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**Numerical Simulation of a Cold Trap
for Sodium Purification**

by

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NUMERICAL SIMULATION OF A COLD TRAP FOR SODIUM PURIFICATION

by

B. C. Goplen, J. C. Biery, and C. C. McPheeters

ABSTRACT

The dynamic behavior of a sodium system cold trap was numerically simulated on a digital computer. The simulation accounted for mixing in the hold tank, delay times in pipes, temperature variation with distance in the cold trap, impurity buildup on the walls of the cold trap, and simultaneous precipitation and dissolution of the impurity in different portions of the cold trap. The main purpose of the simulation was to generate mass transfer coefficients from experimental data taken from an experimental sodium loop. The program can also help in the design of sodium systems containing cold traps.

I. Introduction

A common means of purifying liquid metal systems is the low-temperature precipitation of impurities. The process is referred to as cold trapping. To study the kinetics of cold trap behavior, a series of experiments was performed at the Los Alamos Scientific Laboratory (LASL).¹ Because of the complexity of the cold trap system a numerical simulation program, VASSAR, was written in FORTRAN for the IBM 7030 computer to help analyze the experimental results.

Basically, the two purposes for a program of this type are (1) to calculate mass transfer coefficients, both for precipitation and dissolution, by the direct simulation of experimental data; and (2) to assist in designing sodium systems by testing the effectiveness of various cold traps in the particular system being considered. This report is concerned only with the first purpose.

The VASSAR program uses the Lagrangian coordinate system and finite difference techniques to solve the steady-state heat transfer and unsteady-state mass transfer differential equations.

II. The Experimental System

The sodium test system considered was a closed, forced convection circuit with partial flow through the

cold trap. The test loop, shown in Fig. 1, consisted of (1) a large volume ballast tank to provide a suitable time delay in the circuit; (2) an electromagnetic sodium pump; (3) a vacuum distillation sampler; (4) a plugging meter; (5) a removable cold trap section provided with a NaK

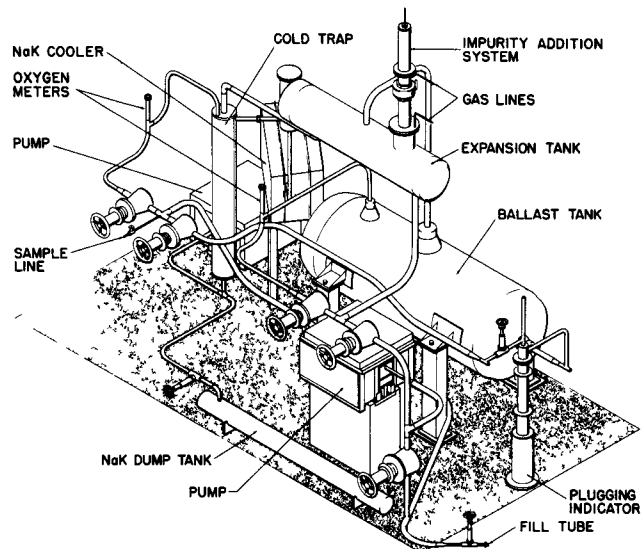


Fig. 1.
Isometric view of cold trap test loop.

alloy cooling circuit consisting of an expansion tank, a NaK-to-air heat exchanger, an electromagnetic pump, a flowmeter, and a diffusion cold trap; (6) two emf liquid metal oxygen meters, one upstream from the cold trap and one downstream; (7) an expansion tank containing the main system heat input and an impurity addition device; (8) two sodium system flowmeters, one immediately upstream from the cold trap, and the other in the plugging meter section; and (9) valving and piping to isolate the cold trap section from the large tank section while maintaining pump flow through the cold trap section.

The system flow is illustrated schematically in Fig. 2. In the primary system, flow proceeded from the ballast tank through the pump to a pipe cross where it divided to go to the vacuum distillation analytical sampler, the plugging meter, and the cold trap. Flow through the distillation sampler was returned to the main stream between the expansion tank and the ballast tank. Flow through the plugging indicator was returned to the ballast tank. Flow to the cold trap passed through the main system flowmeter, oxygen meter No. 1, the cold trap, the expansion tank, oxygen meter No. 2, and returned to the ballast tank.

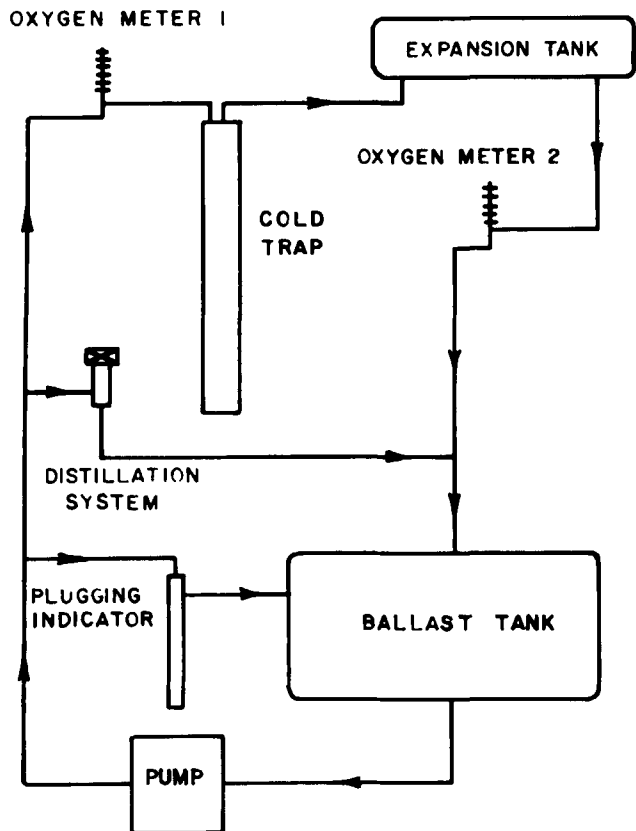


Fig. 2.
Flow diagram of cold trap test loop.

A cutaway view of the cold trap is shown in Fig. 3, with NaK and sodium flows as illustrated. Packing was eliminated to simplify the geometry of the nucleation surfaces. A helical winding of tubing in the NaK annulus provided uniform flow distribution. Six thermocouples in a well in the annulus measured bulk temperatures in the sodium.

III. Calculational Technique

The computer program, VASSAR, uses a Lagrangian coordinate system to follow a "slug" or element of fluid in its routing through the system; the associated impurity concentration is continually recalculated. Thus, the entire physical system is divided into a large number of elements with a "node" number associated with each location in the system.

The simulation program takes into account all aspects of the system including the delay time in pipes, the mixing characteristics of the tank, and the precipitation and dissolution characteristics of the cold trap. Three surfaces on which precipitation can occur in the cold trap are the inner and outer surfaces of the annular space which the sodium contacts as it moves down the cold trap and the cylindrical surface that it contacts as it moves upward out of the cold trap.

