6.3 Simulation and Prediction of Contamination

6.3.1 Relational Expressions

CONTENTS

1. Introduction

The purpose of the MSF-2 is to estimate the quality of the product water in case when the oil contaminated seawater has been fed into the MSF Plant. It has been done through the investigation on the quantitative analysis of the evaporation phenomena of the volatile organic contaminants in the feed sea-water.

The quality of seawater in the Arabian Gulf has been surveyed and reported in 6.1.1. The volatility mechanisms of oil and bromoform, a kind of trihalomethane, has been investigated by preparative experiment and reported in 6.1.2.

The Henry's constant of bromoform in brine, which is the basic physical property necessary for the quantitative analysis of dilute solution, has been measured by the "Vapor/Liquid Equilibrium Experimental Apparatus". The results are reported in 6.2. The Henry's constant obtained in 6.2 showed good agreement with that of 6.1.2. Thus, the Henry's constant, as a function of temperature obtained by 6.2, has been used for the computer simulation.

The flow chart and the formula used for the computer simulation of the evaporation of the organic contaminants in brine are described in this section based on the evaporation mechanisms shown in 6.1 and 6.2.

As this simulation is of the first order estimation, this calculates the amount of evaporated oil and/or bromoform in the MSF test plant but does not include the calculation for the amount of oil and/or bromoform in the product water.

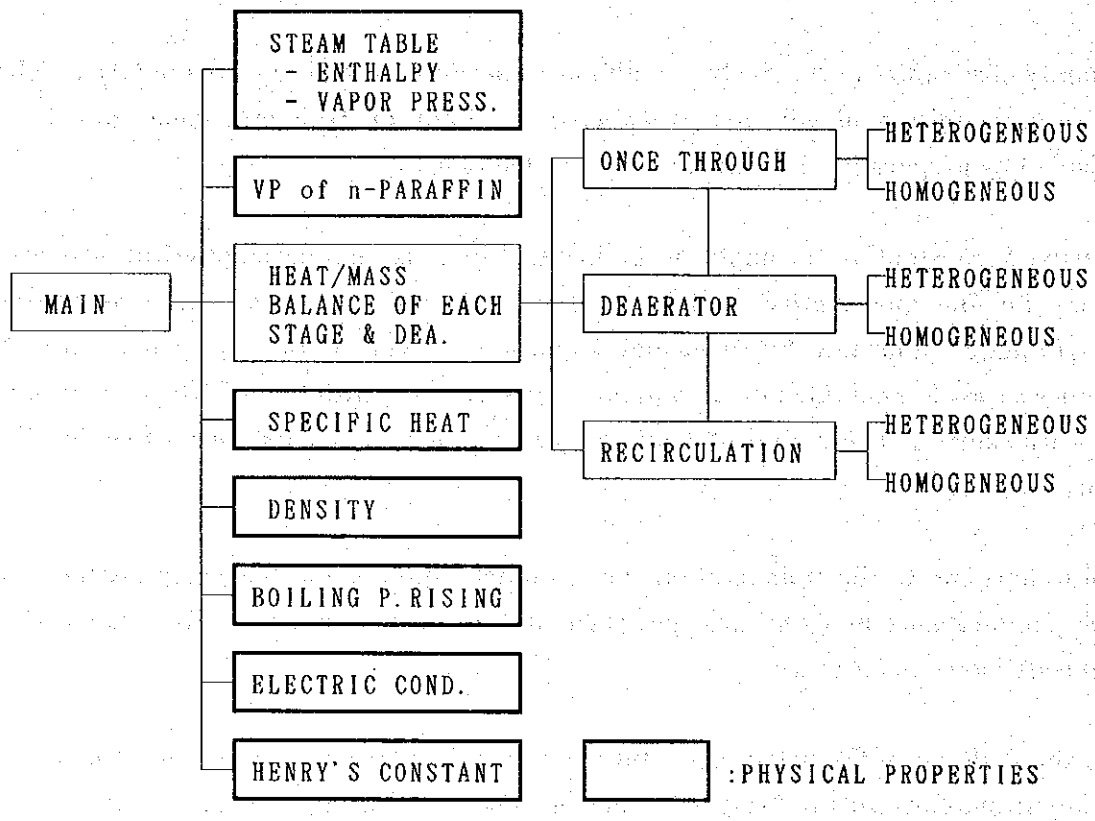
The oil carried-over from the brine can be estimated by the computer program shown in 6.3.2. However, not all of the carried-over oil goes into the product water. Certain amount of the oil will be exhausted out of the system from the ejector, but the unknown factors still remains for the quantitative estimation of the process.

2. Precondition for the computer program

The precondition for the computer program should be the program which can run on the computer owned by SWCC. To satisfy this precondition, followings are taken into account.

- **HARD WARE : PC type IBM Compatible, 486 based machines operating**
- **SOFT WARE : FORTRAN Language**
- **HD Space : less than 200MB**

3. Structure of the Program



4. How to Set Up Symbols for the Formulas

4.1 Fundamental rule for setting up the above mentioned symbols

I	II	III	IV

I	F: Flow rate of brine, water & contaminants	(kg/h)
	C:Concentration of the constituents	(kg/L)
	T:Temperature	(C)
	P:Pressure	(Pa)
	S:Electric conductivity	(S/cm)
	X:Mole fraction	
II	B:Seawater, brine	
	W:Water	
	O:Aliphatic hydrocarbonic & homogeneous contaminants	
III	E:Vapor generated by evaporation & distillation	
	L:Liquid (Water, seawater, brine)	
	M:Liquid (Contaminants to be dosed)	
	S:Solid that phase change do not occures by heating, etc.	

IV	M:Make-up	D:Inlet of deaerator	
	T:Outlet of Last stage	G:Outlet of deaerator	
	C:Recirculation brine	1:#1 stage	4:#4 stage
	B:Blow brine	2:#2 stage	5:#5 stage
	O:Outlet of brine heater	3:#3 stage	6:#6 stage

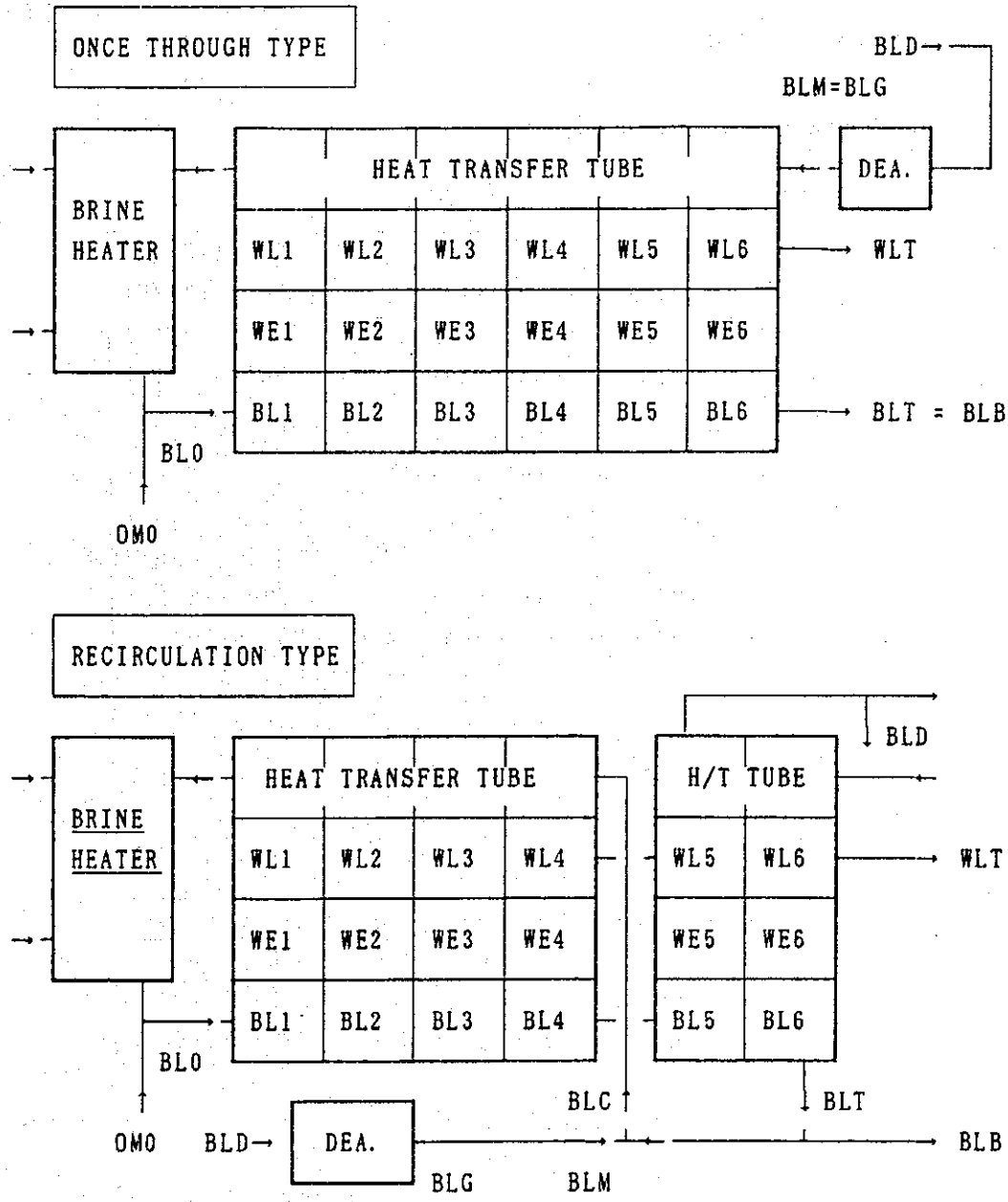
4.2 Physical properties, etc. (The symbols are not treated the same as a fundamental rule)

D	:	Density	(kg/L)
H	:	Henry's constant	{mol/(L•Pa)}
ENT	:	Enthalpy	(kJ/kg)
CP	:	Specific heat	{kJ/(kg•C)}
MW, MO	:	Molecular weight of water & contaminants	
EC	:	Electric conductivity of the brine at 25 ^{O}C	(S/cm)
ONTD	:	Overall NETD	(C)
NTD	:	NETD based on the equipment structure	(C)
BPR	:	Boiling point rising	(C)
N	:	Number of carbons of paraffin (Aliphatic hydrocarbon)	

4.3 Symbols which are Added on the Top or the End of Four Figures

'A' added on the top	:	The assumed value & the value obtained by the convergence caluculation
'B' added on the top	:	The final results obtained by assuming the A
'NE' added on the top	:	The value of #6 stage obtained by calculation based on the once through type
'BB' added on the top	:	The final results obtained by the 'NE'
'1···9, a···z' added on the end	:	Number of carbons in paraffin, where, 'a···z' indicate the number of carbons 10···35

