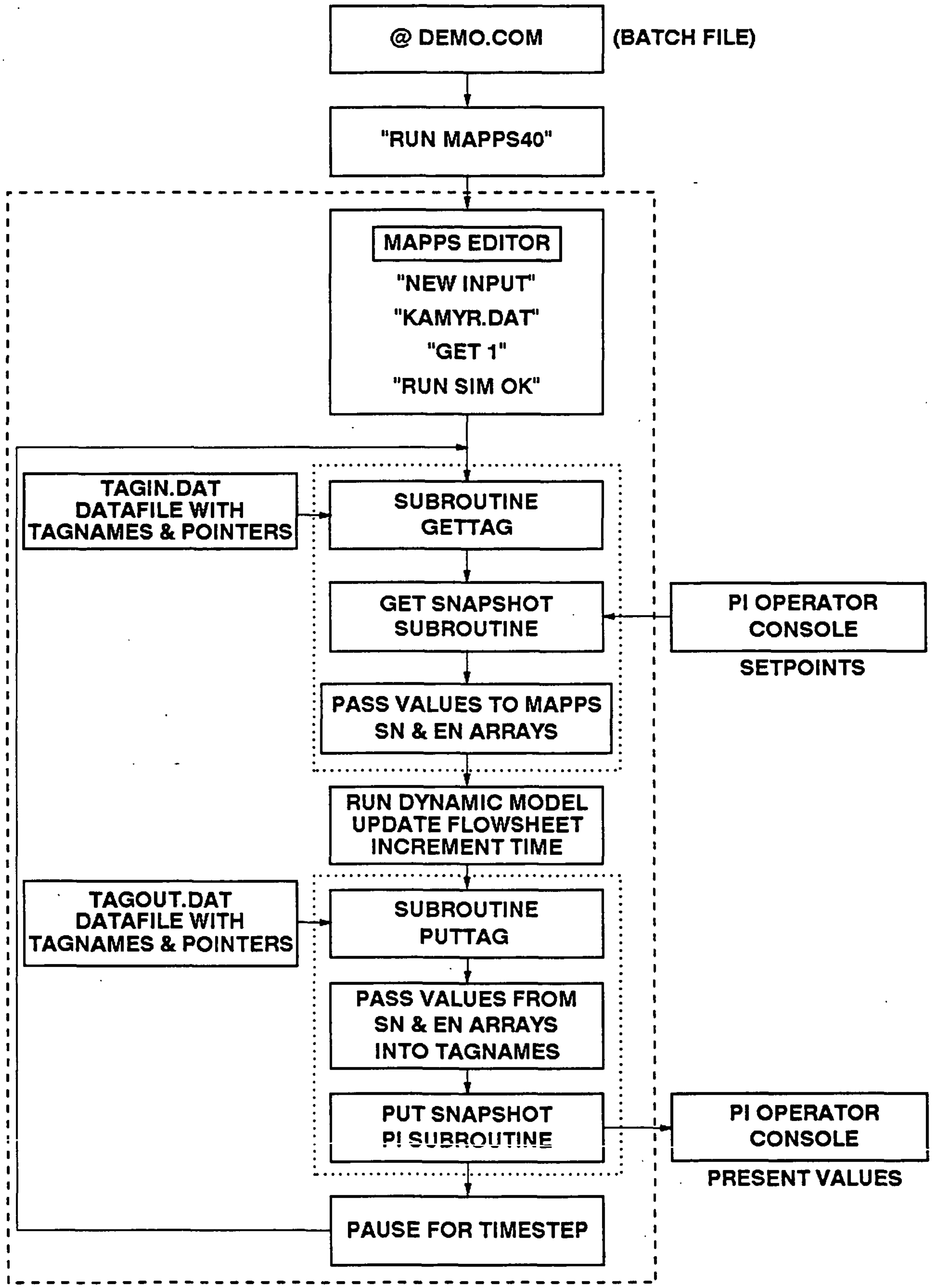
Kamyr Digester Dynamic Model (Continued)