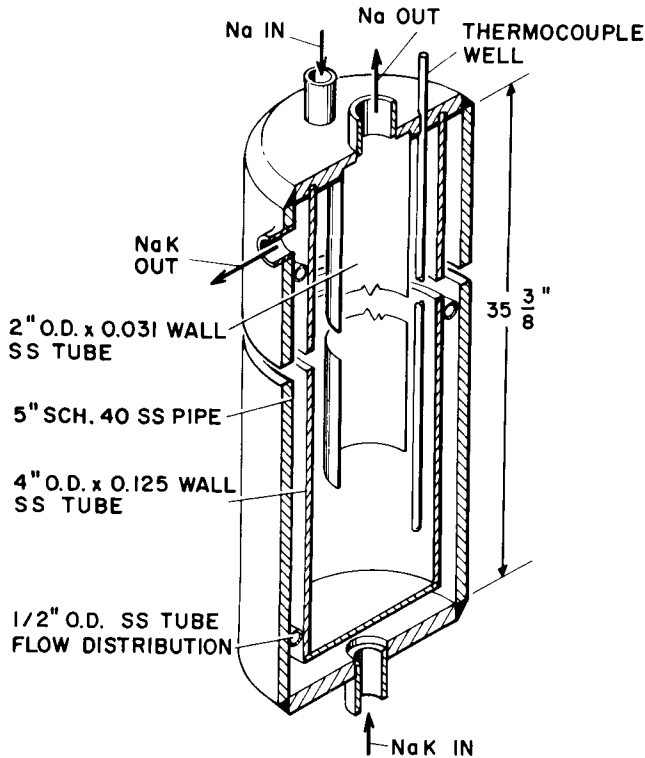


Fig. 3.
Cutaway view of cold trap.

Because the impurity concentration at which precipitation occurs is a function of the cold trap surface temperature, a complete temperature calculation is required in the cold trap. The rest of the system is considered to be isothermal. The NaK annulus, the incoming sodium annulus, and the outgoing sodium cylinder are designated, respectively, as regions A_{NaK} , B_{Na} , and C_{Na} . The law of conservation of energy in each region provides three differential equations, Eqs (1) through (3), that are solved simultaneously in finite difference by relaxation. Boundary conditions are imposed by specifying the NaK and sodium inlet temperatures.

$$\frac{dT_a}{dx} = \frac{h_1 \cdot h_{1+} + \pi d_1}{(h_{1-} + h_{1+}) (m c_p)_a} (T_b - T_a) \quad (1)$$

$$\begin{aligned} \frac{dT_b}{dx} = & \frac{h_1 \cdot h_{1+} + \pi d_1}{(h_{1-} + h_{1+}) (m c_p)_b} (T_a - T_b) \\ & + \frac{h_2 \cdot h_{2+} + \pi d_2}{(h_{2-} + h_{2+}) (m c_p)_b} (T_c - T_b) \quad (2) \end{aligned}$$

and

$$\frac{dT_c}{dx} = \frac{h_2 \cdot h_{2+} + \pi d_2}{(h_{2-} + h_{2+}) (m c_p)} (T_b - T_c) \quad (3)$$

Following solution for the bulk temperature in each region, the wall temperatures for the surfaces of precipitation may be calculated directly. As an option, the code user may input a specific bulk temperature distribution for sodium in Region B. In this case, the code ignores Eq (2), then Eqs (1) and (3) become analytic, and the surface temperatures are calculated as usual.

In the LASL experiments,¹ oxygen was considered to be the main precipitation impurity. Oxygen solubility data were obtained from the Rutkauskas oxygen solubility relationship.² A semilogarithmic function of degree three, Eq (4), was used to fit the data points rather than the traditional I/T fit because the data appear to diverge from linear I/T line in the lower temperature region, which is the primary region of interest. Insertion of the wall temperature distribution into Eq (4) produces the equilibrium oxygen impurity concentration distribution in the cold trap.

$$\log_{10} C_e = DA + ET + FT^2 + GT^3 \quad (4)$$

with

$$\begin{aligned} D &= 3.17871 \times 10^{-1} \\ E &= -5.99152 \times 10^{-3} \\ F &= 2.67916 \times 10^{-5} \\ G &= 1.87669 \times 10^{-8} \end{aligned}$$

The differential mass transfer of the impurities to and from the collection surface in the cold trap can be expressed as

$$\frac{dm}{dt} = ka A_p (C - C_e) \quad (5)$$

where dm/dt is the rate of mass precipitation or dissolution, ka is the mass transfer coefficient, A_p is the area of precipitation, C is the sodium oxide concentration, and C_e is the equilibrium concentration as determined by a solubility curve for the impurity precipitating in a sodium system.

Equation (5) applies for each element of surface. However, to obtain the overall effect on the sodium flowing through the trap, the mass of impurities transferring into and out of an element of moving fluid must be accounted for. The mass balances for elements flowing through Regions B and C are written as

$$\begin{aligned} \frac{DC_b(x,t)}{Dt} = & \frac{-4 \times 10^6}{(d_1^2 - d_2^2)} \frac{ka}{\rho_b} \\ & \left\{ d_1 (C - C_{e1}) + d_2 (C - C_{e2}) \right\} \quad (6) \end{aligned}$$

and

$$\frac{DC_c(x,t)}{Dt} = -4 \times 10^6 \frac{ka}{d_2 \rho_2} (C - C_{e2}) \quad (7)$$

The use of Eqs (6) and (7) allows the calculation of oxygen concentration in the trap as a function of both time and position. The equations were solved simultaneously in finite difference form along with tank mixing and delay functions to generate the impurity concentrations.

The mass precipitated (or dissolved) is related to the concentration change by the elemental volume. A running account is kept of the mass distribution on the wall. Such mass is, of course, free to reenter the system should concentration at the point fall below equilibrium.

Various components of the system are considered in terms of their mixing or delay effects. In the expansion and storage tanks, partial mixing may be in effect. In this case, a certain percentage of the volume is considered to mix perfectly, governed by the relation

$$\frac{dC}{dt} = \frac{m_b}{\rho_b V_m} (C_{in} - C) \quad (8)$$

The remainder of the volume in the hold tank is considered in terms of a time delay, as are the volumes in the pipes and other small elements in the system. Time delays in the program are provided by storing an element's concentration and introducing it to the appropriate component after a suitable time lapse.

The time step used in the program is determined by the mass flow rate and selection of the size of the element.

of fluid as indicated by

$$\Delta t = \frac{\Delta V \rho_b}{m_b} \quad (9)$$

In general, the mass transfer coefficient, k_a , is assumed to be a function of temperature

$$k_a = a e^{\left(\frac{-\Delta E}{RT}\right)} \quad (10)$$

Further, the coefficients for dissolution and precipitation are considered to be different. In practice, the energy, ΔE , is assigned some value and the program is run iteratively to determine the quantity by comparing the computed results with the experimental data after a specified period of time. The quantity a is then revised according to

$$a = a' \left(\frac{C_{\text{calc}}}{C_{\text{exp}}} \right)^n \quad (11)$$

where acceptable values of the exponent n are generally found between 1.0 and 1.3. Satisfactory convergence was normally obtained within five iterations.

The program is versatile in that various types of experimental runs can be duplicated. For example, it is possible to calculate a precipitation run immediately followed by a dissolution run, that is, the precipitation run is calculated as usual and is followed by a temperature recalculation. The masses deposited on the walls of the cold trap as well as the concentrations remaining in the system are unchanged, or if desired, a suitable time delay can be introduced. The dissolution run then follows in which the sodium oxide is reintroduced into the system.

IV Numerical Results

The mass transfer coefficient has generally been considered a function of temperature, however, experimental data and numerical correlations have indicated that the temperature dependence is very slight. This condition is equivalent to stating that the quantity ΔE is generally much less than the quantity RT , see Eq. (10). Also, recent data³ show no significant difference between the precipitation coefficient and the dissolution coefficient. This result was verified in our work by numerical simulation of both types of experimental runs.

