APPENDIX K

LIST OF COMPUTER SOFTWARE CODES

```
1.      // JOB
2.      //*PROCLIB=WYL.PD.AUL.PROCLIB
3.      //STEP1 EXEC FORTXCLG
4.      //FORT.SYSIN DD *
5.            INTEGER RUNID0,RUNID1,TIMES
6.            REAL MOLWT,MOLFRN,NRDMOL,NRCONV
7.            DIMENSION COMP(9),FEED(9),AREA0(9),MOLWT(9),BASIN(9),TCWRF(9)
8.           1          ,AREA1(9),AREA2(9),WTFRN(9),BASOUT(9),CONV(9),MOLFRN(9)
9.           2          ,DMOLES(9)
10.           READ (5,5) (COMP(I), I=1,6)
11.          5 FORMAT(6A5)
12.            READ (5,10) (MOLWT(I), I=1,6)
13.         10 FORMAT(6F10.3)
14.         20 READ (5,30) RUNID0, TIMES, (FEED(I), AREA0(I), I=1,6)
15.         30 FORMAT(2I10/(F10.4,F10.1))
16.            TOLFED = 0.0
17.            DO 40 I=1,6
18.         40 TOLFED = TOLFED + FEED(I)
19.            WRITE (6,45) RUNID0, TOLFED
20.         45 FORMAT(1H1,2X,10H RUN NO.! ,I10,5X,14H TOTAL FEED = ,F10.4,
21.           1          22H MILLIPOUNDS PER HOUR //)
22.            WRITE (6,50)
23.         50 FORMAT(//8X,10HCOMPONENTS,10X,11HGC ANALYSIS,7X,10HTC WEIGHT ,/
24.           1          2X,22H(MILLIPOUNDS PER HOUR),4X,10HPEAK AREAS,4X,
25.           2                                        16HRESPONSE FACTORS//)
26.            DO 60 I=1,6
27.            IF (FEED(I).EQ.0.0) GO TO 70
28.            IF (FEED(3).EQ.0.0) GO TO 70
29.            TCWRF(I) = (FEED(I)/FEED(3))*(AREA0(3)/AREA0(I))
30.            GO TO 61
31.         70 READ(5,65) TCWRF(I)
32.         65 FORMAT(F10.4)
33.         61 BASIN(I) = (FEED(I)/MOLWT(I))*0.4535924
34.         60 WRITE (6,55) COMP(I), FEED(I), AREA0(I), TCWRF(I)
35.         55 FORMAT(4X,A5,1X,F10.4,7X,F10.2,5X,F10.4/)
36.            TRI = BASIN(1) + BASIN(2) + BASIN(5)
37.            DO 777 J=1,TIMES
38.            READ (5,80) RUNID1, (AREA1(I), I=1,6)
39.         80 FORMAT(I10/(F10.1))
40.            SUM = 0.0
```

Figure K.1. List of Computer Program GC.

```
      DO 90 I=1,6
      AREA2(I) = AREA1(I)*TCWRF(I)
   90 SUM = SUM + AREA2(I)
  111 READ (5,110) ORGYD,DENST1,AQUYD,DENST2
  110 FORMAT(4F10.4)
      GASYD = TOLFED*0.4535924 - ORGYD*DENST1 - AQUYD*DENST2
      TOLGAS = 0.0
      DO 100 I=1,6
      WTFRN(I) = AREA2(I)/SUM
      GASOUT(I) = GASYD*WTFRN(I)/MOLWT(I)
      DMOLES(I) = GASIN(I) - GASOUT(I)
      TOLGAS = TOLGAS + GASOUT(I)
      IF (GASIN(I).EQ.0.0) GO TO 100
      CONV(I) = (DMOLES(I)/GASIN(I))*100.0
  100 CONTINUE
      TRO = GASOUT(1) + GASOUT(2) + GASOUT(5)
      NRDMOL = TRI - TRO
      WRITE (6,125) RUNID1
  125 FORMAT(1H1,2X,10H RUN NO.: ,I10)
      WRITE (6,130)
  130 FORMAT(//4X,10HCOMPONENTS,6X,2HIN,9X,3HOUT,7X,3HREL,6X,5HMOLAR
     1          ,8X,10HPERCENTAGE,/
     2           6X,6HIN GAS,10X,21H(GRAM-MOLES PER HOUR),7X,7HPERCENT
     3          ,6X,10HCONVERSION//)
      DO 140 I=1,6
      MOLFRN(I) = (GASOUT(I)/TOLGAS)*100.0
      IF (GASIN(I).EQ.0.0) GO TO 145
      WRITE (6,150) COMP(I), GASIN(I), GASOUT(I), DMOLES(I), MOLFRN(I)
     1              ,CONV(I)
  150 FORMAT(5X,A5,4X,F10.4,3(1X,F10.4),5X,F10.4/)
      GO TO 140
  145 WRITE (6,155) COMP(I), GASIN(I), GASOUT(I), DMOLES(I), MOLFRN(I)
  155 FORMAT(5X,A5,4X,F10.4,3(1X,F10.4),5X,
     1       10H  --------/)
  140 CONTINUE
      NRCONV = (NRDMOL/TRI)*100.0
      WRITE (6,160) TRI, TRO, NRDMOL, NRCONV
  160 FORMAT(/2X,11H**********,/
     1        2X,11H*   NET   *,/
     2        2X,11H* ACTIVE  *,3(1X,F10.4),16X,F10.4,/
```

Figure K.1. (Cont'd.)

```
     3         2X,11H*REACTANTS*,/
     4         2X,11H***********)
   777 CONTINUE
       GO TO 20
   999 STOP
       END
/*
//GO.SYSIN DD *
   H2    CO   CO2   CH4 C2H4 C2H6
2.016     28.01      44.01      16.04      28.05      30.07
1119110413
                7
1.18       44.1
16.0       67.7
13.8       55.3
4.2        51.2
8.8        63.1
0.0        0.0
0.5617
1119115031
55.7
62.8
66.8
118.6
45.4
41.5
0.0        0.75       0.0        0.97
1119121010
55.7
132.2
70.9
77.7
78.5
6.9
0.0        0.75       0.0        0.97
1119123041
56.4
131.9
74.5
77.3
78.4
```

Figure K.1. (Cont'd.)

```
121.      7.3
122.      0.0          0.75        0.0         0.97
123.      1119125046
124.      57.0
125.      130.8
126.      78.0
127.      75.5
128.      77.0
129.      7.0
130.      0.0          0.75        0.0         0.97
131.      1119131019
132.      56.8
133.      131.2
134.      78.6
135.      75.0
136.      77.0
137.      8.2
138.      0.0          0.75        0.0         0.97
139.      1119133036
140.      56.6
141.      131.3
142.      79.5
143.      74.9
144.      77.1
145.      8.4
146.      0.0          0.75        0.0         0.97
147.      1119135147
148.      58.6
149.      111.0
150.      68.4
151.      64.6
152.      70.1
153.      5.3
154.      0.0          0.75        0.0         0.97
155.      1119145304                6
156.      2.36         55.3
157.      32.0         141.1
158.      27.6         63.3
159.      12.0         59.8
160.      17.6         76.4
```

Figure K.1. (Cont'd.)

```
161,      0.0          0.0
162,      0.5310
163,      1119162111
164,      72.3
165,      85.2
166,      45.2
167,      99.7
168,      61.0
169,      22.8
170,      0.0          0.75        0.0         0.97
171,      1119163816
172,      66.0
173,      125.1
174,      68.1
175,      72.4
176,      74.7
177,      5.8
178,      0.0          0.75        0.0         0.97
179,      1119170107
180,      65.4
181,      127.8
182,      78.7
183,      62.0
184,      77.1
185,      2.8
186,      0.0          0.75        0.0         0.97
187,      1119172019
188,      66.2
189,      128.8
190,      78.7
191,      63.9
192,      76.3
193,      3.3
194,      0.0          0.75        0.0         0.97
195,      1119174048
196,      66.8
197,      122.4
198,      75.9
199,      71.3
200,      74.7
```

Figure K.1. (Cont'd.)

```
201,    4,3
202,    0,0         0,75        0,0         0,97
203,    1119180034
204,    67,2
205,    121,9
206,    74,9
207,    71,2
208,    74,3
209,    4,6
210,    0,0         0,75        0,0         0,97
211,    1119194136              6
212,    3,54        28,1
213,    48,0        41,2
214,    41,4        33,2
215,    18,0        31,2
216,    26,4        36,3
217,    0,0         0,0
218,    0,5861
219,    1119202106
220,    60,7
221,    102,9
222,    84,4
223,    73,1
224,    87,2
225,    0,7
226,    0,0         0,75        0,0         0,97
227,    1119204105
228,    64,9
229,    113,1
230,    87,5
231,    71,4
232,    87,9
233,    1,3
234,    0,0         0,75        0,0         0,97
235,    1119210125
236,    61,1
237,    131,3
238,    83,4
239,    68,3
240,    84,3
```