TAGIN.DAT
POINTERS FOR MAPPS INPUTS
PASS VALUES TO MAPPS INTERNAL DATA
MAPPS INTERNAL DATA
PASS VALUES FROM MAPPS TO PI
TAGOUT.DAT
POINTERS FROM MAPPS OUTPUTS
GET TAG BLOCK
MOD 1
MOD 2
MOD N
MAPPS PROCESS MODULES
PUTTAG BLOCK
TAG DATABASE
PI

PI-MAPPS INTERFACE ALGORITHM



Development, Validation, And Sensitivity Study Of A TMP Pulp Mill Simulation

Candidate: Norren Jonason

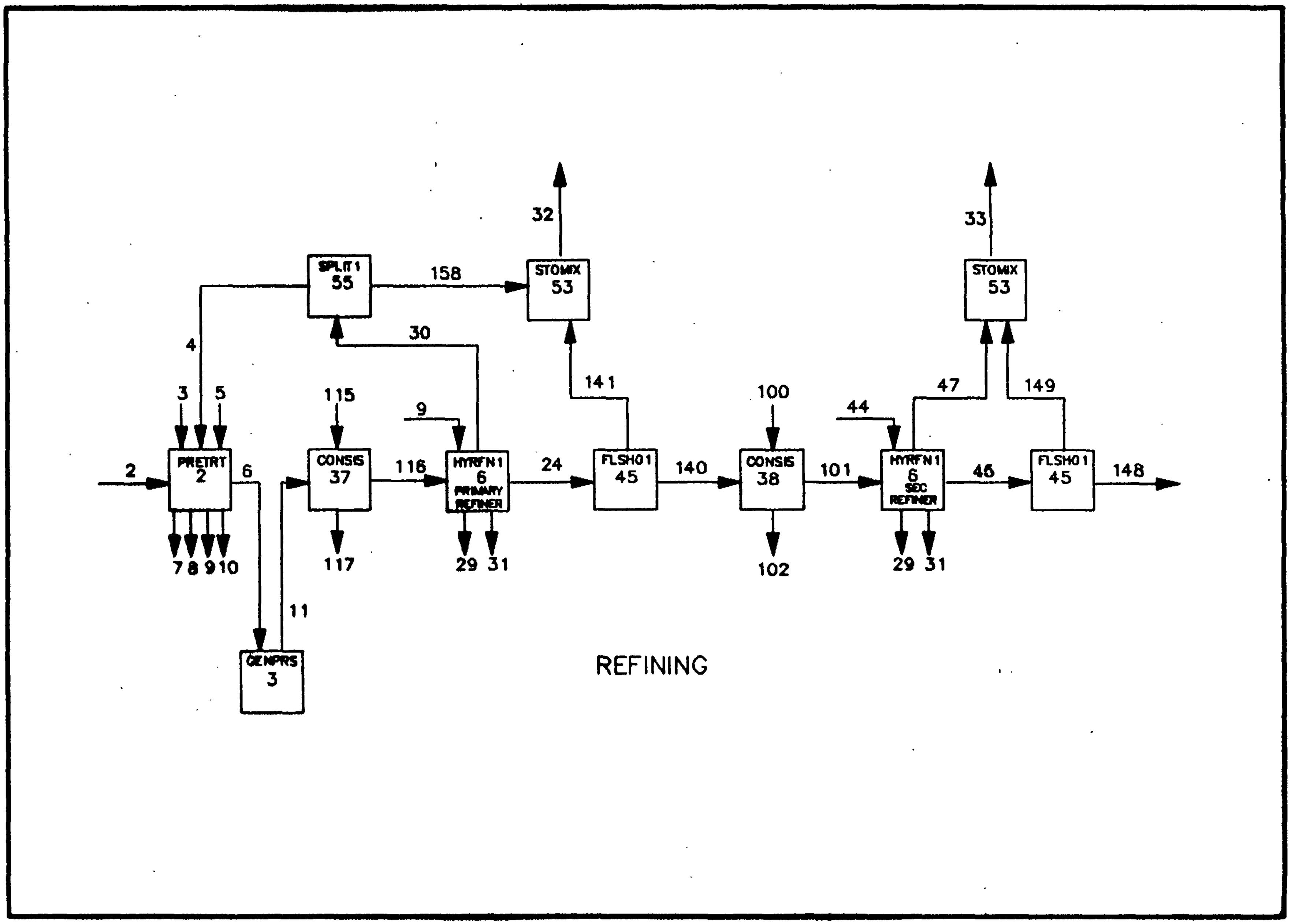
Advisor: Dr. Gary Jones

Completion Date: March 1992

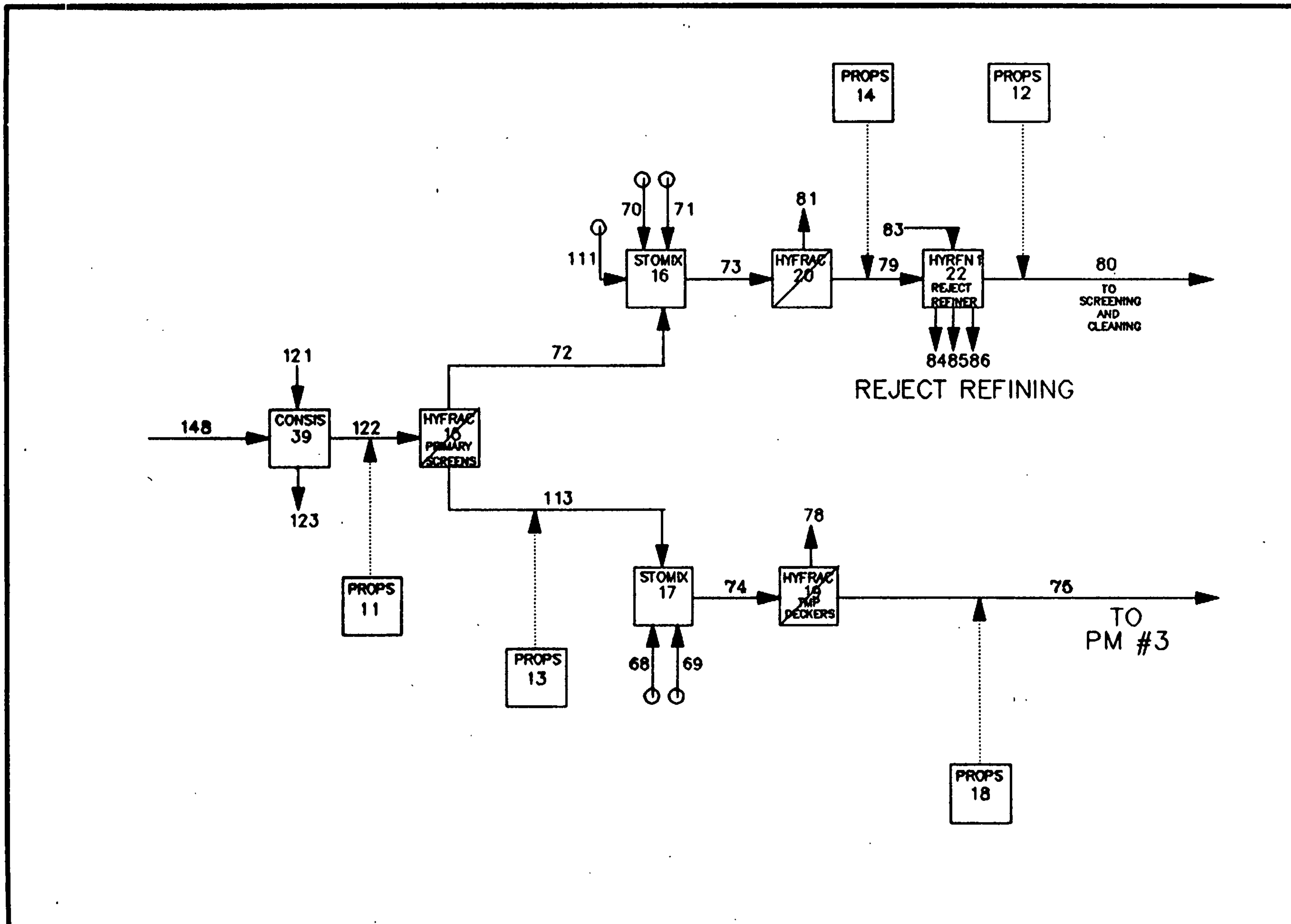
Objectives

- Develop Base Case Simulation Models For The Newsprint And Light-Weight Coated TMP Lines For Bowater's Catawba, South Carolina Mill
- Validate The Base Case Models With Mill Data
- Set Up An Experimental Design To Perform A Sensitivity Study Of The Important Process Parameters And Performance Attributes
- Run Simulations And Collect Data
- Analyze The Data With SAS To Develop Linear Correlations And Sensitivity Coefficients Between The Process And Performance Attributes Parameters And The Simulation Results