Both precipitation and dissolution occur in a typical precipitation run. As sodium oxide precipitates in the cold trap, the overall oxygen concentration is decreased below the saturation concentration in the warmer portions of the cold trap. When this condition occurs, the oxide dissolves from the cold trap surfaces into the sodium and becomes available for precipitation further down the cold trap in the low-temperature regions. This

effect is complicated by the condition that inner and outer surfaces of the sodium annulus may exist at different temperatures. Hence, mass may be simultaneously precipitating from and dissolving into a single fluid element. The general effect is clearly illustrated in Fig. 4, which shows the computed sodium oxide distribution on the outer surface of the cold trap annulus. As time increases, the sodium oxide is dissolving off the leading edge at the warmer portions of the cold trap and is precipitating in the colder zones. Thus, the precipitation zone becomes significantly smaller as the sodium oxide is completely removed from the warmer areas.

The general effect of the cold trap on system concentration is shown in Fig. 5. The two curves represent the oxygen concentration in the sodium entering the cold trap and that in the sodium leaving the cold trap. The discontinuities in the curves are due to an arbitrary introduction of sodium oxide. This oxide introduction feature was added because of experimental evidence that sodium oxide actually breaks loose from portions of the cold trap and is carried back into the sodium system where it redissolves and appears as an addition to the system. This experimental effect, as well as the computer simulation, is illustrated in Fig. 6. The value of the mass transfer coefficient given was determined with the previously described iterative technique.

An attempt was made to gain an analytic solution by defining the term "concentration factor". This is the area-weighted difference between system and equilibrium concentration throughout the cold trap. Use of the concentration factor allows definition of the effective precipitation driving potential in terms of the oxygen concentration in the bulk sodium as it leaves the cold trap and the equilibrium concentration at the coldest point in the trap. Calculated values of the concentration factor and its variation in time are shown in Fig. 7. The upper curve is illustrative of precipitation areas only, whereas

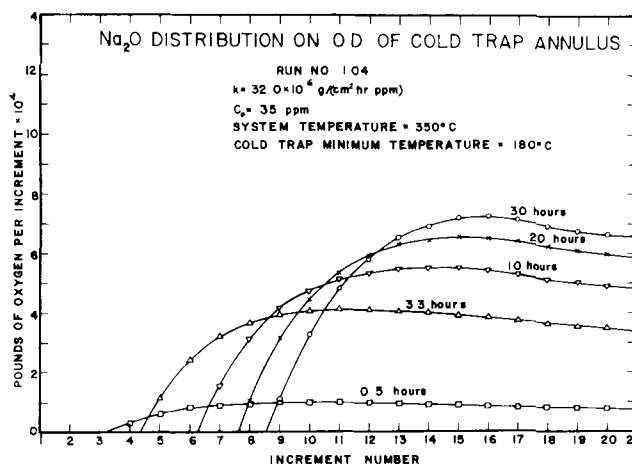


Fig. 4
Computed Na_2O mass distributions on outer wall of cold trap as a function of time

CONCENTRATION CHANGE IN A PRECIPITATION RUN

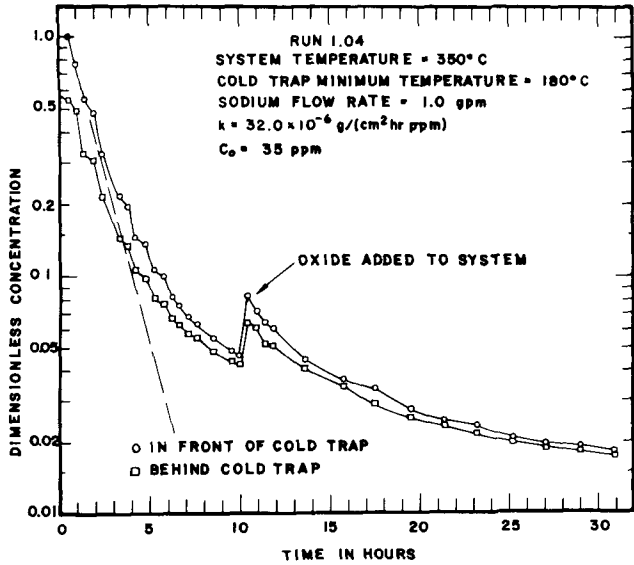


Fig. 5.

Computed oxygen concentrations in cold trap test loop as a function of time.

VARIATION OF COLD TRAP CONCENTRATION FACTOR WITH TIME

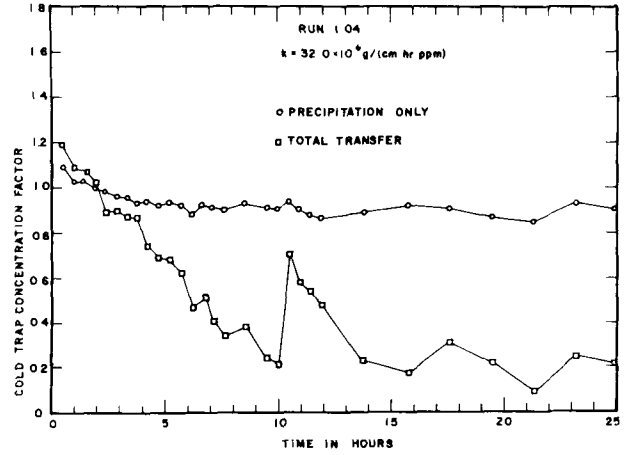


Fig. 7.

Concentration factor as a function of time as computed by the simulation program.

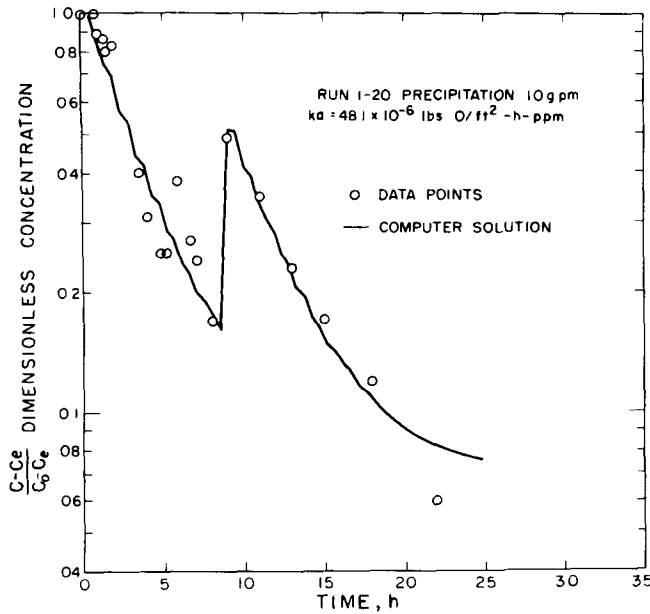


Fig. 6.

Computed and experimental oxygen concentrations as a function of time for runs 1-20 in cold trap test loop.