Figure K.1. (Cont'd.)

```
241.    1.5
242.    0.0         0.75        0.0         0.97
243.    1119212017
244.    61.4
245.    132.2
246.    83.7
247.    67.6
248.    86.3
249.    1.9
250.    0.0         0.75        0.0         0.97
251.    1119214035
252.    61.6
253.    131.9
254.    82.5
255.    68.0
256.    85.8
257.    2.0
258.    0.0         0.75        0.0         0.97
259.    1119220120
260.    61.5
261.    130.9
262.    83.9
263.    68.1
264.    85.6
265.    2.2
266.    0.0         0.75        0.0         0.97
267.    1119230148                      6
268.    4.72        51.8
269.    64.0        80.3
270.    55.2        58.4
271.    24.0        52.9
272.    35.2        61.8
273.    0.0         0.0
274.    0.6056
275.    1120002105
276.    59.2
277.    114.3
278.    86.3
279.    76.9
280.    83.8
```

Figure K.1. (Cont'd.)

```
281.      1,7
282.      0,0          0,75        0,0         0,97
283.      1120004106
284.      62,8
285.      113,8
286.      94,5
287.      72,5
288.      80,2
289.      1,9
290.      0,0          0,75        0,0         0,97
291.      1120010041
292.      63,5
293.      118,1
294.      92,3
295.      72,3
296.      78,8
297.      2,0
298.      0,0          0,75        0,0         0,97
299.      1120012204
300.      63,2
301.      119,9
302.      90,7
303.      72,2
304.      79,3
305.      2,1
306.      0,0          0,75        0,0         0,97
307.      1120014030
308.      62,3
309.      122,7
310.      95,8
311.      70,1
312.      78,7
313.      2,2
314.      0,0          0,75        0,0         0,97
315.      1120020130
316.      64,3
317.      114,8
318.      93,4
319.      72,6
320.      80,6
```

Figure K.1. (Cont'd.)

```
2.7
0.0          0.75          0.0          0.97
1120034115                 6
4.72         52.3
64.0         105.6
55.2         57.0
24.0         78.8
35.2         74.3
0.0          0.0
0.4917
1120052051
42.2
66.9
57.0
56.7
59.2
2.2
0.0          0.75          0.0          0.97
1120054025
65.5
113.2
90.7
69.8
83.6
0.7
0.0          0.75          0.0          0.97
1120060039
65.3
115.7
89.6
76.2
80.3
0.7
0.0          0.75          0.0          0.97
1120062109
61.9
126.1
89.4
73.1
81.0
```

Figure K.1. (Cont'd.)

```
361.      0.5
362.      0.0          0.75        0.0         0.97
363.      1120070634
364.      57.3
365.      129.7
366.      88.1
367.      72.7
368.      80.0
369.      0.5
370.      0.0          0.75        0.0         0.97
371.      1120072335
372.      63.0
373.      133.0
374.      87.5
375.      71.6
376.      77.0
377.      0.4
378.      0.0          0.75        0.0         0.97
379.      1120084122                6
380.      3.54         60.4
381.      48.0         114.9
382.      41.4         76.3
383.      18.0         61.4
384.      26.4         88.7
385.      0.0          0.0
386.      0.5513
387.      1120100051
388.      33.8
389.      78.2
390.      52.8
391.      52.6
392.      60.5
393.      1.2
394.      0.0          0.75        0.0         0.97
395.      1120102154
396.      57.5
397.      126.5
398.      85.3
399.      67.9
400.      84.9
>
```

Figure K.1. (Cont'd.)

```
401.    0.7
402.    0.0         0.75        0.0         0.97
403.    1120104059
404.    59.2
405.    129.1
406.    89.1
407.    68.9
408.    85.6
409.    0.9
410.    0.0         0.75        0.0         0.97
411.    1120110012
412.    59.0
413.    130.2
414.    90.9
415.    69.3
416.    86.2
417.    0.8
418.    0.0         0.75        0.0         0.97
419.    1120112043
420.    58.4
421.    129.5
422.    94.2
423.    69.0
424.    85.4
425.    0.8
426.    0.0         0.75        0.0         0.97
427.    1120114013
428.    58.8
429.    130.4
430.    93.7
431.    69.3
432.    84.8
433.    0.7
434.    0.0         0.75        0.0         0.97
435.    1120132014                5
436.    2.36        58.9
437.    32.0        130.1
438.    27.6        84.1
439.    12.0        68.0
440.    17.6        78.1
```

Figure K.1. (Cont'd.)

```
441.    0.0         0.0
442.    0.6901
443.    1120144035
444.    31.9
445.    51.8
446.    37.9
447.    44.5
440.    34.6
449.    5.0
450.    0.0         0.75        0.0         0.97
451.    1120150031
452.    55.5
453.    136.9
454.    98.9
455.    66.9
456.    74.7
457.    0.8
458.    0.0         0.75        0.0         0.97
459.    1120152018
460.    55.9
461.    137.9
462.    98.4
463.    70.0
464.    74.9
465.    0.8
466.    0.0         0.75        0.0         0.97
467.    1120154022
468.    56.4
469.    136.3
470.    99.1
471.    69.0
472.    74.3
473.    0.8
474.    0.0         0.75        0.0         0.97
475.    1120160018
476.    56.8
477.    136.4
478.    100.9
479.    68.8
480.    74.0
```

Figure K.1. (Cont'd.)

```
481.      0.8
482.      0.0          0.75       0.0        0.97
483.      1120165516             6
484.      1.18         55.0
485.      16.0         113.6
486.      13.8         94.0
487.      4.2          76.7
488.      8.8          92.8
489.      0.0          0.0
490.      0.6491
491.      1120182126
492.      47.4
493.      107.2
494.      91.5
495.      79.2
496.      84.0
497.      2.2
498.      0.0          0.75       0.0        0.97
499.      1120184207
500.      56.1
501.      114.0
502.      94.6
503.      77.6
504.      88.2
505.      1.7
506.      0.0          0.75       0.0        0.97
507.      1120190026
508.      57.8
509.      115.6
510.      93.6
511.      81.2
512.      87.4
513.      1.6
514.      0.0          0.75       0.0        0.97
515.      1120192026
516.      56.2
517.      112.2
518.      100.6
519.      78.7
520.      89.7
>
```

Figure K.1. (Cont'd.)

```
521.      1.7
522.      0.0          0.75          0.0          0.97
523.      1120194021
524.      56.6
525.      111.6
526.      98.6
527.      78.4
528.      91.5
529.      1.7
530.      0.0          0.75          0.0          0.97
531.      1120200058
532.      54.8
533.      108.5
534.      94.2
535.      76.0
536.      108.1
537.      2.0
538.      0.0          0.75          0.0          0.97
539.      1121040311                 1
540.      1.12         49.2
541.      16.0         108.8
542.      13.0         94.6
543.      5.0          73.7
544.      8.5          95.5
545.      0.0          0.0
546.      0.6510
547.      1121031132
548.      28.9
549.      0.9
550.      6.1
551.      32.7
552.      21.0
553.      1.0
554.      0.0          0.75          0.0          0.97
555.      1121053148                 1
556.      1.12         53.7
557.      16.0         97.0
558.      13.0         103.1
559.      4.2          81.4
560.      7.7          94.3
```

Figure K.1. (Cont'd.)

```
561.      0.0         0.0
562.      0.6509
563.      1121045526
564.      57.6
565.      7.0
566.      6.9
567.      58.6
568.      31.5
569.      10.9
570.      0.0         0.75        0.0         0.97
571.      1121082006              1
572.      1.18        48.8
573.      16.0        108.3
574.      13.8        100.1
575.      4.2         73.0
576.      7.2         85.3
577.      0.0         0.0
578.      0.6154
579.      1121074844
580.      4.9
581.      0.0
582.      0.3
583.      8.4
584.      2.5
585.      0.0
586.      0.0         0.75        0.0         0.97
587.      1121102859              1
588.      1.28        52.1
589.      16.6        109.7
590.      13.0        93.7
591.      5.6         68.6
592.      6.7         97.0
593.      0.0         0.0
594.      0.5004
595.      1121094318
596.      31.4
597.      2.2
598.      3.2
599.      25.8
600.      14.4
>
```

Figure K.1. (Cont'd.)

```
0,1
0,0          0,75          0,0          0,97
1121140900                 1
1,24         51,4
19,0         106,8
18,1         85,0
5,6          78,9
8,0          102,6
0,0          0,0
0,3680
1121133315
48,7
0,0
2,1
36,9
35,7
3,7
0,0          0,75          0,0          0,97
1121152312                 1
1,21         50,8
16,8         107,6
14,6         93,9
8,0          82,9
7,0          91,2
0,0          0,0
0,4961
1121145136
12,7
0,0
4,9
15,7
11,8
0,9
0,0          0,75          0,0          0,97
1121172010                 1
1,18         52,7
16,0         99,3
13,8         102,9
4,2          72,3
8,8          101,8
>
```