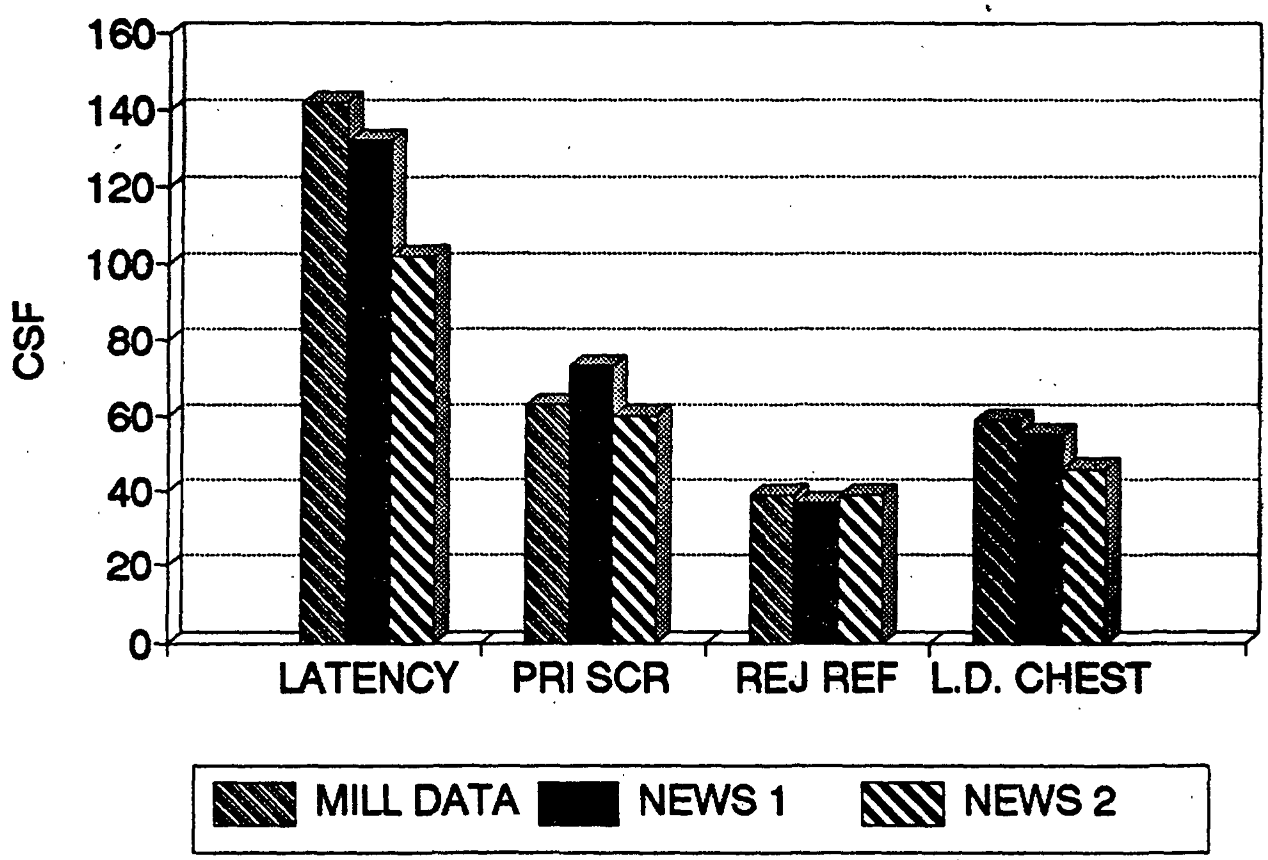
BOWATER NEWSPRINT LINES 4-7



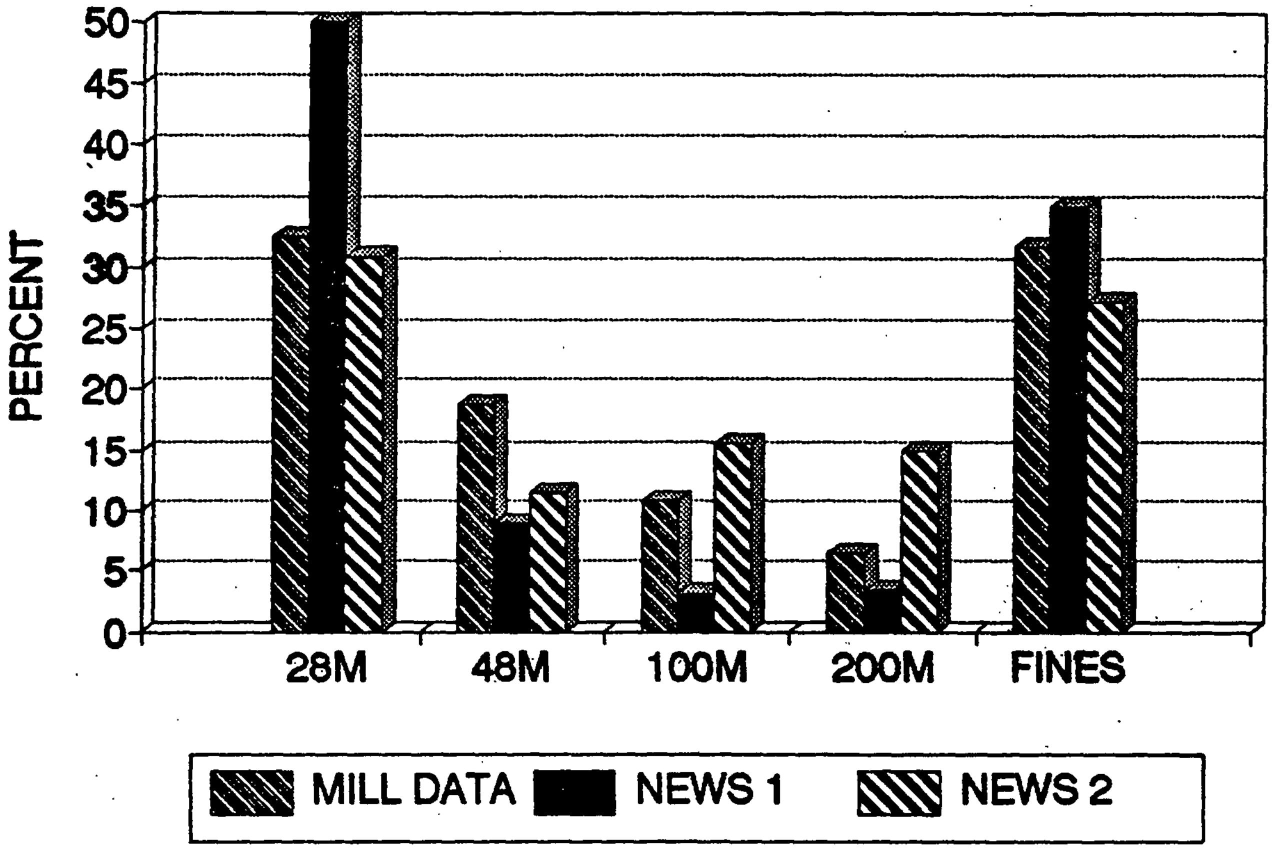