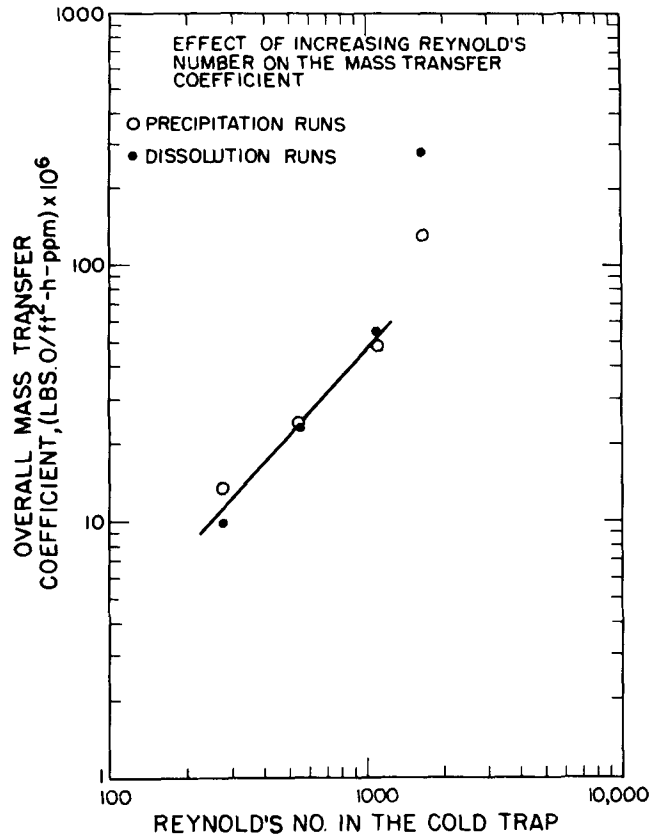


Fig. 8.

Mass transfer coefficient as a function of Reynolds number for packless trap in cold trap test loop.

the lower curve considers the transfer area of the entire cold trap.

The results of the experimental program are shown in Fig. 8 where the change in mass transfer coefficient with Reynolds number is presented. These coefficients were generated by using the simulation program.

V. Summary and Conclusions

The computer program, VASSAR, has sufficient versatility to adequately describe the precipitation and dissolution processes that occur in the experimental system. Numerical correlation with experimental data has been successful, and has allowed the generation of mass transfer coefficients.

The program also can assist in the design of cold traps for sodium systems of this type. With the knowledge of mass transfer coefficient as a function of Reynolds number, the rate of system cleanup as a function of cold trap physical parameters and modes of operation can be studied with the simulation program. By reformulation of the mathematical model, the effects of packing can also be studied.

Nomenclature

A_{NaK}	Annular region in cold trap through which NaK flows.
A_p	Area on which impurity precipitation occurs, cm^2 .
B_{Na}	Annular region in cold trap through which sodium flows.
C	Concentration of oxide impurity in sodium stream, ppm.
C_{calc}	Calculated concentrations in hold tank at some specified time, ppm.
C_e	Impurity saturation concentration, ppm
C_{exp}	Experimental concentration in hold tank at some specified time during run, ppm.
C_{in}	Concentrations entering perfectly mixed volume, ppm.
C_{Na}	Cylindrical region in cold trap through which sodium flows.
C_p	Specific heat, $cal/g^{\circ}C$.
D/Dt	Substantial derivative; change within a flowing fluid element with respect to time.
d	Diameter, cm.
h	Heat transfer coefficient, $\frac{Btu}{h\ ft^2\ ^{\circ}F}$, $\frac{cal}{sec\ cm^2\ ^{\circ}C}$.
ka	Mass transfer coefficient, $g\ impurity/(cm^2\ \cdot h\ \cdot ppm\ of\ impurity)$ or $lbs\ impurity/(ft^2\ \cdot h\ \cdot ppm)$. (First rate constant $\times 2.06 =$ second rate constant.)

m	Mass of impurity precipitating or dissolving, g.
\dot{m}	Sodium mass flow rate, g/sec , lb/h .
n	Exponent in iteration process used to correct a as indicated in Eq. (11).
T	Temperature, $^{\circ}C$.
t	Time, h.
V_m	Volume in which perfect mixing occurs, cm^3 .
x	Axial distance along cold trap, cm.

Subscripts

a	Region A_{NaK} in cold trap; annular region through which NaK flows.
b	Region B_{Na} in cold trap; annular region through which sodium flows into trap.
c	Region C_{Na} in cold trap; cylindrical region through which sodium flows out of trap.
1	Outer surface of annular space containing sodium.
2	Inner surface of annular space containing sodium.
1-	NaK side of outer surface.
1+	Sodium side of outer surface.
2-	Annular sodium side of inner surface.
2+	Cylindrical sodium side of inner surface.

Greek Symbols

a	Constant in mass transfer coefficient temperature function, Eq. (10).
a'	Constant adjusted by Eq. (11) to produce the best a to fit experimental data.
ΔE	Activation energy, in Eq. (10), $cal/(mole\ ^{\circ}K)$.
Δt	Time increment used in numerical integration, h.
ΔV	Incremental volume of liquid used in numerical simulation, cm^3 .
ρ_b	Density of sodium, g/cm^3 .



References

- 1 C C McPheeters, "Mass Transfer of Oxygen in Sodium Cold Traps," LA-3936, Los Alamos Scientific Laboratory (May 1968)
- 2 V J Rutkauskas, "Determination of the Solubility of Oxygen in Sodium by Vacuum Distillation," LA-3607-MS, Los Alamos Scientific Laboratory (September 1968)
- 3 C C McPheeters and J C Biery, "Oxygen Transport in Sodium," Proceedings of the International Conference on Sodium Technology and Large Fast Reactor Design, ANL-7520, Pt 1, pp 471-477, Argonne National Laboratory (November 1968)

APPENDIX

COLD TRAP SIMULATION PROGRAM (VASSAR)

I. Input Data

<u>Card Number</u>	<u>Data Description</u>	<u>Format</u>
-13 - 0	Mass of precipitate on each Δx of cold trap wall surface Surface areas 1+, 2-, and 2+. Masses read into program in direction of sodium flow (This input is used only if a precipitation run preceeded the present run.), lbs.	6E13.6
1	Run Number.	E13.6
2	A tag to adjust dissolution mass transfer coefficient in the iteration process. ± 1 0 = Adjust, 0 0 = No adjust	E13.6
3	Tag, + 1.0 = all Δx nodes in cold trap will be used, 0.0 = all Δx nodes above C_o saturation temperature will be dis- carded	E13.6
4	Precipitation rate constant, lbs/(h-ppm-ft ²).	E13.6
5	Constants a and ΔE in Eq (10) for calculation of dissolution mass transfer coefficient lb/(h-ft ² -ppm) and cal/mol/°K	2E13.6
6	Initial concentration of impurity in hold tank, ppm	E13.6
7	Number of Δt calculations before a printout	15
8	Number of increments on 1- and 2+ surfaces and length of increment, in	215, E13.6
9	Gallon/min of NaK flow, gal/min of sodium flow	2E13.6
10	Tank mixing factor = fraction of tank perfectly mixed	E13.6
11	Temperature of NaK entering cold trap, and temperature of sodium entering cold trap, °C.	2E13.6
12	Maximum time of run, h	E13.6
13	Number of iterations to adjust mass transfer coefficients	15
14	Time at which ΔC ppm of impurity is added to system.	2E13.6
15	Time at which number of Δt calculations per printout is changed	E13.6, 15