4.4 Flow of MSF Test Plant and Symbols of II, III, IV Groups



(FUNDAMENTAL MASS BALANCE OF MSF PROCESSES)

$$FBLM = FBLB + FWLT + \alpha$$

$$(FBLM)(CBLM) = (FBLB)(CBLB)$$

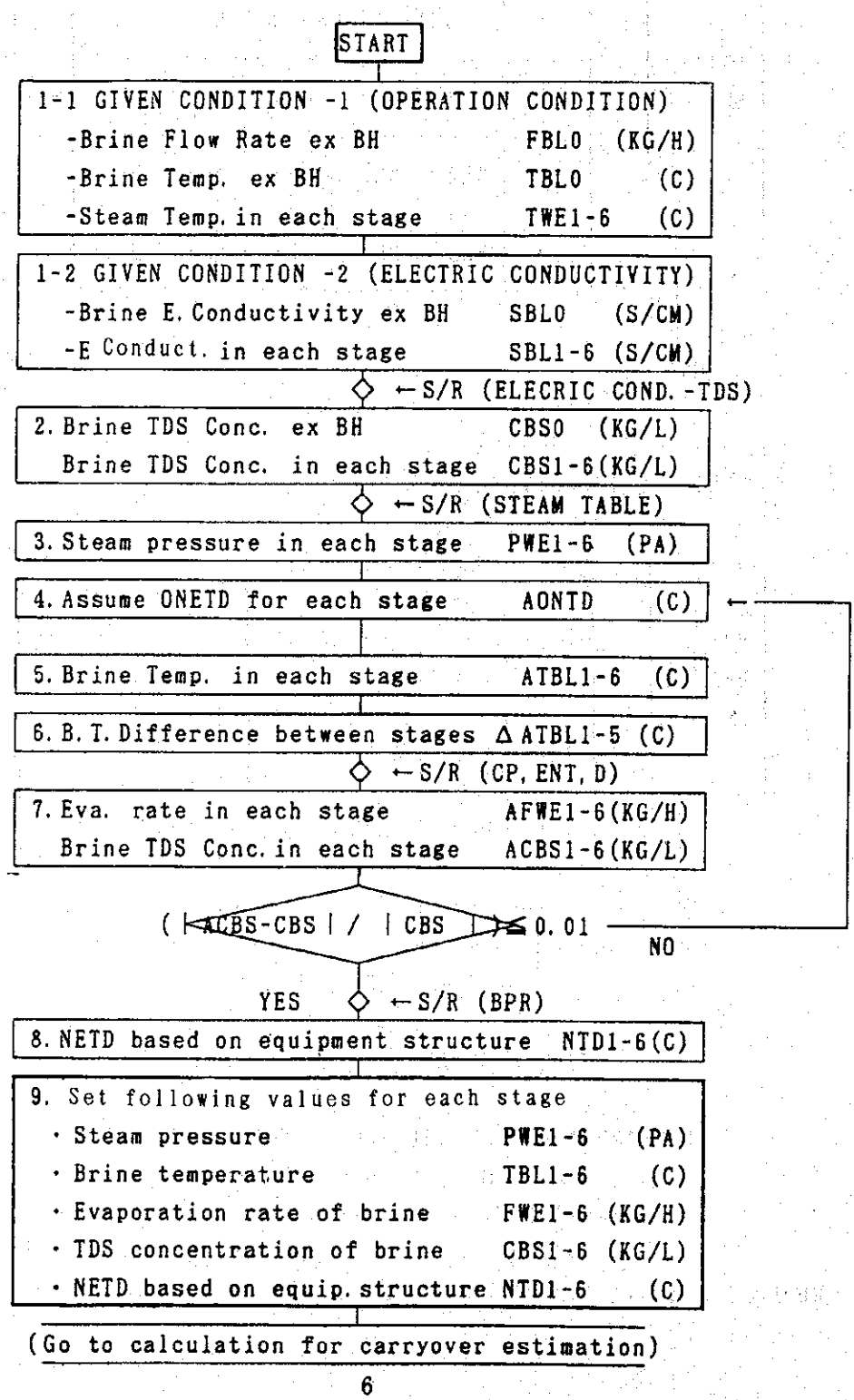
$$FBLB = FBLM(CBLM/CBLB) = FBLM - FWLT$$

Where, α indicates the amount of non-condensible gasses.