Figure K.1. (Cont'd.)

```
641,      0.0          0.0
642,      0.6478
643,      1121160716
644,      4.5
645,      0.0
646,      1.8
647,      9.0
648,      4.7
649,      0.1
650,      0.0          0.75          0.0          0.97
651,      1121185026                 1
652,      2.36         63.1
653,      32.0         108.0
654,      27.5         77.1
655,      12.0         75.4
656,      17.5         95.6
657,      0.0          0.0
658,      0.5158
659,      1121181453
660,      47.9
661,      1.3
662,      5.1
663,      54.8
664,      26.9
665,      12.7
666,      0.0          0.75          0.0          0.97
667,      1121200137                 1
668,      1.85         57.2
669,      23.1         117.0
670,      22.5         85.6
671,      10.3         77.2
672,      14.4         89.4
673,      0.0          0.0
674,      0.6159
675,      1121192901
676,      88.5
677,      2.5
678,      24.0
679,      66.1
680,      28.8
```

Figure K.1. (Cont'd.)

```
681.     13,5
682.     0,0        0,75        0,0         0,97
683.     /*
684.     //
>
```

Figure K.1. (Cont'd.)

```
//  JOB
//*PROCLIB=WYL,PD,AUL,PROCLIB
//   EXEC  FORTXCLG
//FORT.SYSIN  DD  *
      INTEGER C,M,A(3,74)
      REAL NP1(74),N(74),NN(74),LAM,NP1T,NT,NNT,LAMH,MF(74),LL
      DIMENSION PI(3),B(3),AA(4,4),CC(4),CONV(74),
     1          GRT(74),DEL(74),RHO(74),DFDL(11),DELH(74),
     2          PN(74),X(40),Y(40),D(40,3),WKAREA(8)
      LOGICAL CHECK
      R = 1.987
      READ (5,4) T
    4 FORMAT(1F10.2)
      DELTA = 1.0E-03
      ITMAX = 200
   10 READ (5,20) C,M
   20 FORMAT(2I10)
      DO 30 J = 1,M
      READ (5,40) (A(J,I), I = 1,C)
   40 FORMAT(16I5)
   30 CONTINUE
   50 READ (5,60) (NN(I), I=1,C)
   60 FORMAT(5E15.8)
      DO 62 I = 1,C
   62 GRT(I) = 0.0
      WRITE (6,64)
   64 FORMAT(1H1,2X,29H INPUT OF THERMODYNAMIC DATA ///)
      DO 70 I = 1,C
      READ (5,71) NX
      IC = NX
      READ (5,72) (X(J), Y(J), J = 1,NX)
      WRITE (6,69) (X(J), Y(J), J = 1,NX)
   69 FORMAT(2(5X,F10.4))
      CALL IQH8CU(X,Y,NX,D,IC,IER1)
      READ (5,71) K
      V = T - X(K)
      W = ((D(K,3)*V + D(K,2))*V + D(K,1))*V + Y(K)
      GRT(I) = 1000.0*W/(R*T)
   71 FORMAT(1I2)
   72 FORMAT(2F10.4)
```

Figure K.2. List of Computer Program THERMODY.

```
      70 CONTINUE
      73 READ (5,60) (N(I), I=1,C)
         WRITE (6,74) T
      74 FORMAT(1H1,' FOR COMPLEX REACTION SYSTEM  AT TEMP = ',F10.3,
     1           ' K '//)
         WRITE (6,21) C,M
      21 FORMAT(6X,8HCONTAINS,I5,23H CHEMICAL COMPONENTS OF,I5,
     1          17H ATOMIC SPECIES. ///)
         WRITE (6,75)
      75 FORMAT(26H THE COEFFICIENT MATRIX IS//)
         DO 76 J = 1,M
      76 WRITE (6,40) (A(J,I), I=1,C)
         WRITE (6,77) (NN(I), GRT(I), N(I), I=1,C)
      77 FORMAT(//36H THE NN(I), GRT(I), N(I) VECTORS ARE///(3(5X,F10.4)))
         WRITE (6,78)
      78 FORMAT(1H1,30H ATOMIC SPECIES BALANCE CHECK ///)
         CHECK = .FALSE.
      80 DO 100 J = 1,M
      85 B(J) = 0.0
     130 BCHECK = 0.0
      90 DO 99 I = 1,C
         B(J) = B(J) + A(J,I)*NN(I)
         BCHECK = BCHECK + A(J,I)*N(I)
      99 WRITE (6,102) B(J),BCHECK
     102 FORMAT(2(10X,E15.8))
     160 IF (ABS(BCHECK - B(J)).LE.DELTA) GO TO 100
         CHECK = .TRUE.
     100 CONTINUE
     170 IF (.NOT.CHECK) GO TO 220
     180 WRITE (6,190)
     190 FORMAT(///46H BAD INITIAL GUESSES, B VECTORS DO NOT CHECK. )
     200 GO TO 73
     220 IT = 1
     225 NT = 0.0
     226 DO 227 I = 1,C
         PN(I) = N(I)
         NT = NT + N(I)
     227 PNT = NT
     230 DO 290 J = 1,M
     235 CC(J) = 0.0
```

Figure K.2. (Cont'd.)

```
 81.       240 DO 270 I = 1,M
 82.       250 AA(J,I) = 0.0
 83.       260 DO 270 L = 1,C
 84.       270 AA(J,I) = AA(J,I) + A(J,L)*A(I,L)*N(L)
 85.       279 DO 280 I = 1,C
 86.       280 CC(J) = CC(J) + A(J,I)*N(I)*(GRT(I) + ALOG(N(I)/NT))
 87.           MP1 = M + 1
 88.       290 AA(J,MP1) = B(J)
 89.       310 DO 320 I = 1,M
 90.       320 AA(MP1,I) = B(I)
 91.       330 AA(MP1,MP1) = 0.0
 92.       340 CC(MP1) = 0.0
 93.       350 DO 360 I = 1,C
 94.       360 CC(MP1) = CC(MP1) + N(I)*(GRT(I) + ALOG(N(I)/NT))
 95.           IJOB = 3
 96.           D1 = -1.0
 97.           CALL LINV3F(AA,CC,IJOB,MP1,MP1,D1,D2,WKAREA,IER2)
 98.       380 DO 390 J = 1,M
 99.       390 PI(J) = CC(J)
100.       400 U = CC(MP1)
101.       410 NP1T = NT*(U + 1.0)
102.       420 DO 460 I = 1,C
103.       430 NP1(I) = NP1T*N(I)/NT - N(I)*(GRT(I) + ALOG(N(I)/NT))
104.       440 DO 450 J = 1,M
105.       450 NP1(I) = NP1(I) + N(I)*PI(J)*A(J,I)
106.       460 DEL(I) = NP1(I) - N(I)
107.       465 DELN = NP1T - NT
108.       473 LAM = 1.0
109.       480 DO 520 I = 1,C
110.       490 IF (NP1(I).GT.0.0) GO TO 520
111.       500 LL = .99999*N(I)/(N(I)-NP1(I))
112.       510 IF (LL.LT.LAM) LAM = LL
113.       520 CONTINUE
114.       514 DO 515 I = 1,C
115.       515 RHO(I) = N(I) + DEL(I)*LAM
116.       550 DO 610 L = 1,11
117.       560 LL = LAM*(1.0 - (L-1)/10.)
118.       570 DFDL(L) = 0.0
119.       580 DO 590 I = 1,C
120.       590 DFDL(L) = DFDL(L) + DEL(I)*(GRT(I) +
```

Figure K.2. (Cont'd.)

```
     1              ALOG((N(I) + LL*DEL(I))/(NT + LL*DELN)))
     1 610 CONTINUE
       607 L = 1
       600 IF (DFDL(L).LE.0.0) GO TO 650
       599 L = L+1
       598 IF (L.EQ.11) GO TO 640
       597 GO TO 600
       640 LLL = LLL + 1
       641 DO 642 I = 1,C
       642 N(I) = PN(I) - LLL*LAMH*DELH(I)/10.
       643 NT = PNT - LLL*LAMH*DELNH/10.
       644 IF (LLL.NE.11) GO TO 230
       620 WRITE (6,630)
       630 FORMAT(40H NO LAMBDA FOUND, TRY NEW CALCULATION,  )
       645 GO TO 73
       650 LAM = LAM*(1. - (L - 1)/10.)
       651 LLL = 0
       660 DO 670 I = 1,C
       670 N(I) = N(I) + LAM*DEL(I)
       680 NT = NT + LAM*DELN
       690 IT = IT + 1
           ITM1 = IT - 1
       700 WRITE (6,710) ITM1, LAM, (N(I), I=1,C)
       710 FORMAT(1H1,6H AFTER,I5,17H ITERATIONS LAM =,F6.3,
     1                17H THE NEW N'S ARE ///(55X,E15.8))
       720 CHECK = .TRUE.
       730 DO 740 I = 1,C
       740 IF (ABS((N(I) - PN(I))/N(I)).GT.DELTA) CHECK = .FALSE.
       750 IF (CHECK) GO TO 800
       751 LAMH = LAM
       752 DO 753 I = 1,C
       755 PN(I) = N(I)
       753 DELH(I) = DEL(I)
       754 DELNH = DELN
       756 PNT = NT
       760 IF (IT.LT.ITMAX) GO TO 230
       770 WRITE (6,780)
       780 FORMAT(40H ITERATION FAILED TO CONVERGE, BAIL OUT.)
       790 GO TO 820
       800 WRITE (6,810) (N(I), I = 1,C)
>
```