<u>Card Number</u>	<u>Data Description</u>	<u>Format</u>
16, 17, 18, and 19	Temperatures in Region B _{Na} . Read in from cold to hot end. Each temperature at center of Δx .	6E13.6
20	Experimental concentration and time measured. (Used in mass transfer coefficient iteration process.)	2E13.6
21	Exponent, n, for adjusting mass transfer coefficient. Used in Eq. (11).	E13.6
22	Tag to indicate whether or not to adjust precipitation mass transfer coefficient, $\pm 1.0 = \text{yes}$, $0.0 = \text{no}$.	E13.6

II. Program Printout

```

C      VASSAR IS A FINITE DIFFERENCE TRANSIENT MASS
C      TRANSFER CODE FOR COLD TRAP ANALYSIS.
C
C      THIS PARTICULAR VERSION CONSIDERS THE TYPE OF
C      COLD TRAP INITIALLY DESIGNED BY MCPHEETERS.
C
C      BEGIN WITH A STEADY STATE HEAT TRANSFER SOLUTION.
C
C      DIMENSION  DX(50),TA(50),TB(50),TC(50),AA(50),AC(50),
1CA(50),CC(50),T(100),CE(50),C(1000),XM(50),XK(50),AKT(50),CØ(50)
2,A(50),TW(50),TWC(50),TTC(50),CEC(50),AAC(50),AKTC(50),
3XMI(50),CØØ(50),CØNC(50),XMC(50),CECC(50),AKTCC(50),
4XMM(50),XMMI(50),XMMC(50),
5XKD(50),XKDC(50),AKTD(50),AKTCD(50),AKTDC(50),XKDCC(50),
6XKCC(50)
C
C
C
1  FORMAT(1H0,10(F8.3,2X))
2  FORMAT(1H1)
3  FORMAT(53H1RESULTS OF TEMPERATURE CALCULATION. T(A), T(B), T(C))
4  FORMAT(66H1EQUILIBRIUM CONCENTRATION AND WALL TEMPERATURE, PPM AND
1  DEGREES F)
5  FORMAT(15H0REGION B ONLY.)
6  FORMAT(1H0)
7  FORMAT(10(2X,E10.3))
8  OFORMAT(69H0AVERAGE CONC. DIFF. (PPM),NØ. OF NØDES ACTIVE, AND AVG.
1  CONC. FACTØR)
9  FORMAT(1H , 22X, E13.6, 22X, I5, 22X, E13.6)
10  FORMAT(6E13.6)
11  FORMAT(43H0DIMENSIONLESS EXP. CONC. AND TIME OF CONC.)
12  FORMAT(47H1PPTN K, INIT. CONC., PPM, TIME INC., HR., ADIS)
13  FORMAT(37H0VOLUMES, IN3, NØDE, TANK, LEG1, LEG2)
14  FORMAT(21H0NØ. OF ITERATIONS = , I5)

```

```

15  FORMAT(21H1DT, TIMAX, TIME, HRS)
16  FORMAT(27HONA CONC. IN COLD TRAP, PPM)
17  FORMAT(34HONA CONC. IN LEG1, TANK, LEG2, PPM)
18  OFORMAT(58HO TANK CONC., TANK DIM. CONC., TIME, XMASS(LB), XMASS(L
    1B))
19  FORMAT(29HOPPTD. MASS IN COLD TRAP(LBS))
20  FORMAT(26HOFRACTION OF TANK MIXED = ,F8.5)
21  FORMAT(14HOREGION C ONLY)
22  OFORMAT(70HJAVG. CONC. DIFF., NO. PPTN. ZONES, CONC. FACTOR INCLUDI
    ING DISSOLUTION)
23  FORMAT(23HOCNC. IN REGION C, PPM)
24  FORMAT(43HOMASS PRECIPITATED ON INSIDE OF ZONE B, LBS)
25  FORMAT(33HOMASS PRECIPITATED IN ZONE C, LBS)
26  FORMAT(39HOOXIDE IN SYSTEM, LBS., INITIAL AND NOW)
27  FORMAT(51HOEQUIL. CONC. IN ZONE C, XKCC, XKDCC, AKTCC, AKTCDC)
28  FORMAT(34HOPPTN. CONSTANT, LB/HR/FT2/PPM, = , E13.6)
29  FORMAT(22HOINITIAL CONC., PPM = , E13.6)
30  FORMAT(5I5)
31  FORMAT(26HONO. OF LOOPS PER PRINT = , I5)
32  FORMAT(2I5, E13.6)
33  FORMAT(RHOJAMX = , I5, 9H JCMX = , I5, 15H DEL X, IN, = ,E13.6)
34  FORMAT(8HOGPM1 = , E13.6, 9H GPM2 = , E13.6)
35  FORMAT(12HOTINA, C, = , E13.6 , 13H TINB, C, = ,E13.6)
36  FORMAT(15HOTIMAX, HR., = , E13.6)
37  FORMAT(30HOEXP. TEMPS. IN ZONE B, DEG. C)
38  FORMAT(36HONO. OF ITER. LOOPS TO CHANGE XK0 = , I5)
39  FORMAT(11HIRLUN NO. = , F6.3)
40  FORMAT(32HODIM. CONC. EXITING COLD TRAP = , E13.6)
41  FORMAT(16HOAT TIME, HR, = , E13.6, 13H INC. PPM = , E13.6)
42  FORMAT(42HOSIGNAL FOR TEMP. CHANGE 1 = YES 0 = NO = , E13.6)
43  FORMAT(16HOAT TIME, HR, = , E13.6, 21H CHANGE NPRINT TO = , I5)
44  FORMAT(E13.6, I5)
45  OFORMAT(67HOEQN. FACTOR BASED ON ACTIVE PPN. NODES AND 3 ZONES OF P
    1PN. AREA = , E13.6)
46  OFORMAT(77HOEQN. FACTOR BASED ON ACTIVE PPN. AND DIS. NODES AND 3 Z
    1ONES OF OXIDE AREA = , E13.6)
47  OFORMAT(50HOK DISS. AS FNC. OF TEMP., LB/HR FT2 PPM, ADIS, = ,
    1E13.6, 23H DELTA ENERGY, KCAL = , E13.6)
48  FORMAT(33HOK DIS. FOR ZONE B, LB/HR FT2 PPM)
49  FORMAT(1HO, (9E13.6))
50  FORMAT(33HOK DIS. FOR ZONE C, LB/HR FT2 PPM)
51  OFORMAT(69HOTAG TO INDICATE IF ADIS CONSTANT TO BE ADJUSTED, 0 = NO
    1, 1 = YES, = , E13.6)
52  FORMAT(48HOTAG TO ADJUST XK0 FOR PPN., 0 = NO, 1 = YES, = , E13.6)
53  FORMAT(39HOEXPONENT FOR ADJUSTING XK0 AND ADIS = , E13.6)
54  OFORMAT(48H1MASS OXYGEN, LBS, ON OD OF ANNULUS INITIALLY = , /,
    1(9E13.6))
55  OFORMAT(48HOMASS OXYGEN, LBS, ON ID OF ANNULUS INITIALLY = , /,
    1(9E13.6))
56  OFORMAT(52HOMASS OXYGEN, LBS, ON ID OF INSIDE PIPE INITIALLY = ,
    1/, (9E13.6))