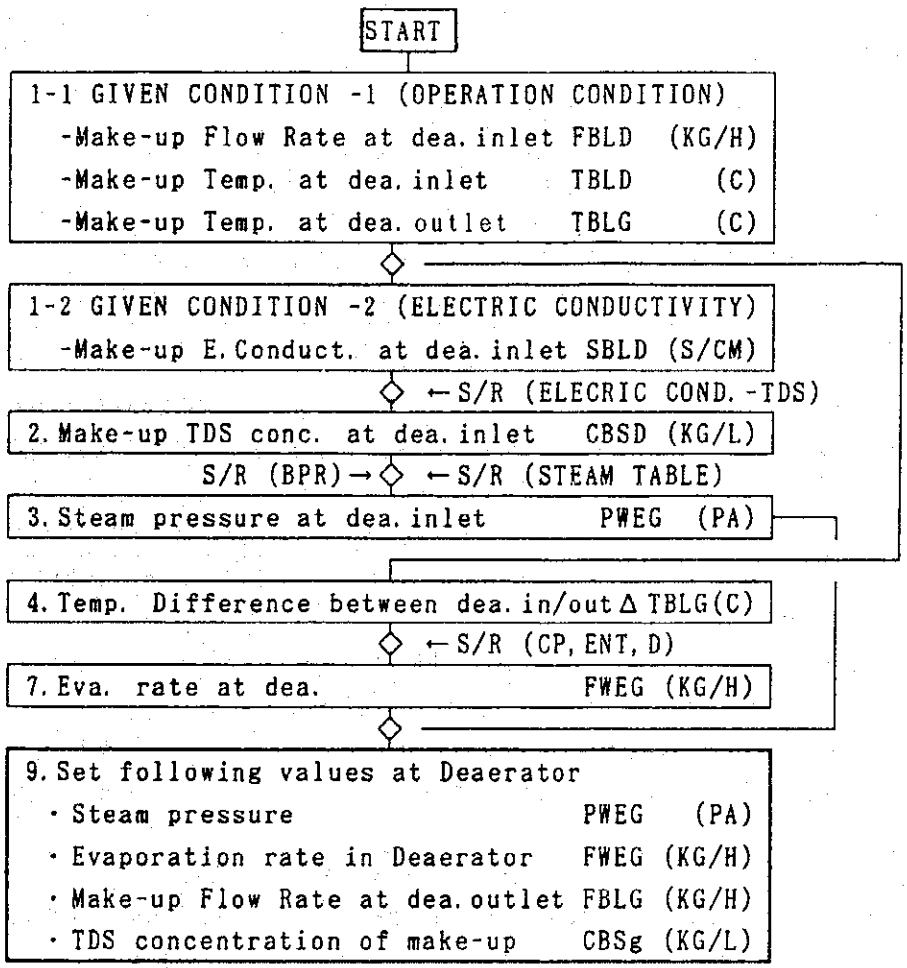
5. Flow Chart

5.1 Heat & Mass Balance

5.1.1 Once Through/Recirculation Type

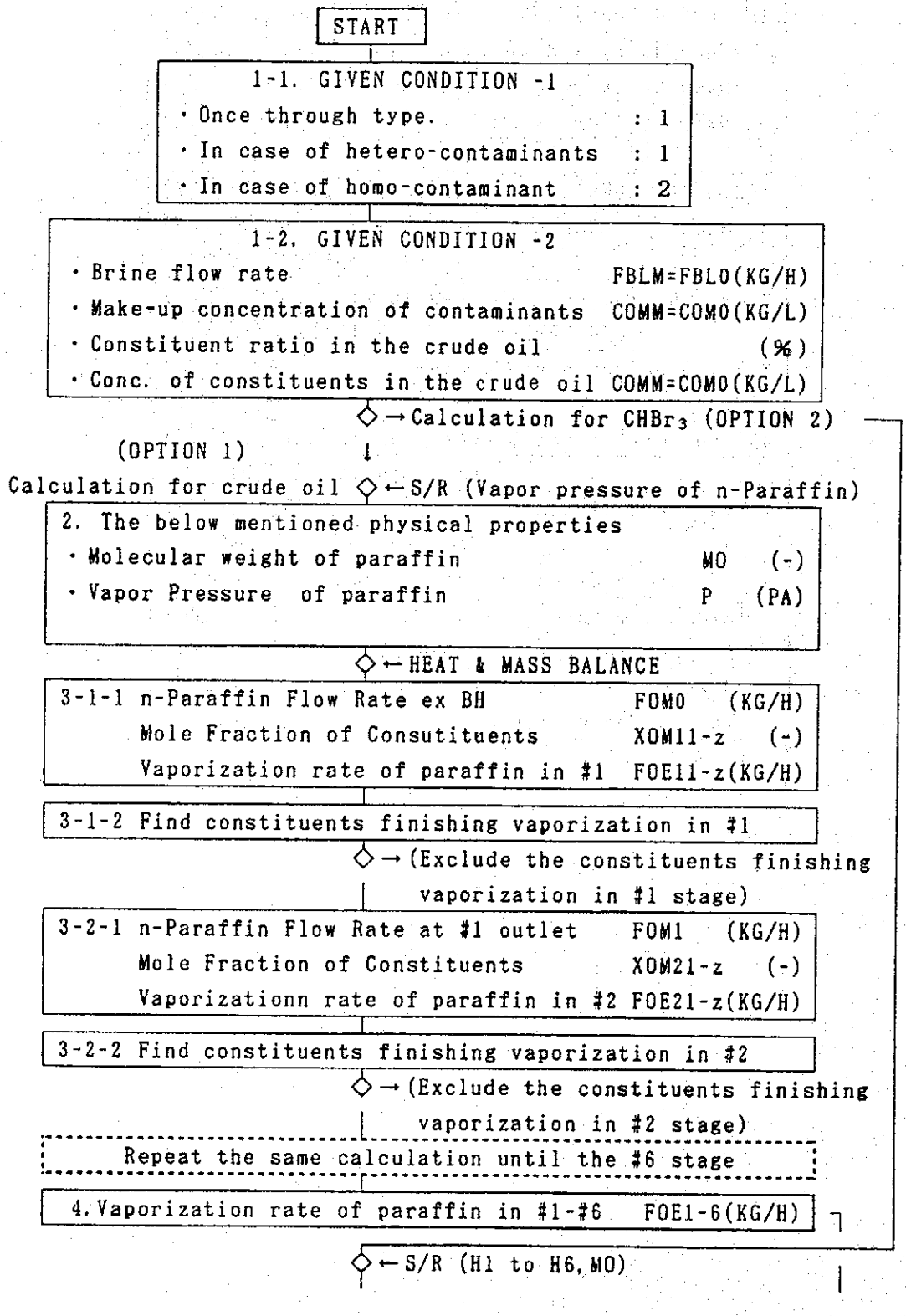


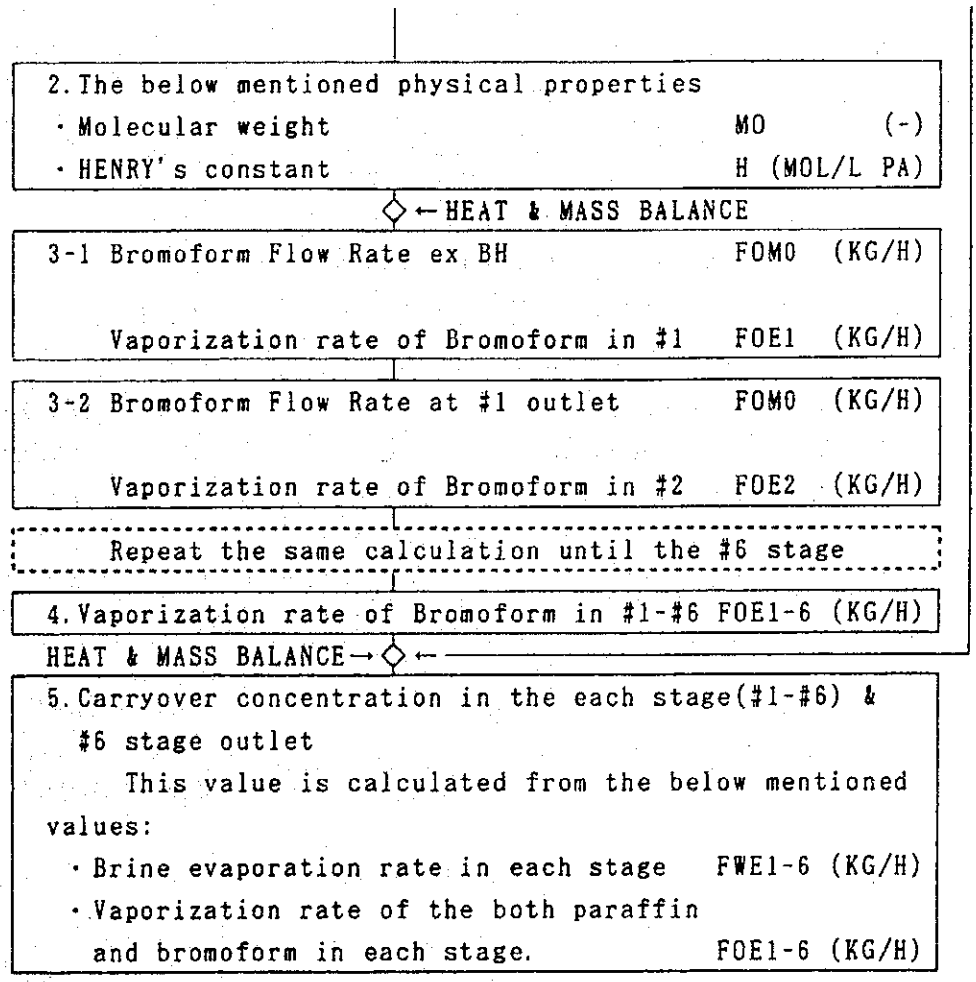
5.1.2 Deaerator



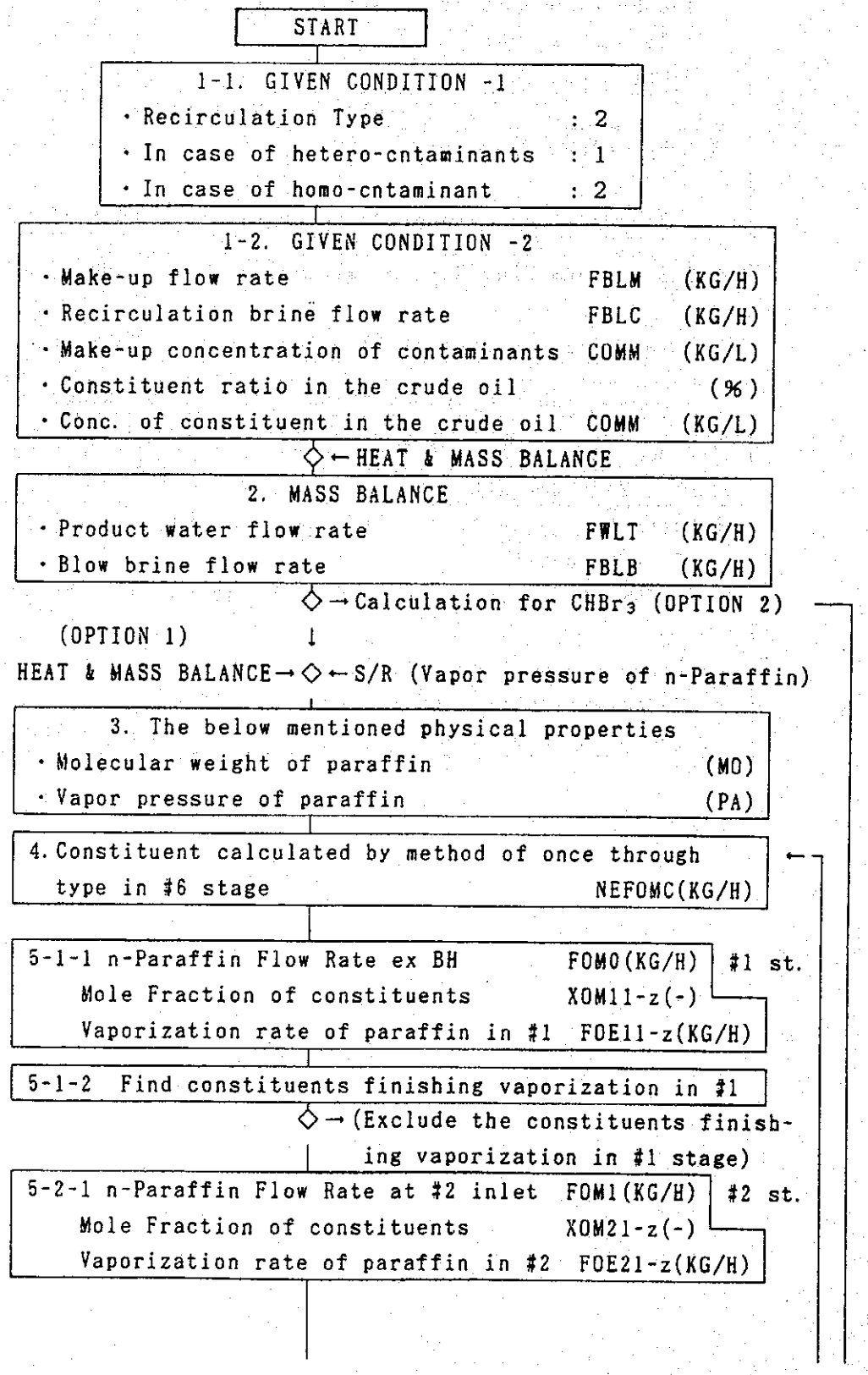
5.2 Carryover Estimation of Contaminants