Figure K.2. (Cont'd.)

```
      810 FORMAT(1H1,46H CONVERGENCE ORTAINED, FINAL MOLE NUMBERS ARE ///
     1          (50X,E15.8))
      814 DO 815 I = 1,C
      815 MF(I) = N(I)/NT
      816 WRITE (6,817) (MF(I), I = 1,C)
      817 FORMAT(1H1,26H FINAL MOLE FRACTIONS ARE ///(30X, E15.8))
          WRITE (6,900)
      900 FORMAT(1H1,48H PERCENTAGE CONVERSIONS OF ACTIVE REACTANTS ARE ///)
          DO 910 I = 1,C
          IF (I.EQ.1.OR.I.EQ.49.OR.I.EQ.71.OR.I.EQ.72.OR.I.EQ.74) GO TO 920
          GO TO 910
      920 CONV(I) = ((NN(I) - N(I))/NN(I))*100.
          WRITE (6,930) CONV(I)
      930 FORMAT(30X,F10.4/)
      910 CONTINUE
      820 STOP
          END
//LKED,SYSLIB  DD
//             DD
//             DD
//             DD   DSN=WYL.AG.DCL.LIB,DISP=SHR
//GO.SYSIN   DD  *
553.16
          70           3
     1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16
     4    5    6    6    7    7    8    8    8    8    9    9   10   10   10   11
    12   13   14   15   16   11   12   13   11   13    7    8    2    6    7    8
     9   10   11   12   13    6    7    8    8    8    9    9    9    9    2    3
     3    4    1    1    0    0
     4    6    8   10   12   14   16   18   20   22   24   26   28   30   32   34
    10   12   14   14   16   16   18   18   18   18   20   20   22   22   22   24
    26   28   30   32   34   24   26   28   24   28   14   16    4   12   14   16
    18   20   22   24   26    6    8   10   10   10   12   12   12   12    6    8
     8   10    0    0    2    2
     0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
     0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
     0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
     0    0    0    0    0    0    0    0    0    0    0    0    0    0    1    1
     1    1    1    2    1    0
 0.40524000E+010.0          0.0          0.0          0.0
```

Figure K.2. (Cont'd.)

```
201.      0.0              0.0              0.0              0.0              0.0
202.      0.0              0.0              0.0              0.0              0.0
203.      0.0              0.0              0.0              0.0              0.0
204.      0.0              0.0              0.0              0.0              0.0
205.      0.0              0.0              0.0              0.0              0.0
206.      0.0              0.0              0.0              0.0              0.0
207.      0.0              0.0              0.0              0.0              0.23992900E+02
208.      0.0              0.0              0.0              0.0              0.0
209.      0.0              0.0              0.0              0.0              0.0
210.      0.0              0.0              0.0              0.0              0.0
211.      0.0              0.0              0.0              0.0              0.0
212.      0.0              0.0              0.0              0.0              0.33978200E+02
213.      0.0     0.17536600E+02 0.93161000E+01 0.0
214.      18
215.      0.0          -15.987
216.      250.0        -12.987
217.      298.16       -12.140
218.      300.0        -12.105
219.      350.0        -11.113
220.      400.0        -10.048
221.      450.0        -8.969
222.      500.0        -7.841
223.      600.0        -5.49
224.      700.0        -3.05
225.      800.0        -0.55
226.      900.0        2.01
227.      1000.0       4.61
228.      1100.0       7.22
229.      1200.0       9.85
230.      1300.0       12.50
231.      1400.0       15.14
232.      1500.0       17.79
233.       8
234.      18
235.      0.0          -16.517
236.      250.0        -9.731
237.      298.16       -7.860
238.      300.0        -7.785
239.      350.0        -5.664
240.      400.0        -3.447
```

Figure K.2. (Cont'd.)

```
241.      450.0       -1.165
242.      500.0       1.168
243.      600.0       5.97
244.      700.0       10.90
245.      800.0       15.92
246.      900.0       21.00
247.      1000.0      26.13
248.      1100.0      31.28
249.      1200.0      36.45
250.      1300.0      41.62
251.      1400.0      46.79
252.      1500.0      51.99
253.       8
254.      18
255.      0.0         -19.482
256.      250.0       -8.549
257.      298.16      -5.614
258.      300.0       -5.541
259.      350.0       -2.218
260.      400.0       1.191
261.      450.0       4.674
262.      500.0       8.230
263.      600.0       15.50
264.      700.0       22.93
265.      800.0       30.45
266.      900.0       38.05
267.      1000.0      45.68
268.      1100.0      53.34
269.      1200.0      61.01
270.      1300.0      68.68
271.      1400.0      76.35
272.      1500.0      84.08
273.       8
274.      18
275.      0.0         -23.67
276.      250.0       -8.10
277.      298.16      -4.10
278.      300.0       -3.94
279.      350.0       0.50
280.      400.0       5.09
```

Figure K.2. (Cont'd.)

```
281,      450.0       9.76
282,      500.0       14.54
283,      600.0       24.28
284,      700.0       34.19
285,      800.0       44.21
286,      900.0       54.34
287,      1000.0      64.50
288,      1100.0      74.67
289,      1200.0      84.84
290,      1300.0      95.04
291,      1400.0      105.24
292,      1500.0      115.42
293,       8
294,      18
295,      0.0         -27.23
296,      250.0       -7.08
297,      298.16      -2.00
298,      300.0       -1.80
299,      350.0       3.81
300,      400.0       9.60
301,      450.0       15.50
302,      500.0       21.51
303,      600.0       33.76
304,      700.0       46.20
305,      800.0       58.77
306,      900.0       71.46
307,      1000.0      84.18
308,      1100.0      96.91
309,      1200.0      109.63
310,      1300.0      122.39
311,      1400.0      135.13
312,      1500.0      147.86
313,       8
314,      11
315,      0.0         -31.08
316,      200.0       -12.67
317,      298.15      -0.04
318,      300.0       0.21
319,      400.0       13.98
320,      500.0       28.32
>
```

Figure K.2. (Cont'd.)

```
321,      600.0       43.0
322,      700.0       58.0
323,      800.0       73.1
324,      900.0       88.2
325,      1000.0      103.5
326,       6
327,      11
328,      0.0         -34.84
329,      200.0       -12.91
330,      298.15      1.93
331,      300.0       2.22
332,      400.0       18.36
333,      500.0       35.14
334,      600.0       52.4
335,      700.0       69.8
336,      800.0       87.4
337,      900.0       105.2
338,      1000.0      123.0
339,       6
340,      11
341,      0.0         -38.71
342,      200.0       -13.26
343,      298.15      3.78
344,      300.0       4.11
345,      400.0       22.63
346,      500.0       41.86
347,      600.0       61.6
348,      700.0       81.6
349,      800.0       101.7
350,      900.0       122.0
351,      1000.0      142.3
352,       6
353,      11
354,      0.0         -42.31
355,      200.0       -13.35
356,      298.15      5.91
357,      300.0       6.28
358,      400.0       27.17
359,      500.0       48.84
360,      600.0       71.0
```

Figure K.2. (Cont'd.)

```
361,      700.0       93.5
362,      800.0       116.2
363,      900.0       139.0
364,      1000.0      161.9
365,       6
366,      11
367,      0.0         -46.06
368,      200.0       -13.58
369,      298.15      7.88
370,      300.0       8.30
371,      400.0       31.56
372,      500.0       55.67
373,      600.0       80.3
374,      700.0       105.3
375,      800.0       130.6
376,      900.0       155.9
377,      1000.0      181.4
378,       6
379,      15
380,      0.0         -49.13
381,      298.16      9.95
382,      300.0       10.41
383,      400.0       36.06
384,      500.0       62.66
385,      600.0       89.87
386,      700.0       117.46
387,      800.0       145.25
388,      900.0       173.27
389,      1000.0      201.31
390,      1100.0      229.35
391,      1200.0      257.34
392,      1300.0      285.39
393,      1400.0      313.39
394,      1500.0      341.38
395,       5
396,      15
397,      0.0         -52.77
398,      298.16      11.96
399,      300.0       12.47
400,      400.0       40.49
>
```

Figure K.2. (Cont'd.)

```
401,      500.0       69.55
402,      600.0       99.26
403,      700.0       129.37
404,      800.0       159.71
405,      900.0       190.28
406,      1000.0      220.88
407,      1100.0      251.48
408,      1200.0      282.02
409,      1300.0      312.62
410,      1400.0      343.15
411,      1500.0      373.70
412,       5
413,      15
414,      0.0         -56.42
415,      298.15      13.97
416,      300.0       14.52
417,      400.0       44.92
418,      500.0       76.42
419,      600.0       108.64
420,      700.0       141.27
421,      800.0       174.15
422,      900.0       207.27
423,      1000.0      240.44
424,      1100.0      273.59
425,      1200.0      306.67
426,      1300.0      339.84
427,      1400.0      372.92
428,      1500.0      406.00
429,       5
430,      15
431,      0.0         -60.07
432,      298.16      15.97
433,      300.0       16.56
434,      400.0       49.34
435,      500.0       83.30
436,      600.0       118.01
437,      700.0       153.18
438,      800.0       188.60
439,      900.0       224.28
440,      1000.0      260.00
>
```