```

```

C
C   THIS IS THE INPUT SECTION.
C

```

```

NCASE=1
NTEMP=1
PPMAS1 = 0.0
SIG1 = 0.0
DØ 300 J = 1, 50
XM(J)=0.
XMI(J) = 0.0
XMC(J) = 0.0
300 CONTINUE
READ(10,10)(XM(J), J = 1, 36)
READ(10,10)(XMI(J), J = 1, 36)
READ(10,10)(XMC(J), J = 1, 12)
WRITE(9,54)(XM(J), J = 1, 36)
WRITE(9,55)(XMI(J), J = 1, 36)
WRITE(9,56)(XMC(J), J = 1,12)
200 CONTINUE
DØ 201 J = 1,50
XMM(J) = XM(J)
XMMI(J) = XMI(J)
XMMC(J) = XMC(J)
201 CONTINUE
READ(10,10)RUNNØ
WRITE(9,39)RUNNØ
READ(10,10)DISTAG
WRITE(9,51)DISTAG
READ(10,10)SIGTEM
WRITE(9,42)SIGTEM
READ(10,10)XKØ
WRITE(9,28)XKØ
READ(10,10)ADIS, DELEND
WRITE(9,47)ADIS,DELEND
READ(10,10)CS
WRITE(9,29)CS
READ(10,30)NPRINT
WRITE(9,31)NPRINT
EPST=.001
READ(10,32)JAMX, JCMX, DXX
WRITE(9,33)JAMX, JCMX, DXX
D1 = 3.75
D2=2.
HNU1=4.35
HNU2=4.35
HNU3=4.35
HNU4=4.35
HK1=14.3
HK2=46.0
CP1 = 0.215
CP2 = 0.315
RØ1 = 51.0
RØ2 = 56.0
READ(10,10)GPM1,GPM2
WRITE(9,34)GPM1,GPM2
VLEG1=117.5
VLEG2=185.

```

```

VTANK=13318.
READ(10,10)TANKFR
WRITE(9,20)TANKFR
VLEG1 = VLEG1 + (1.0-TANKFR)*VTANK
VTANK = VTANK*TANKFR
READ(10,10)TINA,TINB
WRITE(9,35)TINA,TINB
TINA = TINA*(9./5.)+32.
TINB = TINB*(9./5.)+32.
READ(10,10)TIMAX
WRITE(9,36)TIMAX
READ(10,30)NØITP1
WRITE(9,38)NØITP1
READ(10,10)CHTIME,DELPPM
WRITE(9,41)CHTIME,DELPPM
READ(10,44)CHTIM2,NPRIN2
WRITE(9,43)CHTIM2,NPRIN2
READ(10,10)(TB(I),I = 1, JAMX)
WRITE(9,37)
WRITE(9,6)
WRITE(9,7)(TB(I), I = 1, JAMX)
READ(10,10)REFCØN,REFTIM
WRITE(9,11)
WRITE(9,10) REF CØN,REFTIM
READ(10,10)ADJEXP
WRITE(9,53)ADJEXP
READ(10,10)PPNTAG
WRITE(9,52)PPNTAG
DØ1000J=1, JAMX
DX(J) = DXX

```

```
1000 CONTINUE
```

```

C
C
C
C

```

```
END ØF INPUT.
```

```

JBMX=JAMX-JCMX
JA=JBMX+1
JB=JCMX+1
NK=0
D1=D1/12.
D2=D2/12.
PI=3.14159
PI4=3.14159/4.
A1=PI4*(D1**2)
A2=PI4*(D2**2)
H1=HNU1*HK1/D1
H2=HNU2*HK2/D1
H3=HNU3*HK2/D2
H4=HNU4*HK2/D2

```

```

C
C

```

```

DØ1010J=1, JAMX
TA(J)=465.
TC(J)=465.

```

```

DX(J)=DX(J)/12.
AA(J)=PI*D1*DX(J)
AC(J)=PI*D2*DX(J)
CA(J)=(H1*H2)*AA(J)/(H1+H2)
CC(J)=(H3*H4)*AC(J)/(H3+H4)
1010 CONTINUE
VNODE=(A1-A2)*DX(JAMX)*1728.
C
C   THE TIME STEP IS BASED UPON THE JAMX NODE.
C
DT=VNODE/(GPM2*60.*231.)
C
W1=R01*GPM1*231.*60./1728.
W2=R02*GPM2*231.*60./1728.
CW1=2.*CP1*W1
CW2=2.*CP2*W2
I1=IFIX(VLEG1/VNODE)
I2=IFIX(VLEG2/VNODE)
C
C   TEMPERATURE ITERATION LOOP.  LFLAG=0 WILL EXIT.
C
REGION B
C
NTEMP=0 INDICATES ANALYTICAL SOLUTION IN REGION B.
INPUT TB(J) IN DEGREES C.
C
1012 IF(NTEMP)1015,1020,1015
1015 CONTINUE
C
D01165J=1,JAMX
TB(J)=(9./5.)*TB(J)+32.
1165 CONTINUE
TOUT=(TB(JBMX)+TB(JA))/2.
LFLAG=0
GOTO1085
C
C
1020 TIN=TINB
LFLAG=0
D01050J=1,JCMX
I=JAMX+1-J
TP=(CA(I)*TA(I)+CC(I)*TC(I)+CW2*TIN)
I  /((CA(I)+CC(I)+CW2)
E=ABS(TP-TB(I))
IF(E-EPST)1040,1030,1030
1030 LFLAG=1
1040 TB(I)=TP
TIN=2.*TP-TIN
1050 CONTINUE
TOUT=TIN
C

```



```

D01080J=JB,JAMX
I=JAMX+1-J
TP=(CA(I)*TA(I)+CW2*TIN)/(CA(I)+CW2)
E=ABS(TP-TB(I))
IF(E-LPST)1070,1060,1060
1060 LFLAG=1
1070 TB(I)=TP
TIN=2.*TP-TIN
1080 CONTINUE
C
C REGION C
C
1085 TIN=TOUT
D01110J=JA,JAMX
TP=(CC(J)*TB(J)+CW2*TIN)/(CC(J)+CW2)
E=ABS(TP-TC(J))
IF(E-EPST)1100,1090,1090
1090 LFLAG=1
1100 TC(J)=TP
TIN=2.*TP-TIN
1110 CONTINUE
C
C REGION A
C
TIN=TINA
D01140J=1,JAMX
TP=(CA(J)*TB(J)+CW1*TIN)/(CA(J)+CW1)
E=ABS(TP-TA(J))
IF(E-EPST)1130,1120,1120
1120 LFLAG=1
1130 TA(J)=TP
TIN=2.*TP-TIN
1140 CONTINUE
C
C CONVERGENCE
C
IF(NTEMP)1150,1142,1150
C
1142 IF(LFLAG)1145,1150,1145
1145 LFLAG=0
GOTO1020
1150 WRITE(9,3)
D01160J=1,JAMX
WRITE(9,1)TA(J),TB(J),TC(J)
1160 CONTINUE
C
C CALCULATE WALL TEMPERATURES IN REGION B.
C
D01170J=1,JAMX
TW(J)=TB(J)-(CA(J)/(H2*AA(J)))*(TB(J)-TA(J))
1170 CONTINUE
C CALCULATE WALL TEMP IN REGION C