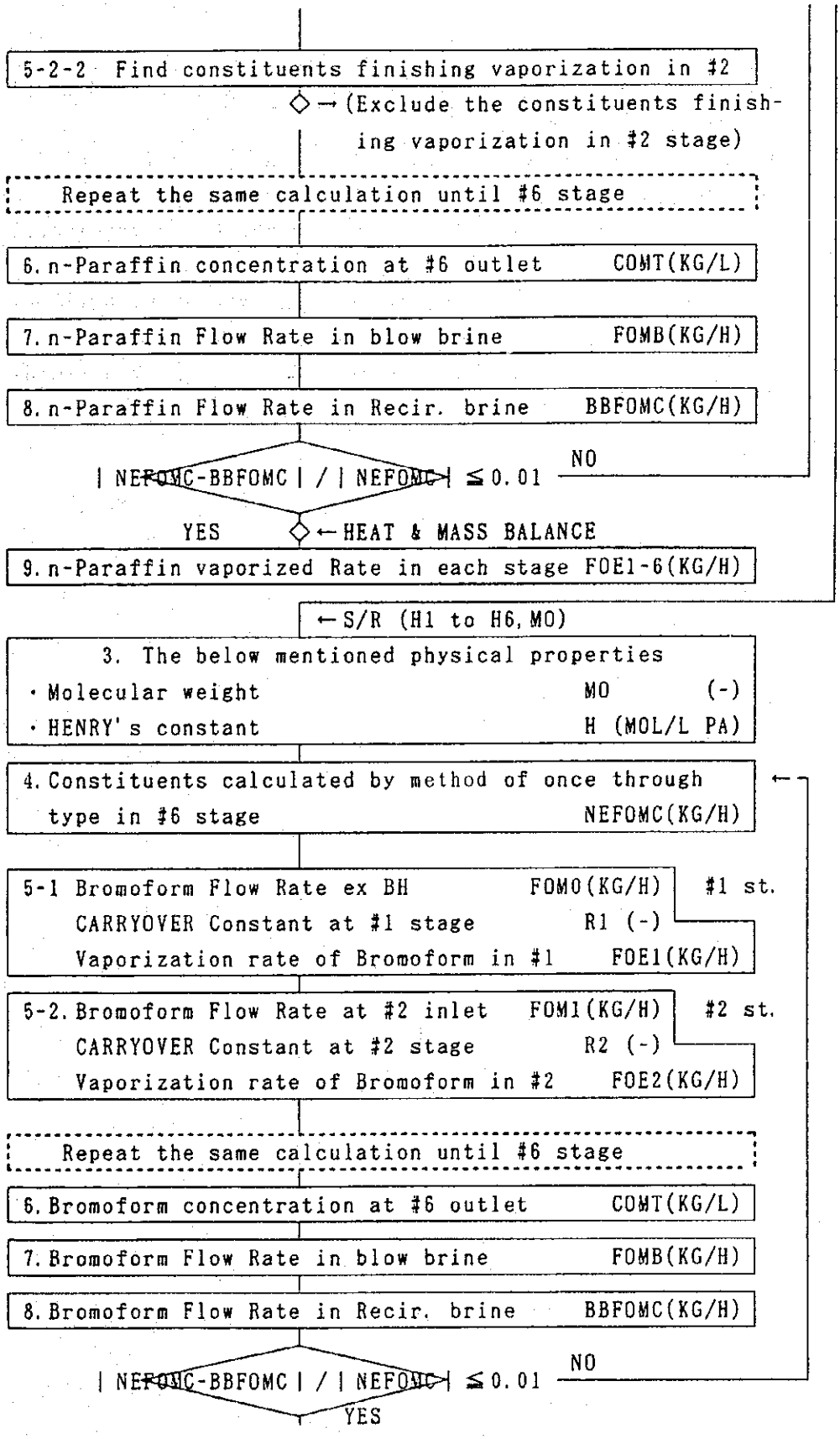
5.2.1 Once Through Type




2. The below mentioned physical properties
・Molecular weight MO (-)
・HENRY's constant H (MOL/L PA)
◇←HEAT & MASS BALANCE
3-1 Bromoform Flow Rate ex BH FOM0 (KG/H)
Vaporization rate of Bromoform in #1 FOE1 (KG/H)
3-2 Bromoform Flow Rate at #1 outlet FOM0 (KG/H)
Vaporization rate of Bromoform in #2 FOE2 (KG/H)
Repeat the same calculation until the #6 stage
4. Vaporization rate of Bromoform in #1-#6 FOE1-6 (KG/H)
HEAT & MASS BALANCE→◇←
5. Carryover concentration in the each stage(#1-#6) & #6 stage outlet
This value is calculated from the below mentioned values:
・Brine evaporation rate in each stage FWE1-6 (KG/H)
・Vaporization rate of the both paraffin and bromoform in each stage. FOE1-6 (KG/H)

5.2.2 Recirculation Type




5-2-2 Find constituents finishing vaporization in #2
→ (Exclude the constituents finishing vaporization in #2 stage)
Repeat the same calculation until #6 stage
6. n-Paraffin concentration at #6 outlet COMT(KG/L)
7. n-Paraffin Flow Rate in blow brine FOMB(KG/H)
8. n-Paraffin Flow Rate in Recir. brine BBFOMC(KG/H)
| NEFOMC-BBFOMC | / | NEFOMC | ≦ 0.01
NO
YES
← HEAT & MASS BALANCE
9. n-Paraffin vaporized Rate in each stage FOE1-6(KG/H)
← S/R (H1 to H6, MO)
3. The below mentioned physical properties
・Molecular weight MO (-)
・HENRY's constant H (MOL/L PA)
4. Constituents calculated by method of once through type in #6 stage NEFOMC(KG/H)
5-1 Bromoform Flow Rate ex BH FOMO(KG/H) #1 st.
CARRYOVER Constant at #1 stage R1 (-)
Vaporization rate of Bromoform in #1 FOE1(KG/H)
5-2. Bromoform Flow Rate at #2 inlet FOM1(KG/H) #2 st.
CARRYOVER Constant at #2 stage R2 (-)
Vaporization rate of Bromoform in #2 FOE2(KG/H)
Repeat the same calculation until #6 stage
6. Bromoform concentration at #6 outlet COMT(KG/L)
7. Bromoform Flow Rate in blow brine FOMB(KG/H)
8. Bromoform Flow Rate in Recir. brine BBFOMC(KG/H)
| NEFOMC-BBFOMC | / | NEFOMC | ≦ 0.01
NO
YES

9. Bromoform vaporization Rate in each stage FOE1-6(KG/H)

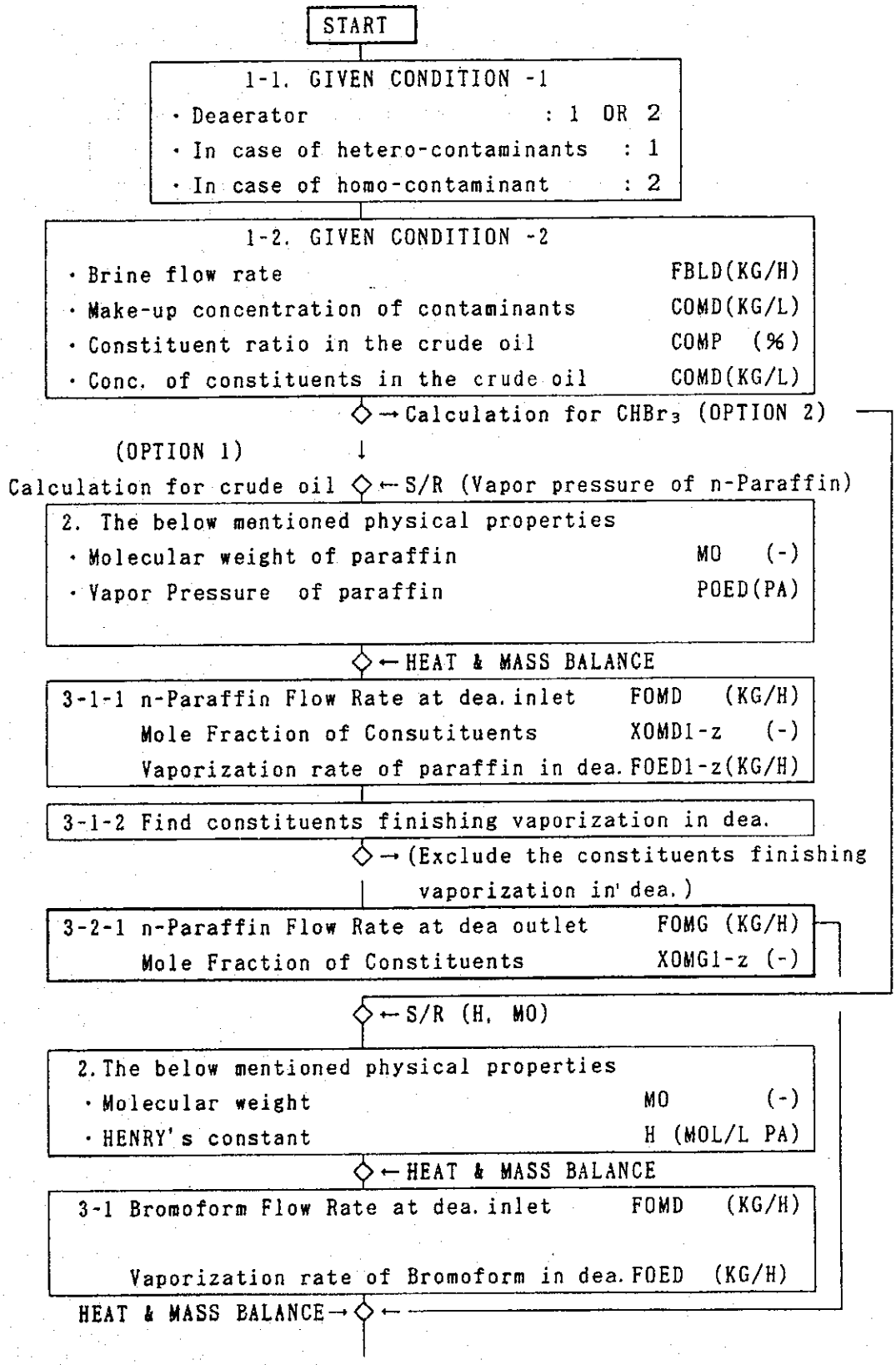
HEAT & MASS BALANCE→◇

10. Carryover concentration in the each stage(#1-#6) & #6 stage outlet

This value is calculated from the below mentioned values:

- Brine evaporation rate in each stage FWE1-6 (KG/H)
- Vaporization rate of the both paraffin and bromoform in each stage. FOE1-6 (KG/H)

5.2.3 Deaerator



5. Concentration of the both paraffin and bromoform in the dearator outlet : COMM1-Z

This value is calculated from the below mentioned values:

- Brine evaporation rate in deaerator FWEG (KG/H)
- Vaporization rate of the both paraffin and bromoform in deaerator FOEG1-z(KG/H)

6. The formulas adopted for Calculation/Estimation

6.1 The formulas adopted for Heat/Mass Balance Calculation

(1) PWE1～PEW6 (Steam Pressure in each stage) (PA)
Eash value read corresponds to from TWE1 to TWE6 of the STEAM TABLE

(2) ONTD1～ONTD6 (Overall NETD for each stage) (C)
AONTD = ATBL – TWE = 0～+5.0 (C)

(3) TBL1～TBL6 (Brine Temp. in each stage) (C)
ATBL1–6 = TWE1–6 + AONTD1–6

(4) △ATBL (Temperature difference of brine between this stage and the preceding stage) (C)
△ATBL1 = TBL0 – ATBL1
△ATBL2 = ATBL1 – ATBL2
△ATBL3 = ATBL2 – ATBL3
△ATBL4 = ATBL3 – ATBL4
△ATBL5 = ATBL4 – ATBL5
△ATBL6 = ATBL5 – ATBL6

(5) AFWE (Evaporation flow rate in each stage)
(KG/H)(KJ/KG•C)(C)/(KJ/KG)=(KG/H)
AFWE1 = (FBL0)(CP1)(△ATBL1/ENT1)
AFWE2 = (AFBL1)(CP2)(△ATBL2/ENT2)
AFWE3 = (AFBL2)(CP3)(△ATBL3/ENT3)
AFWE4 = (AFBL3)(CP4)(△ATBL4/ENT4)
AFWE5 = (AFBL4)(CP5)(△ATBL5/ENT5)
AFWE6 = (AFBL5)(CP6)(△ATBL6/ENT6)
AFWLT = AFWE1+AFWE2+AFWE3+AFWE4+AFWE5+AFWE6
(Flow rate of produced water)

(6) AFBL (Brine flow rate in each stage) (KG/H)
AFBL1 = FBLO – AFWE1

AFBL2 = AFBL1 – AFWE2
AFBL3 = AFBL2 – AFWE3
AFBL4 = AFBL3 – AFWE4
AFBL5 = AFBL4 – AFWE5
AFBL6 = AFBL5 – AFWE6
AFBLT = AFBL6 (Brine flow rate in the last stage)

(7) CBS (Concentration of TDS in each stage)

(KG/L)(KG/H)(H/KG)(KG/L)(L/KG)=(KG/L)
ACBS1 = CBS0(FBL0/AFBL1)(DB1/DB0)
ACBS2 = ACBS1(AFBL1/AFBL2)(DB2/DB1)
ACBS3 = ASBS2(AFBL2/AFBL3)(DB3/DB2)
ACBS4 = ACBS3(AFBL3/AFBL4)(DB4/DB3)
ACBS5 = ACBS4(AFBL4/AFBL5)(DB5/DB4)
ACBS6 = ACBS5(AFBL5/AFBL6)(DB6/DB5)
ACBST = ACBS6 (TDS Concentration in the last stage)

(8) CONVERGENCE CALCULATION

The difference between TWE and TBL during the normal operation is due to three reasons: the first is the temperature distribution of both phases (gaseous and liquid at the stage), the second is BPR and the third is the diversion from the equilibrium based on the equipment structure.