Figure K.2. (Cont'd.)

```
441.      1100.0      295.71
442.      1200.0      331.33
443.      1300.0      367.05
444.      1400.0      402.68
445.      1500.0      438.31
446.       5
447.      15
448.      0.0         -63.71
449.      298.16      17.98
450.      300.0       18.62
451.      400.0       53.77
452.      500.0       90.19
453.      600.0       127.40
454.      700.0       165.09
455.      800.0       203.05
456.      900.0       241.29
457.      1000.0      279.57
458.      1100.0      317.83
459.      1200.0      356.01
460.      1300.0      394.27
461.      1400.0      432.45
462.      1500.0      470.64
463.       5
464.      15
465.      0.0         -67.35
466.      298.16      20.02
467.      300.0       20.68
468.      400.0       58.21
469.      500.0       97.07
470.      600.0       136.78
471.      700.0       177.01
472.      800.0       217.51
473.      900.0       258.31
474.      1000.0      299.14
475.      1100.0      339.95
476.      1200.0      380.68
477.      1300.0      421.51
478.      1400.0      462.23
479.      1500.0      502.96
480.       5
```

Figure K.2. (Cont'd.)

```
481,      18
482,      0.0           -25.30
483,      250.0         -9.17
484,      298.16        -5.00
485,      300.0         -4.83
486,      350.0         -0.20
487,      400.0         4.57
488,      450.0         9.44
489,      500.0         14.39
490,      600.0         24.48
491,      700.0         34.74
492,      800.0         45.12
493,      900.0         55.59
494,      1000.0        66.09
495,      1100.0        76.62
496,      1200.0        87.16
497,      1300.0        97.69
498,      1400.0        108.20
499,      1500.0        118.74
500,       8
501,      18
502,      0.0           -28.81
503,      250.0         -8.70
504,      298.16        -3.54
505,      300.0         -3.33
506,      350.0         2.35
507,      400.0         8.22
508,      450.0         14.21
509,      500.0         20.26
510,      600.0         32.63
511,      700.0         45.19
512,      800.0         57.88
513,      900.0         70.68
514,      1000.0        83.51
515,      1100.0        96.37
516,      1200.0        109.21
517,      1300.0        122.02
518,      1400.0        134.85
519,      1500.0        147.69
520,       8
```

Figure K.2. (Cont'd.)

```
521.      11
522.      0.0           -32.36
523.      200.0         -14.13
524.      298.15        -1.33
525.      300.0         -1.07
526.      400.0         12.88
527.      500.0         27.40
528.      600.0         42.3
529.      700.0         57.4
530.      800.0         72.6
531.      900.0         87.9
532.      1000.0        103.3
533.       6
534.      11
535.      0.0           -31.67
536.      200.0         -13.59
537.      298.15        -0.84
538.      300.0         -0.59
539.      400.0         13.32
540.      500.0         27.81
541.      600.0         42.7
542.      700.0         57.7
543.      800.0         73.0
544.      900.0         88.3
545.      1000.0        103.7
546.       6
547.      11
548.      0.0           -35.97
549.      200.0         -14.23
550.      298.15        0.78
551.      300.0         1.07
552.      400.0         17.39
553.      500.0         34.35
554.      600.0         51.7
555.      700.0         69.3
556.      800.0         87.1
557.      900.0         104.9
558.      1000.0        122.9
559.       6
560.      11
```

Figure K.2. (Cont'd.)

```
561.      0.0         -35.04
562.      200.0       -13.67
563.      298.15      1.19
564.      300.0       1.48
565.      400.0       17.68
566.      500.0       34.50
567.      600.0       51.8
568.      700.0       69.2
569.      800.0       86.9
570.      900.0       104.6
571.      1000.0      122.4
572.       6
573.      11
574.      0.0         -38.92
575.      200.0       -14.04
576.      298.15      3.02
577.      300.0       3.36
578.      400.0       21.91
579.      500.0       41.19
580.      600.0       61.0
581.      700.0       81.0
582.      800.0       101.1
583.      900.0       121.4
584.      1000.0      141.8
585.       6
586.      11
587.      0.0         -39.71
588.      200.0       -14.45
589.      298.15      2.76
590.      300.0       3.10
591.      400.0       21.80
592.      500.0       41.20
593.      600.0       61.0
594.      700.0       81.1
595.      800.0       101.4
596.      900.0       121.9
597.      1000.0      142.3
598.       6
599.      11
600.      0.0         -41.54
```

Figure K.2. (Cont'd.)

```
601.      200.0       -15.38
602.      298.15      2.47
603.      300.0       2.82
604.      400.0       22.15
605.      500.0       42.17
606.      600.0       62.6
607.      700.0       83.3
608.      800.0       104.2
609.      900.0       125.1
610.      1000.0      146.1
611.       6
612.      11
613.      0.0         -41.00
614.      200.0       -14.77
615.      298.15      3.30
616.      300.0       3.66
617.      400.0       23.22
618.      500.0       43.47
619.      600.0       64.1
620.      700.0       85.0
621.      800.0       106.1
622.      900.0       127.3
623.      1000.0      148.4
624.       6
625.      11
626.      0.0         -42.80
627.      200.0       -14.41
628.      298.15      4.87
629.      300.0       5.25
630.      400.0       26.18
631.      500.0       47.89
632.      600.0       70.1
633.      700.0       92.6
634.      800.0       115.3
635.      900.0       138.2
636.      1000.0      161.0
637.       6
638.      11
639.      0.0         -43.42
640.      200.0       -14.64
>
```

Figure K.2. (Cont'd.)

```
641.      298.15      4.78
642.      300.0       5.16
643.      400.0       26.23
644.      500.0       48.07
645.      600.0       70.4
646.      700.0       93.1
647.      800.0       115.9
648.      900.0       138.9
649.      1000.0      161.9
650.       6
651.      11
652.      0.0         -47.64
653.      200.0       -15.75
654.      298.15      6.00
655.      300.0       6.42
656.      400.0       30.00
657.      500.0       54.43
658.      600.0       79.4
659.      700.0       104.7
660.      800.0       130.2
661.      900.0       155.8
662.      1000.0      181.5
663.       6
664.      11
665.      0.0         -46.55
666.      200.0       -14.64
667.      298.15      6.85
668.      300.0       7.27
669.      400.0       30.57
670.      500.0       54.73
671.      600.0       79.4
672.      700.0       104.5
673.      800.0       129.7
674.      900.0       155.1
675.      1000.0      180.6
676.       6
677.      11
678.      0.0         -47.18
679.      200.0       -14.88
680.      298.15      6.75
```

Figure K.2. (Cont'd.)

```
681,      300.0       7.18
682,      400.0       30.61
683,      500.0       54.90
684,      600.0       79.8
685,      700.0       104.9
686,      800.0       130.3
687,      900.0       155.8
688,      1000.0      181.4
689,       6
690,      11
691,      0.0         -50.29
692,      200.0       -14.86
693,      298.15      8.83
694,      300.0       9.30
695,      400.0       34.97
696,      500.0       61.57
697,      600.0       88.7
698,      700.0       116.4
699,      800.0       144.1
700,      900.0       172.0
701,      1000.0      200.1
702,       6
703,      11
704,      0.0         -54.03
705,      200.0       -15.08
706,      298.15      10.81
707,      300.0       11.33
708,      400.0       39.37
709,      500.0       68.41
710,      600.0       98.1
711,      700.0       128.2
712,      800.0       158.5
713,      900.0       188.9
714,      1000.0      219.5
715,       6
716,      11
717,      0.0         -57.77
718,      200.0       -15.30
719,      298.15      12.79
720,      300.0       13.36
>
```

Figure K.2. (Cont'd.)

```
721.      400.0       43.77
722.      500.0       75.25
723.      600.0       107.4
724.      700.0       140.1
725.      800.0       172.8
726.      900.0       205.9
727.      1000.0      239.0
728.       6
729.      11
730.      0.0         -61.51
731.      200.0       -15.52
732.      298.15      14.77
733.      300.0       15.39
734.      400.0       48.17
735.      500.0       82.09
736.      600.0       116.7
737.      700.0       151.9
738.      800.0       187.2
739.      900.0       222.8
740.      1000.0      258.5
741.       6
742.      11
743.      0.0         -65.25
744.      200.0       -15.74
745.      298.15      16.75
746.      300.0       17.42
747.      400.0       52.57
748.      500.0       88.93
749.      600.0       126.1
750.      700.0       163.8
751.      800.0       201.6
752.      900.0       239.7
753.      1000.0      277.9
754.       6
755.      11
756.      0.0         -68.99
757.      200.0       -15.96
758.      298.15      18.73
759.      300.0       19.45
760.      400.0       56.97
>
```