```

```

DØ 1171 J = 1, JAMX
1171 TWC(J) = TB(J) - CC(J)/(H3*AC(J))*(TB(J)-TC(J))
C
C THIS CØMPLETES THE TEMPERATURE CALCULATION.
C
C DISCARD ALL NØDES IN WHICH THE TEMPERATURE IS ABOVE
C THAT ASSØCIATED WITH INITIAL SYSTEM CØNCENTRATION.
C
C CALCULATE EQUILIBRIUM CØEFFICIENTS.
C
C
C CS AND TØ ARE INITIAL CØNCENTRATION AND ASSØCIATED
C TEMPERATURE.
C
C
C REGION B.
2002 K=0
NK=NK+1
DØ1190J=1, JAMX
I=JAMX+1-J
CEPR =-1.87669E-08
CEPC =-1.87669E-08
CEPR=CEPR*TW(I)+2.67916E-05
CEPC=CEPC*TWC(I)+2.67916E-05
CEPR=CEPR*TW(I)-5.99152E-03
CEPC=CEPC*TWC(I)-5.99152E-03
CEPR=CEPR*TW(I)+0.317871
CEPC=CEPC*TWC(I)+0.317871
CEPR =10.**CEPR
CEPC =10.**CEPC
IF(SIGTEM) 1180,1181,1180
1181 IF(CEPC-CS)1180,1190,1190
1180 K=K+1
A(K)=AA(I)
T(K)=TW(I)
CE(K)=CEPR
AAC(K) = AC(I)
TTC(K) = TWC(I)
CEC(K) = CEPC
1190 CØNTINUE
KMAX=K
KBMX = KMAX- JBMX + 1
DØ 1191 J = KBMX, KMAX
1191 AAC(J) = 0.0
IF(SIG1 )1192,1193,1192
1193 A(KMAX) = A(KMAX) + A1
I2 = I2 + JAMX - KMAX
AI2 = I2
VLEG2 = VNØDE*AI2
AJAMX = JAMX
SMASSØ = (VTANK+VLEG1+VLEG2+VNØDE*AJAMX*1.33)*CS*RØ2*1.0E-06/1728.
1192 CØNTINUE
SIG1 = 1.0
C REGIONS B AND C ARE INCLUDED.

```

C

```
WRITE(9,4)
WRITE(9,5)
DO1200K=1,KMAX
WRITE(9,1)CF(K),T(K)
1200 CONTINUE
WRITE(9,4)
WRITE(9,21)
DO 1202 K = 1, KMAX
1202 WRITE(9,1)CEC(K), TTC(K)
NOKIT = 0
1201 CONTINUE
DO 1203 J = 1, 50
XM(J) = XMM(J)
XMI(J) = XMMI(J)
XMC(J) = XMMC(J)
1203 CONTINUE
K1=1
K2=KMAX
K3=K2+1
K4=K3+I1-1
K5=K4+2
K6=K5+I2-1
K7=K4+1
K8 = K2 - JBMX
WRITE(9,12)
WRITE(9,10)XK0,CS, DT, ADIS
WRITE(9,6)
WRITE(9,13)
WRITE(9,7)VN0DE,VTANK,VLEG1,VLEG2
DO2000J=K1,K6
C(J)=CS
2000 CONTINUE
DO 2300 J = 1, K8
CONC(J) = CS
C00(J) = CS
2300 CONTINUE
DO2005J=K1,K2
C0(J)=CS
XK(J)=XK0
XKD(J) = ADIS*EXP(-DELEND/1.987/(T(J)+459.0)*1.80)
XKDC(J) = ADIS*EXP(-DELEND/1.987/(TTC(J)+459.)*1.80)
AKTD(J) = (1.E+06)*XKD(J)*A(J)/W2
AKTCD(J) = (1.0E+06)*XKDC(J)*AAC(J)/W2
AKT(J)=(1.E+06)*XK(J)*A(J)/W2
AKTC(J) =(1.0E+06)*XK(J)*AAC(J)/W2
DIFXK = XK(J) - XKD(J)
IF(DIFXK)2006,2007,2007
2006 XKD(J) = XK(J)
2007 CONTINUE
DIFXKC = XK(J) - XKDC(J)
IF(DIFXKC)2008,2009,2009
2008 XKDC(J) = XK(J)
2009 CONTINUE
```

```

2005 CONTINUE
WRITE(9,48)
WRITE(9,49) (XKD(J), J = 1, K2)
WRITE(9,50)
WRITE(9,49)(XKDC(J), J = 1, K2)
II = 0
DO 2241 J = K1, K8, 3
I = K8 - J
IF(I-1)2241,2245,2245
2245 II = II + 1
CECC(II) = CEC(I)
AKTCC(II) = AKTC(I)*3.0
AKTDC(II) = AKTC(I)*3.0
XKDC(II) = XKDC(I)
XKCC(II) = XK(I)
2241 CONTINUE
KMAXC = II
WRITE(9,27)
DO 2243 J = 1, KMAXC
2243 WRITE(9,10) CECC(J), XKCC(J), XKDC(J), AKTCC(J), AKTDC(J)
C
C THIS COMPLETES THE CALCULATION IN THE COLD TRAP.
C
C
C BEGIN TRANSIENT ANALYSIS.
C
TIME=0.
ITER=0
NPR=0
N1=K3-1
N2=K5-1
2010 ITER=ITER+1
NPR=NPR+1
N1=N1+1
N2=N2+1
IF(N1-K4)2030,2030,2020
2020 N1=K3
2030 IF(N2-K6)2050,2050,2040
2040 N2=K5
2050 CONTINUE
TIME=TIME+DT
C
C START AT THE MIXING TANK.
C
CIN=C(N2)
C(N2)=C(K7)
C(K7)=(C(K7)*(VTANK-VNODE)+VNODE*C(N1))/VTANK
C
C GO TO THE COLD TRAP. CIN HAS BEEN SET.
C
XMASS=0.
DO2140J=K1,K2
DELTA = CIN-CE(J)
IF(DELTA)2060,2061,2061

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```

2061 XKK= XK(J)
      AKKT = AKT(J)
      GO TO 2062
2060 XKK = XKD(J)
      AKKT = AKTD(J)
2062 CONTINUE
      DELTAC = CIN - CEC(J)
      IF(DELTAC)2063,2064,2064
2064 XKKC= XK(J)
      AKKTC = AKTC(J)
      GO TO 2065
2063 XKKC = XKDC(J)
      AKKTC = AKTDC(J)
2065 CONTINUE
      C(J) =(AKKT*CE(J)+2.0*CIN+AKKTC*CEC(J))/(AKKT+AKKTC+2.0)
      DM = XKK*A(J)*(C(J)-CE(J))*DT
      DMI = XKKC*AAC(J)*(C(J)-CEC(J))*DT
      XMI = XMI(J)
      IF(DMI)2111,2131,2131
2111 IF(DMI+XMI(J))2121,2131,2131
2121 DMI = -XMI(J)
      C(J)=(-DMI*1.0E+06/(W2*DT)+2.*CIN+AKKT*CE(J))/(2.+AKKT)
      DM= XKK*A(J)*(C(J)-CE(J))*DT
2131 XMI(J) = XMI(J) + DMI
      IF(DM)2110,2130,2130
2110 IF(DM+XM(J))2120,2130,2130
2120 DM=-XM(J)
      C(J)=(-DM*1.0E+06/(W2*DT)+2.0*CIN+AKKTC*CEC(J))/(2.0+AKKTC)
      DMI = XKKC*AAC(J)*(C(J)-CEC(J))*DT
2130 XM(J)=XM(J)+DM
2112 IF(DMI+XMI) 2122,2132,2132
2122 DMI= -XMI
2132 XMI(J) = XMI + DMI
      C(J) = CIN - (DM+DMI)/(2.0*W2*DT*1.0E-06)
      CINP=CIN
      CIN=C0(J)
      C0(J)=2.*C(J)-CINP
      XMASS=XMASS+XM(J)+ XMI(J)
C
2140 CONTINUE
C   CALCULATE PRECIPITATION AND TRANSFER IN ZONE C
      XCMASS = 0.0
      DO 2242 J = 1, KMAXC
      DELTCC = CIN- CECC(J)
      IF(DELTCC) 2250,2251,2251
2251 XKKCC = XKCC(J)
      AKKTC = AKTCC(J)
      GO TO 2252
2250 XKKCC = XKDCC(J)
      AKKTC = AKTDC(J)
2252 CONTINUE
      CONC(J) = (AKKTC*CECC(J)+2.0*CIN)/(AKKTC+2.0)
      DMC = 2.0*(CIN-CONC(J))*W2*DT*1.0E-06
      IF(DMC)2210,2230,2230

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```

2210 IF(DMC+XMC(J))2220,2230,2230
2220 DMC = - XMC(J)
      C0NC(J) = CIN - DMC/(2.0*W2*DT*1.0E-06)
2230 XMC(J) = XMC(J) + DMC
      CINP = CIN
      CIN = C00(J)
      C00(J) = 2.0*C0NC(J)-CINP
      XCMAS = XCMAS + XMC(J)
2242 C0NTINUF
      CRAT=(C(K7)-CE(K2))/(CS-CE(K2))
C      ST0RE C0LT TRAP 0UTFLOW IN THE FIRST LEG.
C
      C(N1)=CIN
      DCACT = (C(N1) - CE(K2))/(CS-CE(K2))
C
C      PRINT AND EXIT ROUTINE.
C
C      CALCULATE AVERAGE C0NCENTRATI0N FACT0R
      N0ACT = KMAX
      N0PPNZ = KMAX
      AVCDI = 0.0
      AVCDP = 0.0
      D0 2141 J = K1, K2
      CDI = C(J) - CE(J)
      IF(XM(J))2144,2144,2145
2144 N0PPNZ = N0PPNZ - 1
      G0 T0 2146
2145 AVCDP = CDI + AVCDP
2146 C0NTINUE
      IF(CDI ) 2142,2143,2143
2142 N0ACT = N0ACT - 1
      G0 T0 2141
2143 AVCDI = CDI + AVCDI
2141 C0NTINUE
      AN0ACT = N0ACT
      AVCDI = AVCDI /AN0ACT
      AVCDP = AVCDP/AN0ACT
      C0NFAC = AVCDI / (C(KMAX)-CE(KMAX))
      C0NFAP = AVCDP / (C(KMAX) - CE(KMAX))
      N0ACTC = N0ACT - JBMX
      AN0ACC = N0ACTC
      AREA = AN0ACT*AA(4) + AN0ACC*AC(4)*2.0 + A1
      PPMAS = XMAS + XCMAS
      DIFTIM = TIME - TIM1
      DIFPPN = PPMAS - PPMAS1
      PPMAS1 = PPMAS
      TIM1 = TIME
      DMDT = DIFPPN/DIFTIM
      IF(DISTAG)2147,2148,2147
2148 XKZ = XK(KMAX)
      G0 T0 2149
2147 XKZ = XKD(KMAX)
2149 C0NTINUE