Generally speaking, this diversion is defined by the name of ONETD (Symbol:ONTD) and its value is obtained by convergence calculation.

a) Caluculate values of ACBS1～ACBS6, assume ONTD = 0 at stage #1.
b) Compare the results of (1) with proceeding data from CBS1 to CBS6.
c) Try the convergence calculation going down the ratio of the difference between ACBS and CBS within 1 %.
d) Obtain the values of TBL1～TBL6 from the convergent ONTD.

(9) NETD

Divide ONTD into the parts : BPR and that based on the equipment structure.
NTD1–6 = ONTD1–6 – BPR1–6
BPR1–6 = f(CBS.TBL)·····S/R

6.2 The Formulas added for Carryover Estimation

6.2.1 Heterogeneous, Once Through Type

(1) XOM (Mole fraction of paraffin consisted of 35 kinds <1–9, A–Z>)

XOM11–z

XOM11=(COM01/MO1)/{(COM01/MO1)+···+(COM0z/MOz)}

XOM1a=(COM0a/MOa)/{(COM01/MO1)+···+(COM0z/MOz)}

XOM1z=(COM0z/MOz)/{(COM01/MO1)+···+(COM0z/MOz)}

XOM21–z

XOM21=(COM11/MO1)/{(COM11/MO1)+···+(COM1z/MOz)}

XOM2a=(COM1a/MOa)/{(COM11/MO1)+···+(COM1z/MOz)}

XOM2z=(COM1z/MOz)/{(COM11/MO1)+···+(COM1z/MOz)}

XOM31–z

XOM31=(COM21/MO1)/{(COM21/MO1)+···+(COM2z/MOz)}

XOM3a=(COM2a/MOa)/{(COM21/MO1)+···+(COM2z/MOz)}

XOM3z=(COM2z/MOz)/{(COM21/MO1)+···+(COM2z/MOz)}

XOM41–z

XOM41=(COM31/MO1)/{(COM31/MO1)+···+(COM3z/MOz)}

XOM4a=(COM3a/MOa)/{(COM31/MO1)+···+(COM3z/MOz)}

XOM4z=(COM3z/MOz)/{(COM31/MO1)+···+(COM3z/MOz)}

XOM5–z

XOM51=(COM41/MO1)/{(COM41/MO1)+···+(COM4z/MOz)}

XOM5a=(COM4a/MOa)/{(COM41/MO1)+···+(COM4z/MOz)}

XOM5z=(COM4z/MOz)/{(COM41/MO1)+···+(COM4z/MOz)}

XOM6–z

XOM61=(COM51/MO1)/{(COM51/MO1)+···+(COM5z/MOz)}

XOM6a=(COM5a/MOa)/{(COM51/MO1)+···+(COM5z/MOz)}

XOM6z=(COM5z/MOz)/{(COM51/MO1)+···+(COM5z/MOz)}

(2) FOE, FOM (Evaporation/Flow rate of paraffin in each stage) (KG/H)

FOE11–z = (XOM11–z)(R11–z)(FWE1), FOM11–z = FOM01–z – F0E11–z

FOE21–z = (XOM21–z)(R21–z)(FWE2), FOM21–z = FOM11–z – F0E21–z

FOE31–z = (XOM31–z)(R31–z)(FWE3), FOM31–z = FOM21–z – F0E31–z

FOE41–z = (XOM41–z)(R41–z)(FWE4), FOM41–z = FOM31–z – F0E41–z

FOE51–z = (XOM51–z)(R51–z)(FWE5), FOM51–z = FOM41–z – F0E51–z

FOE61-z = (XOM61-z)(R61-z)(FWE6), FOM61-z = FOM51-z - F0E61-z

(3) COM (Paraffin concentration in the brine at each stage)

(The symbols '1' through 'z' were omitted.)

(KG/L){(KG/H)(KG/L)(L/KG)−(KG/H)}/(KG/H)=(KG/L)

COM1=DB1(FBL0 · COM0/DB0 - FOE1)/FBL1

COM2=DB2(FBL1 · COM1/DB1 - FOE2)/FBL2

COM3=DB3(FBL2 · COM2/DB2 - FOE3)/FBL3

COM4=DB4(FBL3 · COM3/DB3 - FOE4)/FBL4

COM5=DB5(FBL4 · COM4/DB4 - FOE5)/FBL5

COM6=DB6(FBL5 · COM5/DB5 - FOE6)/FBL6

(4) COE (Paraffin concentration in the product water at each stage)

(The symbols '1' through 'z' for 'COE' & 'FOE' were omitted.)

(KG/H)/(KG/H)(KG/L)=(KG/L)

COE1=(FOE1/FWE1)(DW1)

COE2={(FOE1+FOE2)/FWE1+FWE2)} DW2

COE3={(FOE1+FOE2+FOE3)/(FWE1+·····+FWE3)} DW3

COE4={(FOE1+FOE2+FOE3+FOE4)/(FWE1+·····+FWE4)} DW4

COE5={(FOE1+FOE2+FOE3+FOE4+FOE5)/(FWE1+·····FWE5)} DW5

COE6={(FOE1+FOE22+FOE3+FOE44+FOE5+FOE6)/(FWE1+·····+FWE6)} DW6

(5) R (CARRYOVER'S CONSTANTS)

R11-z = (M01-z/MW)(POE11-z/PWE1)

R21-z = (M01-z/MW)(POE21-z/PWE2)

R31-z = (M01-z/MW)(POE31-z/PWE3)

R41-z = (M01-z/MW)(POE41-z/PWE4)

R51-z = (M01-z/MW)(POE51-z/PWE5)

R61-z = (M01-z/MW)(POE61-z/PWE6)

MW = 18.02

MO1-z = 14.027N + 2.016

PWE : STEAM TABLE

POE11-z : Be calculated by using ANTOINE'S equation.

POE21-z : Be calculated by using ANTOINE'S equation.

POE31-z : Be calculated by using ANTOINE'S equation.

POE41-z : Be calculated by using ANTOINE'S equation.

POE51-z : Be calculated by using ANTOINE'S equation.
POE61-z : Be calculated by using ANTOINE'S equation.

6.2.2 Homogeneous, Once Through Type

(1) **FOE, FOM : Be the same equation in case of 'HETEROGENEOUS'. However, the symbols '1' through 'z' were not necessary.**

(2) **COM : Be the same equation in case of 'HETEROGENEOUS'. However, the symbols '1' through 'z' were not necessary.**

(3) **COE : Be the same equation in case of HETEROGENEOUS'. However, the symbols '1' through 'z' were not necessary.**

(4) **R (CARRYOVER'S CONSTANTS)**

R1=(MO/MW)(POE1/PWE1)
R2=(MO/MW)(POE2/PWE2)
R3=(MO/MW)(POE3/PWE3)
R4=(MO/MW)(POE4/PWE4)
R5=(MO/MW)(POE5/PWE5)
R6=(MO/MW)(POE6/PWE6)
MW=18.02 (Molecular weight of H_2O)
MO=252.718 (Molecular weight of $CHBr_3$)
PWE:STEAM TABLE
POE1=1000 • COM0/(H1 • MO) (KG/L)/{(KG/MOL)(MOL/L)(1/PA)}=(PA)
POE2=1000 • COM1/(H2 • MO)
POE3=1000 • COM2/(H3 • MO)
POE4=1000 • COM3/(H4 • MO)
POE5=1000 • COM4/(H5 • MO)
POE6=1000 • COM5/(H6 • MO)

6.2.3 Heterogeneous, Recirculation Type

(1) MASS BALANCE

FBLB = FBLM – FWLT = FBLM(CBLM/CBLB)

FWLT (value obtained by 5 in 5.1)

(2) R (CARRYOVER's constant)

R11–z = (MO1–z)(POE11–z)/{(MW)(PWE1)}

R21–z = (MO1–z)(POE21–z)/{(MW)(PWE2)}

R31–z = (MO1–z)(POE31–z)/{(MW)(PWE3)}

R41–z = (MO1–z)(POE41–z)/{(MW)(PWE4)}

R51–z = (MO1–z)(POE51–z)/{(MW)(PWE5)}

R61–z = (MO1–z)(POE61–z)/{(MW)(PWE6)}

MO = 14.027N + 2.016, MW = 18.02

POE : Be calculated by using ANTOINE'S equation

PWE : STEAM TABLE

(3) FOMM (Dosing rate of paraffin) (KG/L)(KG/H)(L/KG)=(KG/H)

FOMM1–z = (COMM1–z)(FBLM)(1/DBT)

(4) NEFOMC (Constituent flow rate calculated by method of once through type in #6 stage)

MAX.NEFOMC1–z =(COMM1–z)(1/DBT)(FBLM) (KG/L)(L/KG)(KG/H)=(KG/H)

MIN. NEFOMC1–z = 0

(5) Mass balance in each stage

(5)–1 #1 stage

(5)–1–1 FOM0 (n–Paraffin flow rate ex brine heater) (KG/H)

MAX. : FOM01–z = (FOMM1–z) + (NEFOMC1–z)

MTN. : FOM01–z = (F0MM1–z)

(5)–1–2 XOM11–z (Mole fraction of constituents at #1 stage)

XOM11 = (COM01/MO1)/{(COM01/MO1)+……+(COM0z/MOz)}

XOM1a = (COM0a/MOa)/{(COM01/MO1)+……+(COM0z/MOz)}

XOM1z = (COM0z/MOz)/{(COM01/MO1)+·····+(COM0z/MOz)}

(5)–1–3 FOE1, FOM1 (Vaporization rate of paraffin at #1 stage) (KG/H)

FOE11 = (XOM11)(R11)(FWE1) FOM11 = FOM01 – F0E11

FOE1a = (XOM1a)(R1a)(FWE1) FOM1a = FOM0a – F0E1a

FOE1z = (XOM1z)(R1z)(FWE1) FOM1z = FOM0z – F0E1z

(5)–1–4 △FOM1 (Exclude the constituents finishing vaporization at #1 stage)

△FOM11 = FOM01 – FOM11

△FOM1a = FOM0a – FOM1a

△FOM1z = FOM0z – FOM1z

No calculation for the below #2 stage is carred out about each paraffin which is △FOM1 ≧FOM0.