Figure K.2. (Cont'd.)

```
761.      500.0       95.77
762.      600.0       135.4
763.      700.0       175.6
764.      800.0       216.0
765.      900.0       256.6
766.      1000.0      297.4
767.       6
768.      11
769.      0.0         -53.04
770.      200.0       -16.31
771.      298.15      8.16
772.      300.0       8.64
773.      400.0       35.09
774.      500.0       62.44
775.      600.0       90.3
776.      700.0       118.6
777.      800.0       147.1
778.      900.0       175.7
779.      1000.0      204.3
780.       6
781.      11
782.      0.0         -54.78
783.      200.0       -16.53
784.      298.15      10.14
785.      300.0       10.67
786.      400.0       39.49
787.      500.0       69.28
788.      600.0       99.6
789.      700.0       130.5
790.      800.0       161.4
791.      900.0       192.6
792.      1000.0      223.7
793.       6
794.      11
795.      0.0         -60.52
796.      200.0       -16.75
797.      298.15      12.12
798.      300.0       12.70
799.      400.0       43.89
800.      500.0       76.12
>
```

Figure K.2. (Cont'd.)

```
801.      600.0       109.0
802.      700.0       142.3
803.      800.0       175.8
804.      900.0       209.5
805.      1000.0      243.2
806.       6
807.      11
808.      0.0         -50.31
809.      200.0       -14.77
810.      298.15      9.20
811.      300.0       9.67
812.      400.0       35.65
813.      500.0       62.55
814.      600.0       90.0
815.      700.0       117.9
816.      800.0       146.0
817.      900.0       174.2
818.      1000.0      202.5
819.       6
820.      11
821.      0.0         -57.79
822.      200.0       -15.21
823.      298.15      13.16
824.      300.0       13.73
825.      400.0       44.45
826.      500.0       76.23
827.      600.0       108.7
828.      700.0       141.6
829.      800.0       174.7
830.      900.0       208.1
831.      1000.0      241.4
832.       6
833.      15
834.      0.0         -26.30
835.      298.16      6.52
836.      300.0       6.79
837.      400.0       21.84
838.      500.0       37.51
839.      600.0       53.55
840.      700.0       69.80
```

Figure K.2. (Cont'd.)

```
841.      800.0       86.16
842.      900.0       102.59
843.      1000.0      119.03
844.      1100.0      135.43
845.      1200.0      151.83
846.      1300.0      168.13
847.      1400.0      184.43
848.      1500.0      200.65
849.       5
850.      15
851.      0.0         -28.94
852.      298.16      9.38
853.      300.0       9.69
854.      400.0       27.12
855.      500.0       45.19
856.      600.0       63.72
857.      700.0       82.50
858.      800.0       101.37
859.      900.0       120.28
860.      1000.0      139.23
861.      1100.0      158.17
862.      1200.0      177.11
863.      1300.0      195.93
864.      1400.0      214.71
865.      1500.0      233.36
866.       5
867.      15
868.      0.0         14.522
869.      298.16      16.282
870.      300.0       16.305
871.      400.0       17.675
872.      500.0       19.245
873.      600.0       20.918
874.      700.0       22.676
875.      800.0       24.490
876.      900.0       26.354
877.      1000.0      28.249
878.      1100.0      30.16
879.      1200.0      32.09
880.      1300.0      34.03
```

Figure K.2. (Cont'd.)

```
881.      1400.0      35.97
882.      1500.0      37.92
883.       5
884.      15
885.      0.0         -2.54
886.      298.16      20.94
887.      300.0       21.13
888.      400.0       31.90
889.      500.0       43.08
890.      600.0       54.57
891.      700.0       66.25
892.      800.0       78.02
893.      900.0       89.90
894.      1000.0      101.81
895.      1100.0      113.73
896.      1200.0      125.61
897.      1300.0      137.53
898.      1400.0      149.42
899.      1500.0      161.23
900.       5
901.      15
902.      0.0         -6.18
903.      298.16      22.95
904.      300.0       23.18
905.      400.0       36.33
906.      500.0       49.96
907.      600.0       63.95
908.      700.0       78.16
909.      800.0       92.47
910.      900.0       106.91
911.      1000.0      121.38
912.      1100.0      135.85
913.      1200.0      150.28
914.      1300.0      164.75
915.      1400.0      179.19
916.      1500.0      193.55
917.       5
918.      15
919.      0.0         -9.83
920.      298.16      24.96
```

Figure K.2. (Cont'd.)

```
921.      300.0       25.24
922.      400.0       40.76
923.      500.0       56.84
924.      600.0       73.33
925.      700.0       90.07
926.      800.0       106.92
927.      900.0       123.92
928.      1000.0      140.94
929.      1100.0      157.97
930.      1200.0      174.95
931.      1300.0      191.97
932.      1400.0      208.96
933.      1500.0      225.86
934.       5
935.      15
936.      0.0         -13.47
937.      298.16      26.97
938.      300.0       27.29
939.      400.0       45.19
940.      500.0       63.73
941.      600.0       82.72
942.      700.0       101.98
943.      800.0       121.37
944.      900.0       140.93
945.      1000.0      160.51
946.      1100.0      180.09
947.      1200.0      199.61
948.      1300.0      219.20
949.      1400.0      238.73
950.      1500.0      258.18
951.       5
952.      15
953.      0.0         -17.12
954.      298.16      28.98
955.      300.0       29.34
956.      400.0       49.62
957.      500.0       70.61
958.      600.0       92.10
959.      700.0       113.89
960.      800.0       135.82
>
```

Figure K.2. (Cont'd.)

```
961,      900.0       157.94
962,      1000.0      180.07
963,      1100.0      202.21
964,      1200.0      224.28
965,      1300.0      246.42
966,      1400.0      268.50
967,      1500.0      290.49
968,       5
969,      15
970,      0.0         -20.76
971,      298.16      30.98
972,      300.0       31.40
973,      400.0       54.05
974,      500.0       77.49
975,      600.0       101.48
976,      700.0       125.80
977,      800.0       150.28
978,      900.0       174.95
979,      1000.0      199.64
980,      1100.0      224.33
981,      1200.0      248.95
982,      1300.0      273.64
983,      1400.0      298.26
984,      1500.0      322.81
985,       5
986,      15
987,      0.0         -24.40
988,      298.16      32.99
989,      300.0       33.45
990,      400.0       58.49
991,      500.0       84.37
992,      600.0       110.86
993,      700.0       137.71
994,      800.0       164.73
995,      900.0       191.95
996,      1000.0      219.21
997,      1100.0      246.45
998,      1200.0      273.62
999,      1300.0      300.86
1000,     1400.0      328.03
```

Figure K.2. (Cont'd.)

```
1001,      1500.0      355.13
1002,        5
1003,      15
1004,      0.0         -28.05
1005,      298.16      35.00
1006,      300.0       35.50
1007,      400.0       62.92
1008,      500.0       91.25
1009,      600.0       120.24
1010,      700.0       149.62
1011,      800.0       179.18
1012,      900.0       208.96
1013,      1000.0      238.77
1014,      1100.0      268.57
1015,      1200.0      298.29
1016,      1300.0      328.08
1017,      1400.0      357.80
1018,      1500.0      387.44
1019,        5
1020,      15
1021,      0.0         24.000
1022,      298.16      30.989
1023,      300.0       31.058
1024,      400.0       35.008
1025,      500.0       39.242
1026,      600.0       43.663
1027,      700.0       48.211
1028,      800.0       52.838
1029,      900.0       57.537
1030,      1000.0      62.270
1031,      1100.0      67.02
1032,      1200.0      71.79
1033,      1300.0      76.57
1034,      1400.0      01.34
1035,      1500.0      86.11
1036,        5
1037,      15
1038,      0.0         17.500
1039,      298.16      29.228
1040,      300.0       29.335
```

Figure K.2. (Cont'd.)

```
1041.      400.0       35.390
1042.      500.0       41.811
1043.      600.0       48.477
1044.      700.0       55.306
1045.      800.0       62.236
1046.      900.0       69.255
1047.      1000.0      76.320
1048.      1100.0      83.40
1049.      1200.0      90.50
1050.      1300.0      97.61
1051.      1400.0      104.71
1052.      1500.0      111.81
1053.       5
1054.      15
1055.      0.0         11.096
1056.      298.16      29.177
1057.      300.0       29.329
1058.      400.0       37.883
1059.      500.0       46.852
1060.      600.0       56.103
1061.      700.0       65.548
1062.      800.0       75.110
1063.      900.0       84.777
1064.      1000.0      94.494
1065.      1100.0      104.23
1066.      1200.0      113.99
1067.      1300.0      123.76
1068.      1400.0      133.50
1069.      1500.0      143.24
1070.       5
1071.      15
1072.      0.0         10.926
1073.      298.16      28.405
1074.      300.0       28.554
1075.      400.0       37.008
1076.      500.0       45.906
1077.      600.0       55.099
1078.      700.0       64.492
1079.      800.0       74.006
1080.      900.0       83.630
```