BOWATER NEWSPRINT LINES 4–7



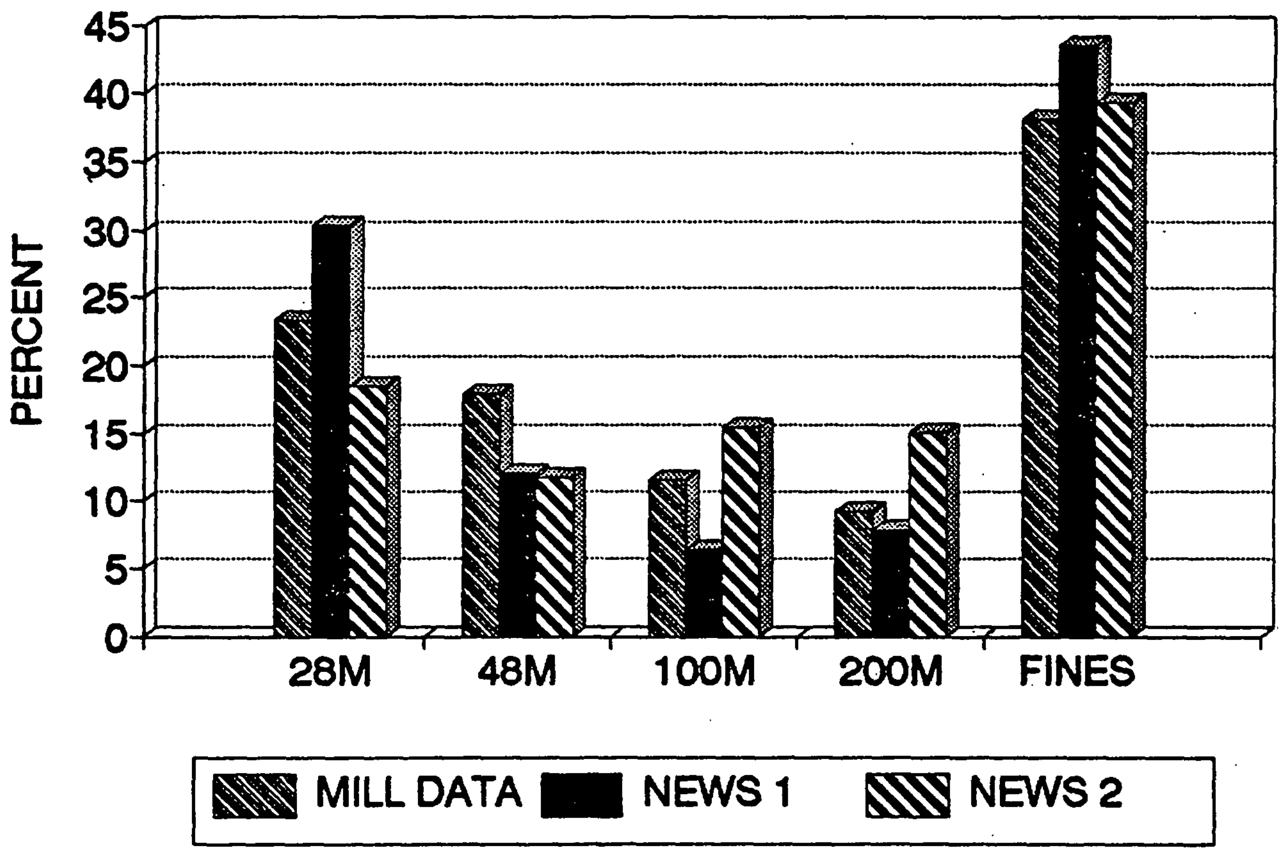
NEWSPRINT CSF COMPARISONS
FOUR LOCATIONS



LATENCY CHEST SAMPLE
FIBER FRACTION COMPARISONS



LOW DENSITY CHEST
FIBER FRACTION COMPARISONS



REJECT REFINER DISCHARGE
FIBER FRACTION COMPARISONS