(5)–2 #2 stage

If calculation results for praffin until N = 9 are FOM1≧FOM0, each formula are as follows;

(5)–2–1 FOM1 (n–Paraffin flow rate at #2 inlet) (KG/H)

The value is the same as FOM1a–z obtained by 5–1–3.

(5)–2–2 XOM2a–z (Mole fraction of constituents at #2 stage)

XOM2a = (COM1a/MOa)/{(COM1a/MOa) +·····+(COM1z/MOz)}

XOM2i = (COM1i/MOi)/{(COM1a/MOa) +·····+(COM1z/MOz)}

XOM2z = (COM1z/MOz)/{(COM1a/MOa)+·····+(COM1z/MOz)}

(5)–2–3 FOE2, (Vaporization rate of paraffin at #2 stage) (KG/H)

FOE2a = (XOM2a)(R2a)(FWE2) FOM2a = FOM1a – F0E2a

FOE2i = (XOM2i)(R2i)(FWE2) FOM2i = FOM1i – F0E2i

FOE2z = (XOM2z)(R2z)(FWE2) FOM2z = FOM1z – F0E2z

(5)–2–4 △FOM2 (Exclude the constituents finishing vaporization at #2 stage)

△FOM2a = FOM1a – FOM2a

△FOM2i = FOM1i – FOM2i

△FOM2z = FOM1z – FOM2z

No calculation for the below #2 stage are carried out about each paraffin which is △FOM2≧FOM1.

Repeat the same calclation until #6 stage

(6) COMT (n-Paraffin concentration at #6 stage) (KG/L)(KG/H)/(KG/H)=(KG/L)

Calculation for #6 stage outlet is carried out about each paraffin (N = i – z) which is excepted on N = 1 – h changing into △AFOM6≧AFOM5.

COMTi = (DBT)(FOM6i)/(FBL0 – FWET)
COMTk = (DBT)(FOM6k)/(FBL0 – FWET)
COMTz = (DBT)(FOM6z)/(FBL0 – FWET)
COMT = (COMTi)+……+(COMTz)

(7) FOMB (n-Paraffin flow rate in blow brine) (KG/L)(KG/H)/(KG/L)=(KG/H)

FOMBi = (COMTi)(FBLB)/(DBT)
FOMBk = (COMTk)(FBLB)/(DBT)
FOMBz = (COMTz)(FBLB)/(DBT)
FOMB = (COMTi)+……+(FOMTz)

(8) BBFOMC (n-Paraffin flow rate in recirculation brine)

BBFOMCi = (FOM6i)-(FOMBi)
BBFOMCk = (FOM6k)-(FOMBk)
BBFOMCz = (FOM6z)-(FOMBz)
BBFOMC = (FOM6i)+……+(FOMCz)

(9) FOMCi-z (Convergence calculation)

| NEFOMCi-BBFOMCi | / | NEFOMCi | ≦0.01
| NEFOMCk-BBFOMCk | / | NEFOMCk | ≦0.01
| NEFOMCz-BBFOMCz | / | NEFOMCz | ≦0.01

However, it is necessary to be satisfied the formulas calculating the below shown values.

XOM11-z
XOM21-z
XOM31-z
XOM41-z

XOM51-z
XOM61-z

(10) COE1-6 (Concentration on the assumption that all of paraffin carring over is dissolved in the evaporated water.)

(KG/H)(KG/L)/(KG/H)=(KG/L)

COE1 = (FOE1/FWE1)(DW1)
COE2 = {(FOE1+FOE2)/(FWE1+FWE2)} DW2
COE3 = {(FOE1+FOE2+FOE3)/(FWE1+·····+FWE3)} DW3
COE4 = {(FOE1+FOE2+FOE3+FOE4)/(FWE1+·····FWE4)} DW4
COE5 = {(FOE1+FOE2+FOE3+FOE4+FOE5)/(FWE1+·····+FWE5)} DW5
COE6 = {(FOE1+FOE22+FOE3+FOE44+FOE5+FOE6)/(FWE1+···+FWE6)} DW6
= COET (n-Paraffin concentration in the product water)

6.2.4 Homogeneous, Recirculation Type

(1) MASS BALANCE

FBLB = FBLM – FWLT = FBLM(CBLM/CBLB)

FWLT (value obtained by 5 in 5.1)

(2) R (CARRYOVER'S constant)

(2)–1 R1 = (MO)(POE1)/{(MW)(PWE1)}

R2 = (MO)(POE2)/{(MW)(PWE2)}

R3 = (MO)(POE3)/{(MW)(PWE3)}

R4 = (MO)(POE4)/{(MW)(PWE4)}

R5 = (MO)(POE5)/{(MW)(PWE5)}

R6 = (MO)(POE6)/{(MW)(PWE6)}

(2)–2 MO as $CHBr_3$ = 252.718, MW as H_2O = 18.02

(2)–3 POE1–6 (Vapor pressure of bromoform) (PA)

POE1 = 1000 • COM0/{(H1)(MO)}

POE2 = 1000 • COM1/{(H2)(MO)}

POE3 = 1000 • COM2/{(H3)(MO)}

POE4 = 1000 • COM3/{(H4)(MO)}

POE5 = 1000 • COM4/{(H5)(MO)}

POE6 = 1000 • COM5/{(H6)(MO)}

(3) FOMM (Dosing rate of bromoform)

(KG/L)(KG/H)(L/KG)=(KG/H)

FOMM = (COMM)(FBLM)(1/DBT)

(4) NEFOMC (Constituent flow rate calculated by method of once through type in #6 stage)

MAX. NEFOMC1–z = (COMM1–z)(1/DBT)(FBLM)

(KG/L)(L/KG)(KG/H)=(KG/H)

MIN. NEFOMC1–z = 0

(5) Mass balance in each stage

(5)-1. #1 stage

(5)-1-1 FOM0 (Bromoform flow rate ex BH) (KG/H)

MAX. : FOM0 = (FOMM) + (FOMC)

MIN. : FOM0 = (FOMM)

(5)-1-2 FOE1 (Vaporization rate of bromoform at #1 stage) (KG/H)

FOM1 = FOM0 - FOE1 FOE1 = (R1)(FWE1)

R1 = (MO)(POE1)/{(MW)(PWE1)}

POE1 = 1000 · COM0/{(H1)(MO)}

OM0 = (AFOM0)(1/FBL1)(DB1)

(5)-1-3 COM1 (Bromoform concentration at #1) (KG/H)(H/KG)(KG/L)=(KG/L)

ACOM1 = (AFOM1)(1/FBL1)(DB1)

(5)-2 #2 stage

(5)-2-1 FOM1 (The value is the same as FOM1 obtained by 5-1-2) (KG/H)

(5)-2-2 FOE2 (Vaporization rate of bromoform at #2 stage) (KG/H)

FOM2 = FOM1 - FOE2 FOE2 = (R2)(FWE2)

R2 = (MO)(POE2)/{(MW)(PWE2)}

POE2 = 1000 · COM1/{(H2)(MO)}

COM1 = (FOM1)(1/FBL2)(DB2)

(5)-2-3 COM2 (Bromoform concentration at #2) (KG/H)(H/KG)(KG/L)=(KG/L)

COM2 = (FOM2)(1/FBL2)(DB2)

Repeat the same calclation until #6 stage

(6) COMT (Bromoform concentration at #6) (KG/L)(KG/H)/(KG/H)=(KG/L)

COMT = (DBT)(AFOM6)/(FBL0 - FWET)

(7) FOMB (Bromoform Flow rate in blow brine) (KG/L)(KG/H)/KG/L)=(KG/H)

FOMB = (COMT)(FBLB)/(DBT)

(8) BBFOMC (Bromoform Flow rate in recirculation brine)

BBFOMC = (FOM6)−(FOMB)

(9) FOMC (Convergence calculation)

$$| NEFOMC-BBFOMC | / | NEFOMC | \leq 0.01$$

(10) COE1−6 (Concentration on the assumption that bromoform carrying over is dissolved in the evaporated water.)

(KG/H)(KG/L)/(KG/H)=(KG/L)

COE1 = (FOE1/FWE1)(DW1)

COE2 = {(FOE1+FOE2)/(FWE1+FWE2)} DW2

COE3 = {(FOE1+FOE2+FOE3)/(FWE1+……+FWE3)} DW3

COE4 = {(FOE1+FOE2+FOE3+FOE4)/(FWE1+……FWE4)} DW4

COE5 = {(FOE1+FOE2+FOE3+FOE4+FOE5)/(FWE1+……+FWE5)} DW5

COE6 = {(FOE1+FOE22+FOE3+FOE44+FOE5+FOE6)/(FWE1+…+FWE6)}DW6

= COET (Bromoform concentration in the product water)

6.2.5 Deaerator

6.2.5.1 HETEROGENEOUS

(1) XOM (Mole fraction of paraffin consisted of 35 kinds <1-9.A-Z>)

XOMG1-z

XOMG1 = (COMD1/MO1)/{(COMD1/MO1)+·····+(COMDz/MOz)}

XOMGa = (COMDa/MOa)/{(COMD1/MO1)+·····+(COMDz/MOz)}

XOMGz = (COM0z/MOz)/{(COMD1/MO1)+·····+(COMDz/MOz)}

(2) FOE, FOM (Evaporatin/Flow rate of paraffin in deaerator)

(KG/H)

FOEG1-z = (XOMG1-z)(RG1-z)(FWEG), FOMG1-z = FOMD1-z - FOEG1-z

(3) COM (Paraffin concentration in the brine at deaerator)

(The symbols '1' through 'z' were omitted.)

(KG/L){(KG/H)(KG/L)(L/KG)-(KG/H)}/(KG/H)=(KG/L)

COMG=DB1(FBLD • COMD/DB0 - FOEG)/FBLG

(4) COE (Paraffin concentration in the ejector drain at dearetor)

(The symbols '1' through 'z' for 'COE' & 'FOE' were omitted.)

(KG/H)/(KG/H)(KG/L)=(KG/L)

COEG = (FOEG/FWEG)(DW1)

(5) R (CARRYOVER'S CONSTANTS)

RG1-z = (MO1-z/MW)(POEG1-z/PWEG)

MW = 18.02

MO1-z = 14.027N + 2.016

PWE : STEAM TABLE

POEG1-z : Be calculated by using ANTIOINE'S equation.

6.2.5.2 HOMOGENEOUS

(1) FOE, FOM : Be the same equation in case of 'HETEROGENEOUS'. However, the symbols '1' through 'z' were not necessary.

(2) COM : Be the same equation in case of 'HETEROGENEOUS'. However, the symbols '1' through 'z' were not necessary.