Figure K.2. (Cont'd.)

```
1081.      1000.0      93.307
1082.      1100.0      103.00
1083.      1200.0      112.72
1084.      1300.0      122.45
1085.      1400.0      132.15
1086.      1500.0      141.85
1087.       5
1088.      15
1089.      0.0         11.064
1090.      298.16      28.952
1091.      300.0       29.104
1092.      400.0       37.688
1093.      500.0       46.724
1094.      600.0       56.060
1095.      700.0       65.604
1096.      800.0       75.275
1097.      900.0       85.058
1098.      1000.0      94.897
1099.      1100.0      104.76
1100.      1200.0      114.64
1101.      1300.0      124.54
1102.      1400.0      134.40
1103.      1500.0      144.27
1104.       5
1105.      15
1106.      0.0         7.593
1107.      298.16      30.217
1108.      300.0       30.406
1109.      400.0       41.05
1110.      500.0       52.20
1111.      600.0       63.68
1112.      700.0       75.38
1113.      800.0       87.20
1114.      900.0       99.14
1115.      1000.0      111.14
1116.      1100.0      123.2
1117.      1200.0      135.2
1118.      1300.0      147.2
1119.      1400.0      159.2
1120.      1500.0      171.2
```

Figure K.2. (Cont'd.)

```
1121.      5
1122.     15
1123.     0.0          5.527
1124.     298.16       29.319
1125.     300.0        29.513
1126.     400.0        40.56
1127.     500.0        52.06
1128.     600.0        63.91
1129.     700.0        76.01
1130.     800.0        88.26
1131.     900.0        100.63
1132.     1000.0       113.07
1133.     1100.0       125.5
1134.     1200.0       138.0
1135.     1300.0       150.6
1136.     1400.0       163.0
1137.     1500.0       175.5
1138.      5
1139.     15
1140.     0.0          4.468
1141.     298.16       27.912
1142.     300.0        28.104
1143.     400.0        39.02
1144.     500.0        50.39
1145.     600.0        62.11
1146.     700.0        74.07
1147.     800.0        86.17
1148.     900.0        98.41
1149.     1000.0       110.71
1150.     1100.0       123.0
1151.     1200.0       135.4
1152.     1300.0       147.8
1153.     1400.0       160.1
1154.     1500.0       172.4
1155.      5
1156.     15
1157.     0.0          4.241
1158.     298.16       28.172
1159.     300.0        28.369
1160.     400.0        39.558
```

Figure K.2. (Cont'd.)

```
1161,      500.0       51.223
1162,      600.0       63.237
1163,      700.0       75.495
1164,      800.0       87.903
1165,      900.0       100.443
1166,      1000.0      113.045
1167,      1100.0      125.67
1168,      1200.0      138.32
1169,      1300.0      150.98
1170,      1400.0      163.60
1171,      1500.0      176.23
1172,       5
1173,      11
1174,      0.0         -51.81
1175,      273.15      -41.44
1176,      298.15      -40.13
1177,      300.0       -40.04
1178,      400.0       -34.52
1179,      500.0       -28.70
1180,      600.0       -22.74
1181,      700.0       -16.64
1182,      800.0       -10.47
1183,      900.0       -6.43
1184,      1000.0      2.09
1185,       6
1186,      11
1187,      0.0         -55.76
1188,      273.15      -40.58
1189,      298.15      -38.75
1190,      300.0       -38.58
1191,      400.0       -30.71
1192,      500.0       -22.48
1193,      600.0       -14.03
1194,      700.0       -5.41
1195,      800.0       3.31
1196,      900.0       12.09
1197,      1000.0      20.92
1198,       6
1199,      11
1200,      0.0         -59.30
```

Figure K.2. (Cont'd.)

```
1201.      273.15      -43.36
1202.      298.15      -41.44
1203.      300.0       -41.28
1204.      400.0       -33.10
1205.      500.0       -24.60
1206.      600.0       -15.87
1207.      700.0       -7.00
1208.      800.0       1.95
1209.      900.0       10.96
1210.      1000.0      20.00
1211.       6
1212.      11
1213.      0.0         -63.02
1214.      273.15      -40.73
1215.      298.15      -40.12
1216.      300.0       -39.95
1217.      400.0       -29.67
1218.      500.0       -18.99
1219.      600.0       -8.05
1220.      700.0       3.07
1221.      800.0       14.30
1222.      900.0       25.60
1223.      1000.0      36.93
1224.       6
1225.      30
1226.      0.0         -27.199
1227.      50.0        -27.86
1228.      100.0       -28.73
1229.      150.0       -29.70
1230.      200.0       -30.71
1231.      273.15      -32.23
1232.      298.15      -32.781
1233.      300.0       -32.82
1234.      400.0       -34.97
1235.      500.0       -37.14
1236.      600.0       -39.30
1237.      700.0       -41.46
1238.      800.0       -43.60
1239.      900.0       -45.73
1240.      1000.0      -47.84
```

Figure K.2. (Cont'd.)

```
1241.       1100.0      -49.95
1242.       1200.0      -52.03
1243.       1300.0      -54.11
1244.       1400.0      -56.16
1245.       1500.0      -58.22
1246.       1750.0      -63.31
1247.       2000.0      -68.33
1248.       2250.0      -73.28
1249.       2500.0      -78.20
1250.       2750.0      -83.07
1251.       3000.0      -87.91
1252.       3500.0      -97.39
1253.       4000.0      -106.81
1254.       4500.0      -116.0
1255.       5000.0      -125.1
1256.       10
1257.       30
1258.       0.0         -93.964
1259.       50.0        -94.03
1260.       100.0       -94.08
1261.       150.0       -94.14
1262.       200.0       -94.19
1263.       273.15      -94.24
1264.       298.15      -94.258
1265.       300.0       -94.26
1266.       400.0       -94.32
1267.       500.0       -94.39
1268.       600.0       -94.44
1269.       700.0       -94.49
1270.       800.0       -94.53
1271.       900.0       -94.57
1272.       1000.0      -94.60
1273.       1100.0      -94.64
1274.       1200.0      -94.65
1275.       1300.0      -94.67
1276.       1400.0      -94.67
1277.       1500.0      -94.69
1278.       1750.0      -94.71
1279.       2000.0      -94.70
1280.       2250.0      -94.66
>
```

Figure K.2. (Cont'd.)

```
1281.      2500.0      -94.64
1282.      2750.0      -94.59
1283.      3000.0      -94.53
1284.      3500.0      -94.28
1285.      4000.0      -94.08
1286.      4500.0      -93.7
1287.      5000.0      -93.3
1288.      10
1289.      30
1290.      0.0         -57.102
1291.      50.0        -56.976
1292.      100.0       -56.552
1293.      150.0       -56.105
1294.      200.0       -55.632
1295.      273.15      -54.903
1296.      298.15      -54.634
1297.      300.0       -54.614
1298.      400.0       -53.515
1299.      500.0       -52.357
1300.      600.0       -51.152
1301.      700.0       -49.911
1302.      800.0       -48.640
1303.      900.0       -47.348
1304.      1000.0      -46.036
1305.      1100.0      -44.708
1306.      1200.0      -43.367
1307.      1300.0      -42.016
1308.      1400.0      -40.655
1309.      1500.0      -39.290
1310.      1750.0      -35.853
1311.      2000.0      -32.392
1312.      2250.0      -28.917
1313.      2500.0      -25.428
1314.      2750.0      -21.927
1315.      3000.0      -18.420
1316.      3500.0      -11.391
1317.      4000.0      -4.335
1318.      4500.0      2.759
1319.      5000.0      9.885
1320.      10
```

Figure K.2. (Cont'd.)

```
1321,      30
1322,      0.0          0.000
1323,      50.0         -0.060
1324,      100.0        -0.008
1325,      150.0        -0.001
1326,      200.0        -0.001
1327,      273.15       -0.001
1328,      298.15       -0.001
1329,      300.0        0.000
1330,      400.0        0.000
1331,      500.0        0.000
1332,      600.0        0.000
1333,      700.0        0.000
1334,      800.0        0.000
1335,      900.0        0.000
1336,      1000.0       0.000
1337,      1100.0       0.000
1338,      1200.0       0.000
1339,      1300.0       0.000
1340,      1400.0       0.000
1341,      1500.0       0.000
1342,      1750.0       0.000
1343,      2000.0       0.000
1344,      2250.0       0.000
1345,      2500.0       0.000
1346,      2750.0       0.000
1347,      3000.0       0.000
1348,      3500.0       0.000
1349,      4000.0       0.000
1350,      4500.0       0.000
1351,      5000.0       0.000
1352,      10
1353,       0.57898000E+01 0.17845600E+02 0.16000000E-02 0.20000000E-02 0.27500000E-01
1354,       0.67100000E-01 0.84100000E-01 0.14240000E+00 0.31100000E-01 0.74700000E-01
1355,       0.72400000E-01 0.49800000E-01 0.38400000E-01 0.33800000E-01 0.17300000E-01
1356,       0.13200000E-01 0.26000000E-02 0.24500000E-01 0.32200000E-01 0.21500000E-01
1357,       0.11700000E-01 0.15600000E-01 0.29500000E-01 0.30200000E-01 0.52000000E-02
1358,       0.20200000E-01 0.22200000E-01 0.23200000E-01 0.81000000E-02 0.17500000E-01
1359,       0.22000000E-01 0.54000000E-02 0.75000000E-02 0.61000000E-02 0.18700000E-01
1360,       0.11300000E-01 0.12400000E-01 0.12000000E-01 0.46000000E-02 0.65000000E-02
```