```

```

EQNFAC = DMDT/(XKZ*AREA*(C0NC(KMAXC)-CE(KMAX)))
N0PPZC = N0PPNZ - JBMX
AN0PPZ = N0PPNZ
AN0PZC = N0PPZC
AREAP = AN0PPZ*AA(4) + AN0PZC*AC(4)*2.0 + A1
EQNFAP = DMDT/(XKZ*AREAP*(C0NC(KMAXC)-CE(KMAX)))
N0IT = N0ITP1 - 1
IF(N0KIT - N0IT)2160,2153,2153
2153 CONTINUE
IF(NPR-NPRINT)2160,2150,2150
2150 NPR=0
WRITE(9,15)
WRITE(9,1)DT,TIMAX,TIME
WRITE(9,16)
WRITE(9,1)(C(J),J=K1,K2)
WRITE(9,23)
WRITE(9,1)(C0NC(I), I = 1, KMAXC)
WRITE(9,6)
WRITE(9,17)
WRITE(9,1)(C(J),J=K3,K6)
WRITE(9,6)
WRITE(9,18)
WRITE(9,7)C(K7),CRAT,TIME,XMASS, XCMASS
WRITE(9,40)DCACT
WRITE(9,6)
WRITE(9,19)
WRITE(9,7)(XM(J),J=K1,K2)
WRITE(9,24)
WRITE(9,7)(XMI(I), I = K1,K2)
WRITE(9,25)
WRITE(9,7)(XMC(I), I = 1, KMAXC)
SMASS = 0.0
D0 2151 I = 1, K6
2151 SMASS = SMASS + VN0DE*R02*C(I)*1.0E-06/1728.
SMASS = SMASS + (VTANK*R02*C(K7)*1.0E-06)/1728.
D0 2152 I = 1, KMAXC
2152 SMASS = SMASS + VN0DE*R02*C0NC(I)*1.0E-06/1728.
SMASS = SMASS + XMASS + XCMASS
WRITE(9,26)
WRITE(9,10)SMASS0, SMASS
WRITE(9,8)
WRITE(9,9)AVCDI,N0ACT,C0NFAC
WRITE(9,22)
WRITE(9,9)AVCDP,N0PPNZ,C0NFAP
WRITE(9,45)EQNFAC
WRITE(9,46)EQNFAP
2160 CONTINUE
C ADJUST PRECIPITATION K FACTOR
IF(TIME-REFTIM)2164,2161,2161
2161 IF(PPNTAG)2167,2168,2167
2167 XK01 = XK0
XK0 = XK01*(CRAT/REFC0N) **ADJEXP
2168 CONTINUE

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```

      IF(DISTAG)2166,2165,2166
2166 ADIS1 = ADIS
      ADIS = ADIS1*(CRAT/REFCON) **ADJEXP
2165 CONTINUE
      WRITE(9,12)
      WRITE(9,10)XK0,CS,DT,ADIS
      NOKIT = NOKIT + 1
      WRITE(9,14)NOKIT
      IF(NOKIT - N0ITP1) 2162,2163,2163
2163 REFTIM = TIMAX + 1.0
      GO TO 2164
2162 GO TO 1201
2164 CONTINUE
      IF(TIME-CHTIME)2173,2171,2171
2171 CHTIME = TIMAX + 1.0
      DO 2172 I = 1, K6
2172 C(I) = C(I) + DELPPM
2173 CONTINUE
      IF(TIME-CHTIM2)2174,2175,2175
2175 CHTIM2 = TIMAX + 1.0
      NPRINT = NPRIN2
2174 CONTINUE
      IF(TIME-TIMAX)2170,2170,2180
2170 GOT02010
2180 CONTINUE
      GO TO 200
C
C      1012 WILL BUY A NEW TEMPERATURE CALCULATION.
C      2002 WILL BUY ONLY A RESET OF CS, C(J), XK0.
C
C
2200 CONTINUE
      END

```