(3) COE : Be the same equation in case of 'HETEROGENEOUS'. However, the symbols '1' through 'z' were not necessary.

(4) R (CARRYOVER'S CONSTANTS)

RG=(MO/MW)(POEG/PWEG)

MW=18.02 (Molecular weight of H_2O)

MO=252.718 (Molecular weight of $CHBr_3$)

PWE:STEAM TABLE

POEG=1000 • COMD/(HG • MO) (KG/L)/{(KG/MOL)(MOL/L)(1/PA)}=(PA)

6.2.5.3 HEAT/MASS BALANCE

(1) PWEG (Steam Pressure in deaerator) (PA)

The value corresponds to TWEG of the steam table.

(2) BPRG (Boiling point rising of feed seawater) (C)

BPRG is calculated from the TDS concentration of the feed seawater.

(3) TWEG (Steam temp. in deaerator) (C)

See the value of TR201 indicated on P/I diagram

(4) △TBLG (Temperature difference of brine between inlet and outlet temp. in deaerator) (C)

TBLG = TWEG + BPRG

△TBLG = TBLD – TBLG

(5) FWEG (Evaporation flow rate in deaerator)

(KG/H)(KJ/KG • C)/(C)/(KJ/KG)=(KG/H)

FWEG = (FBLG)(CPG)(△TBLG/ENTG)

FWLT = FWEG (Condensate flow rate by the ejector condenser)

(6) FBLG (Brine flow rate) (KG/H)

FBLG = FBLD – FWEG

7 Physical Properties

The physical properties used for the calculation are mainly derived from the RESEARCH AND DEVELOPMENT PROGRESS REPORT No.214 (Sep. 1966), OSW, "The Oakridge National Laboratory Conceptional Design of a 250-MGD Desalination Plant". They are shown in 6.3.2.

6.3.2 Simulation for Behaviors of Oil Contaminants

CONTENTS

List of Tables

List of Figures

1. Introduction

The purpose of the MSF-2 is to estimate the quality of the product water in case when the oil contaminated seawater has been fed into the MSF Plant. It has been done through the investigation on the quantitative analysis of the evaporation phenomena of the volatile organic contaminants in the feed seawater.

The Henry's constant of bromoform in brine, which is the basic physical property necessary for the quantitative analysis of the dilute solution, has been measured by the "Vapor/Liquid Equilibrium Experimental Apparatus". The results are reported in 6.2. The Henry's constant obtained in 6.2 showed good agreement with that of 6.1.2. Thus, the Henry's constant, as a function of temperature obtained by 6.2, has been used for the computer simulation.

The flow chart and the formula used for the computer simulation of the evaporation of the organic contaminants in brine are described in 6.3.1 based on the evaporation mechanisms shown in 6.1 and 6.2. In this section the details of the computer programs are described.

2. Structure of the program

The basic structure has been already shown in 6.3.1. The structure comprise of subroutines shown in Figs.1 to 4. The variables used and the dimensions of them are shown in Table 1 with its meanings. The physical properties and the chemical constants are shown in Table 2 as the function of parameters.

The input and output form of the program are shown in Figs.5 and 6.

- Input processing
- Deaerator calculation
- Heat and mass balance calculation
- Carryover calculation
- Output processing

Each part is made up of a number of subordinate subroutines.

3. Variables

Variables are made up primarily of 6 groups:

- **Heat and mass balance calculation**
- **Designate calculation options**
- **Carryover calculation**
- **Store log data**
- **Iteration in heat and mass balance calculation**
- **Deaerator calculation**

4. Physical Properties and Chemical Constants

Physical properties and chemical constants used in the program:

• Function of temperature	:	Henry's constant
		Saturated steam pressure,
		Latent heat of vaporization
• Function of TDC concentration	:	Electric conductivity
		Boiling point elevation of brine
• Function of TDC conc. and temp.	:	Specific heat of brine
		Brine density
• Function of temp. and carbon-number-dependent 3 constants		
	:	Saturated n-paraffin pressure
• Function of molecular weight	:	Carryover constant

Table 1 Variables using in the program

BLOCK NAME	VARIABLE NAME	UNIT	PHYSICAL IDENTITY
SYMBOL	FBL	Kg/H	BRINE FLOW
	TWL	˚C	DISTILATE TEMPERATURE
	TWE	˚C	STEAM TEMPERATURE
	SBL	S/cm	BRINE ELECTRIC CONDUCTIVITY
	CBS	kg/kg	BRINE TDS CONCENTRATION
	PWE	Pa	SATURATED STEAM PRESSURE
	NTD	˚C	NON-EQUILIBRIUM TEMPERATURE
	TBL	˚C	BRINE TEMPERATURE
	FWE	Kg/H	STEAM FLOW
	ONTD	˚C	NTD + BOILING POINT ELEVATION BY TDS IN BRINE
	FWL	Kg/H	DISTILATE FLOW
	FWLT	Kg/H	TOTAL DISTILATE FLOW
OPTION	TYPE	-	CALCULATION TYPE IDENTIFIER
	CONTAM	-	CONTAMINANT TYPE IDENTIFIER
	DEAIR	-	DEAERATOR IDENTIFIER
CARRY	MO	g/mol	MOLECULAR WEIGHT
	POE	Pa	CONTAMINANT SATURATED PRESSURE
	FOM	Kg/H	CONTAMINANT FLOW INTO EACH STAGE
	XOM	-	MOLAR RATIO
	FOE	Kg/H	CONTAMINANT EVAPORATION IN EACH STAGE
	COM	Kg/L	INDIVIDUAL CONTAMINANT CONCENTRATION
	COMM	Kg/L	TOTAL CONTAMINANT CONCENTRATION
	FBLM	Kg/H	MAKEUP BRINE FLOW
	COMP	-	INDIVIDUAL CONTAMINANT COMPOSITION OF COMM
	BROME	Kg/L	BROMOFORM TOTAL CONCENTRATION
	COE	Kg/L	CONTAMINANT CONCENTRATION IN DISTILATE IN EACH STAGE
	SUMFOE	Kg/L	TOTAL CONTAMINANT EVAPORATION
	SUMFWE	Kg/L	TOTAL DISTILATE FLOW
	CWLT	Kg/H	CONTAMINANT FLOW IN SUMFWE
	CBSM	Kg/Kg	TDS CONCENTRATION IN MAKEUP BRINE
	TBLM	˚C	MAKEUP BRINE TEMPERATURE
	FBLB	Kg/H	BLOW BRINE FLOW
	COMO	Kg/L	CONTAMINANT CONCENTRATION IN MAKEUP BRINE
	FOMC	Kg/H	CONTAMINANT FLOW IN RECIRCULATION BRINE
	N_FOMC	Kg/H	FOMC AFTER ONE MORE RECIRCULATION
LOG	RUNNUMBER	-	TEST NUMBER
	DATE	-	TEST DATE
	OPERATOR	-	OPERATOR NAME
	MAXTEMP	˚C	MAXIMUM BRINE TEMPERATURE

(Cont.)

BLOCK NAME	VARIABLE NAME	UNIT	PHYSICAL IDENTITY
A	AONTD	˚C	ASSUMED ONTD IN HEAT/MASS BALANCE CALCULATION
	ATBL	˚C	ASSUMED TBL IN HEAT/MASS BALANCE CALCULATION
	DIFTBL	˚C	BRINE TEMPERATURE DIFFERENCE IN SUCCESIVE STAGES
	AFBL	Kg/H	ASSUMED FBL IN HEAT/MASS BALANCE CALCULATION
	AFWE	Kg/H	ASSUMED FWE IN HEAT/MASS BALANCE CALCULATION
	ACBS	Kg/Kg	ASSUMED CBS IN HEAT/MASS BALANCE CALCULATION
GASNGO	GASNGO	-	LOGICAL VARIABLE TO TALLY COMPLETE EVAPORATION OF OIL
HFACTOR	HFACTOR	-	ARBITRARY INPUT VALUE TO DIVIDE HENRY'S CONSTANT
DEAER	TWEG	˚C	DEAERATOR STEAM TEMPERATURE
	PWEG	Pa	DEAERATOR SATURATED STEAM PRESSURE
	DIFTBLG	˚C	DEAERATOR INLET/OUTLET BRINE TEMPERATURE DIFFERENCE
	TBLD	˚C	DEAERATOR OUTLET TEMPERATURE
	FWEG	Kg/H	DEAERATOR STEAM FLOW
	POED	Pa	DEAERATOR CONTAMINANT SATURATED PRESSURE
	FOMD	Kg/H	DEAERATOR INLET CONTAMINANT FLOW
	XOMD	-	CONTAMINANT MOLAR RATIO IN DEAERATOR
	RG	-	CARRYOVER COEFFICIENT IN DEAERATOR
	FOED	Kg/H	DEAERATOR CONTAMINANT EVAPORATION
	FOMG	Kg/H	DEAERATOR OUTLET CONTAMINANT FLOW
	FBLD	Kg/H	DEAERATOR INLET BRINE FLOW
	COEG	Kg/L	CONTAMINANT CONCENTRATION IN STEAM IN DEAERATOR
	COMD	Kg/L	DEAERATOR OUTLET CONTAMINANT CONCENTRATION
	FBLG	Kg/H	DEAERATOR OUTLET BRINE FLOW

Table 2. Physical Properties and Chemical Constants using in the Program

NAME	HENRY'S CONSTANT[mol/l·Pa](Y)
ARGUMENT	TEMPERATURE[°C](X)
EQUATION	$Y=10^{(0.24-0.024x)}/133.3224$

NAME	TDS CONCENTRATION[g/kg](Y)
ARGUMENT	BRINE ELECTRIC CONDUCTIVITY[S/cm](X)
EQUATION	Y=709.79993X-2.615515

NAME	SATURATED STEAM TEMPERATURE[Pa](Y)
ARGUMENT	TEMPERATURE[°C](X)
EQUATION	$Y=0.006895E6[2.1786818-0.70443622E-1(32+9X/5)+0.93941286E-3(32+9X/5)^2-0.53958083E-5(32+9X/5)^3+0.18139197E-7(32+9X/5)^4]$

NAME	LATENT HEAT of VAPORIZATION [J/Kg](Y)
ARGUMENT	TEMPERATURE[°C](X)
EQUATION	$Y=1.055*2.205[1093.8-0.5703(32+9X/5)+1.2819E-4(32+9X/5)^2-0.8824E-6(32+9X/5)^3]$