Figure K.2. (Cont'd.)

```
1361,      0.60000000E-02 0.80000000E-02 0.89000000E-02 0.15500000E-01 0.65460000E+00
1362,      0.22500000E-01 0.21600000E-01 0.21000000E-01 0.27500000E-01 0.17100000E-01
1363,      0.11400000E-01 0.10000000E-02 0.26000000E-02 0.13800000E-01 0.27600000E-01
1364,      0.25000000E-02 0.40800000E-01 0.40800000E-01 0.89000000E-02 0.67000000E-02
1365,      0.17000000E-01 0.74000000E-02 0.12100000E-01 0.41400000E+00 0.93000000E-02
1366,      0.12500000E-01 0.12150200E+02 0.10676000E+02 0.21056000E+01 0.62579000E+01
1367,    /*
1368,    //
```

Figure K.2. (Cont'd.)

```
1.      // JOB
2.      //STEP1 EXEC WUNPRESB
3.      //SYSUT1 DD DSN=WYL.AG.DCL.FILE1(KINETI5B),DISP=SHR
4.      //SYSUT2 DD DSN=&&TEMP,DISP=(NEW,PASS),SPACE=(TRK,(10,1),RLSE),
5.      // UNIT=SYSDA
6.      //*
7.      //STEP2 EXEC SAS
8.      //SASIN DD DSN=&&TEMP,DISP=(OLD,DELETE)
9.      DATA KINETICS;
10.       INFILE SASIN;
11.       INPUT ID $ 1-4 R 7-12 T 15-20 PH2 25-30 PC2H4 35-40 PCO 45-50
12.                                     PCO2 55-60 PCH4 65-70 PC2H6 75-80
13.     ;
14.       RATIO1=PC2H4/PH2;
15.       RATIO2=PCO/PH2;
16.       LIST;
17.     PROC PRINT;
18.     PROC PLOT;
19.       PLOT R*RATIO1=RATIO2;
20.     PROC NLIN METHOD=MARQUARDT MAXITER=10000000;
21.       PARMS A=28.0 E=0.1 K1=0.1 K2=0.1 K3=0.1 K4=0.1E-20 K5=0.1
22.                          K8=0.1 K10=0.1 K12=0.1 K13=0.1E-20 K14=0.1
23.                          K15=0.1 K17=0.1;
24.       BOUNDS 0<A 0<E 0<=K1 0<=K2 0<=K3 0<=K4 0<=K5 0<=K8 0<=K10
25.                      0<=K12 0<=K13 0<=K14 0<=K15 0<=K17;
26.       R=EXP(-E/(8.3145*T));
27.       P1=K1*PH2;
28.       P2=K2*PCO;
29.       P4=K4*PC2H4;
30.       P14=K14*PCH4;
31.       P15=K15*PC2H6;
32.       P17=K17*PCO2;
33.       S=1.0+SQRT(P1)+P2+SQRT(P4)+(K3/K12)*P2*P2/P17+K12*P17/P2
34.            +K8*P14/SQRT(P1)+K10*P15/SQRT(P1)+P14+P15
35.            +K13*P1*P17/P2+P17;
36.       C=P1*PC2H4-K5*K10*P15;
37.       D=A*R*C;
38.       N=SQRT(P1)*8;
39.       Q1=PH2/K1;
40.       Q4=PC2H4/K4;
```

Figure K.3. List of Computer Program MODEL6B.

```
      MODEL R=D/N;
      DER.A=B*C/N;
      DER.E=(-1.0/(8.3145*T))*D/N;
      DER.K1=A*B*(PH2*PC2H4/N-C/(N*N)*(0.5*SQRT(Q1)*B+
             SQRT(P1)*(0.5*SQRT(Q1)-0.5*(K8/K1)*P14/SQRT(P1)-
             0.5*(K10/K1)*P15/SQRT(P1)+K13*PH2*P17/P2)));
      DER.K2=-D/(N*N)*SQRT(P1)*(PCO+2.0*(K3/K12)*PCO*P2/P17-
             (K12/K2)*P17/P2-(K13/K2)*P1*P17/P2);
      DER.K3=-D/(N*N)*SQRT(P1)*P2*P2/(K12*P17);
      DER.K4=-D/(N*N)*SQRT(P1)*0.5*SQRT(Q4);
      DER.K5=-A*B*K10*P15/N;
      DER.K8=-D/(N*N)*P14;
      DER.K10=A*B*(-K5*P15/N-C/(N*N)*P15);
      DER.K12=-D/(N*N)*SQRT(P1)*(-(K3/(K12*K12))*P2*P2/P17+
              P17/P2);
      DER.K13=-D/(N*N)*SQRT(P1)*P1*P17/P2;
      DER.K14=-D/(N*N)*(K8+SQRT(P1))*PCH4;
      DER.K15=A*B*(-K5*K10*PC2H6/N-D/(N*N)*(K10+SQRT(P1))*PC2H6);
      DER.K17=-D/(N*N)*SQRT(P1)*(-(K3/(K12*K17))*P2*P2/P17+
              K12*PCO2/P2+K13*P1*PCO2/P2+PCO2);
      OUTPUT OUT=OUTLET1 P=PREDICT;
    PROC PRINT;
      VAR ID R PREDICT;
      TITLE SUMMARY OF PREDICTED VALUES VS OBSERVED VALUES;
    PROC PLOT DATA=OUTLET1;
      PLOT PREDICT*R;
```

N1	0.0771	489.82	383.76	150.32	375.61	68.54	83.78	4.58
N4A1	0.0868	503.71	259.96	138.75	295.73	177.83	193.09	1.22
N5A1	0.0762	485.93	288.89	142.62	284.45	205.09	144.71	0.83
N5A2	0.1685	553.71	260.84	146.44	292.28	179.49	183.74	4.60
N5B2	0.1715	554.82	266.93	125.89	295.21	161.43	195.72	21.39
N6B	0.1807	550.37	270.95	128.64	262.31	180.10	201.42	23.18
N8B	0.2144	559.82	267.27	126.35	285.07	167.50	200.80	19.59
N9A	0.0628	496.48	213.82	100.08	271.07	311.09	167.32	3.20
N9B3	0.0975	523.71	218.00	98.94	266.73	320.88	154.94	7.09
N9B4	0.1340	549.82	211.08	91.87	262.14	323.02	163.64	14.83
N9B5	0.2007	577.59	217.03	89.69	250.76	351.71	146.47	10.92
N9B6	0.2689	605.93	207.55	87.97	242.26	370.60	146.81	11.38
N9D	0.0498	494.26	215.20	104.12	277.10	292.21	175.27	2.67
N9E	0.0411	499.82	214.53	108.48	290.61	291.75	155.10	6.11

Figure K.3. (Cont'd.)

81.	N10	0.0435	493.15	152.83	74.41	186.25	443.99	208.61	0.50
82.	N12	0.0513	495.93	179.97	235.28	149.89	329.88	168.45	3.09
83.	N14	0.0193	494.82	126.81	167.72	426.12	221.53	123.78	0.62
84.	N15	0.1048	497.04	331.81	251.99	117.34	224.66	133.24	7.54
85.	N17	0.0432	494.26	211.82	72.41	179.09	392.71	208.23	2.33
86.	N18	0.0126	494.26	157.28	52.50	413.26	276.16	167.37	0.0
87.	N19	0.0113	494.26	140.71	47.27	482.38	244.54	151.68	0.0
88.	N20	0.1295	494.26	367.10	178.22	105.73	258.47	145.05	12.01
89.	N21	0.0670	497.04	302.49	151.86	292.99	202.92	114.87	1.45
90.	N24	0.0293	494.26	83.34	265.33	341.72	237.87	137.22	1.10
91.	N30	0.0590	493.71	153.59	321.95	129.05	291.82	167.22	2.96
92.	N31	0.0382	494.26	125.82	254.07	324.17	226.46	134.87	1.19
93.	N33A	0.0493	494.26	226.31	149.43	309.56	241.63	135.28	4.38
94.	N33B	0.1152	527.59	231.18	128.39	283.76	256.36	146.03	20.85
95.	N33B	0.1473	544.26	230.98	148.61	272.60	260.78	125.01	28.60
96.	N33C	0.0567	499.82	175.85	160.56	361.63	234.41	128.97	5.17
97.	N33C	0.1473	560.93	194.71	113.21	342.84	249.36	139.91	26.55
98.	N34	0.1240	502.59	288.33	168.79	67.10	327.82	181.37	33.18
99.	N35	0.0504	494.82	189.88	130.44	427.03	211.85	106.66	0.72
100.	N39	0.0629	497.04	198.01	278.08	248.59	217.23	120.03	4.65
101.	N40A	0.0442	494.82	237.43	118.39	313.17	244.18	136.52	16.90
102.	N40C	0.0567	493.15	230.67	116.19	332.37	271.71	99.69	15.97

>

Figure K.3. (Cont'd.)