NAME	SPECIFIC HEAT of BRINE[J/Kg·°C](Z)
ARGUMENT	TEMPERATURE[°C](X) BRINE TDS CONCENTRATION[Kg/Kg](,Y)
EQUATION	$Z=1.055*2.205*9/5*[1.005773-0.13280442E-3(32+9X/5)-1.5344907Y+0.39090715E-2(32+9X/5)Y+0.65092605E-6(32+9X/5)^2+2.4955446Y^2-0.11156771E-1(32+9X/5)Y^2-0.88941836E-5(32+9X/5)^2Y+0.3598702E-4(32+9X/5)^2Y^2]$

(Continued)

NAME	BRINE DENSITY[Kg/l](Z)
ARGUMENT	TEMPERATURE[°C](X) BRINE TDS CONCENTRATION[Kg/Kg](Y)
EQUATION	$Z=[62.717753-0.32152986E-2(32+9X/5)$ $+0.44315006E2Y$ $-0.11647394E-1XY$ $-0.48932777E-4(32+9X/5)^2$ $+0.16449945E2Y^2$ $+0.13761984E-1(32+9X/5)Y^2$ $+0.34231326E-5(32+9X/5)^2Y$ $-0.92275301E-4(32+9X/5)^2Y^2]/62.43$

NAME	BRINE BOILING POINT ELEVATION[°C](Z)
ARGUMENT	TEMPERATURE[°C](X) BRINE TDS CONCENTRATION[Kg/Kg](Y)
EQUATION	$Z=5/9[0.1014380E-1+0.1021815E2Y+8.809554Y^2$ $-0.6386588E-4(32+9X/5)$ $+0.6118005E-1(32+9X/5)Y$ $+0.2386759E-6(32+9X/5)^2$ $+0.2214495E-4(32+9X/5)^2Y$ $+0.1714722(32+9X/5)Y^2$ $+0.7173776E2Y^3$ $+0.1170617E-9(32+9X/5)^3$ $+0.1042795E-6(32+9X/5)^3Y$ $+0.3620461(32+9X/5)Y^3$ $+0.7823281E-4(32+9X/5)^2Y^2$ $-0.5218751E-6(32+9X/5)^3Y^2$

NAME	CARRYOVER CONSTANT[-](R)
ARGUMENT	CONTAMINANT MOLECULAR WEIGHT[g/mol](X)SATURATED CONTAMINANT PRESSURE[Pa](Y)SATURATED STEAM PRESSURE[Pa](Z)
EQUATION	$R=(X/18.02)(Y/Z)$

(Continued)

NAME	n-PARRAFIN SATURATED PRESSURE[Pa](Y)			
ARGUMENT	TEMPERATURE[°C](X)			
EQUATION	$Y=133.322*10^{(A-B/(X+C))}$			
CONSTANT	CARBON #	A	B	C
	1	6.61184	389.93000	266.00000
	2	6.80266	656.40000	256.00000
	3	6.82973	813.20000	248.00000
	4	6.83029	945.90000	240.00000
	5	6.85221	1064.63000	232.00000
	6	6.87776	1171.53000	224.36600
	7	6.90240	1268.11500	216.90000
	8	6.92377	1355.12600	209.51700
	9	6.93513	1428.81100	201.61900
	10	6.95367	1501.25800	194.48000
	11	6.97674	1572.47700	188.02200
	12	6.98059	1625.92800	180.31100
	13	7.00339	1669.09300	174.28300
	14	7.01245	1739.62300	167.53400
	15	7.02445	1789.65800	161.29100
	16	7.03044	1831.31700	154.52800
	17	7.04237	1880.60000	150.02000
	18	7.04823	1920.60000	144.53000
	19	7.05710	1961.60000	139.60000
	20	7.06640	1994.00000	133.20000
	21	7.07380	2026.00000	128.20000
	22	7.07950	2052.00000	123.00000
	23	7.08570	2078.00000	119.00000
	24	7.09240	2104.00000	114.00000
	25	7.09910	2132.00000	109.00000
	26	7.10610	2158.00000	106.00000
	27	7.11300	2184.00000	102.00000
	28	7.11950	2218.00000	98.00000
	29	7.12690	2240.00000	94.00000
	30	7.13280	2264.00000	91.00000

(6.3.2)

MAIN and below program structure

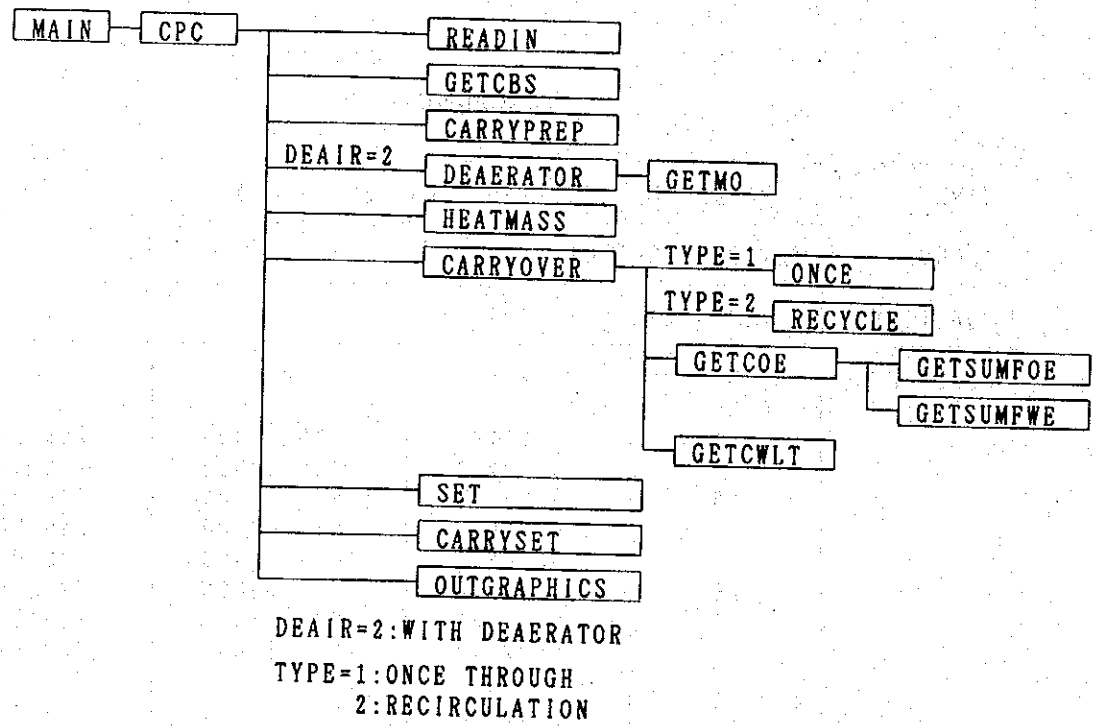


Fig. 1 MAIN and below Program Structure

HEATMASS and below program structure

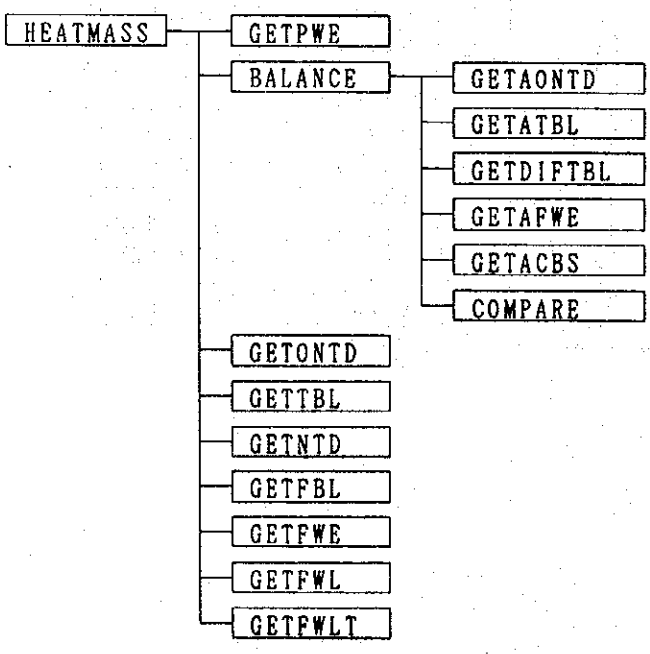


Fig. 2 HEATMASS and below Program Structure

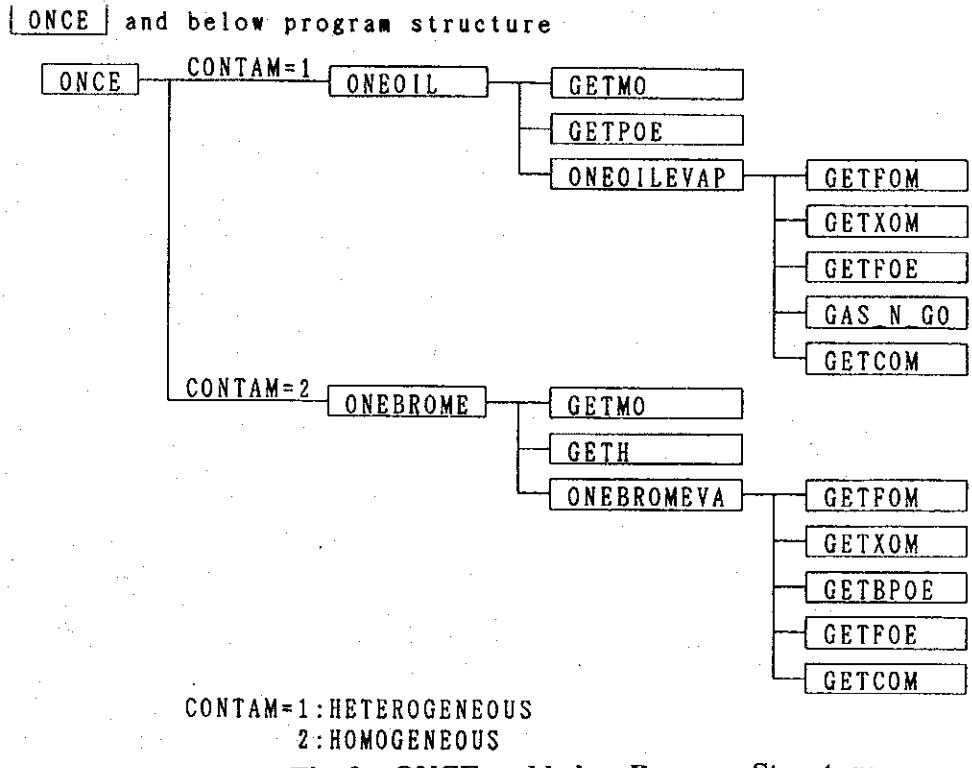


Fig. 3 ONCE and below Program Structure

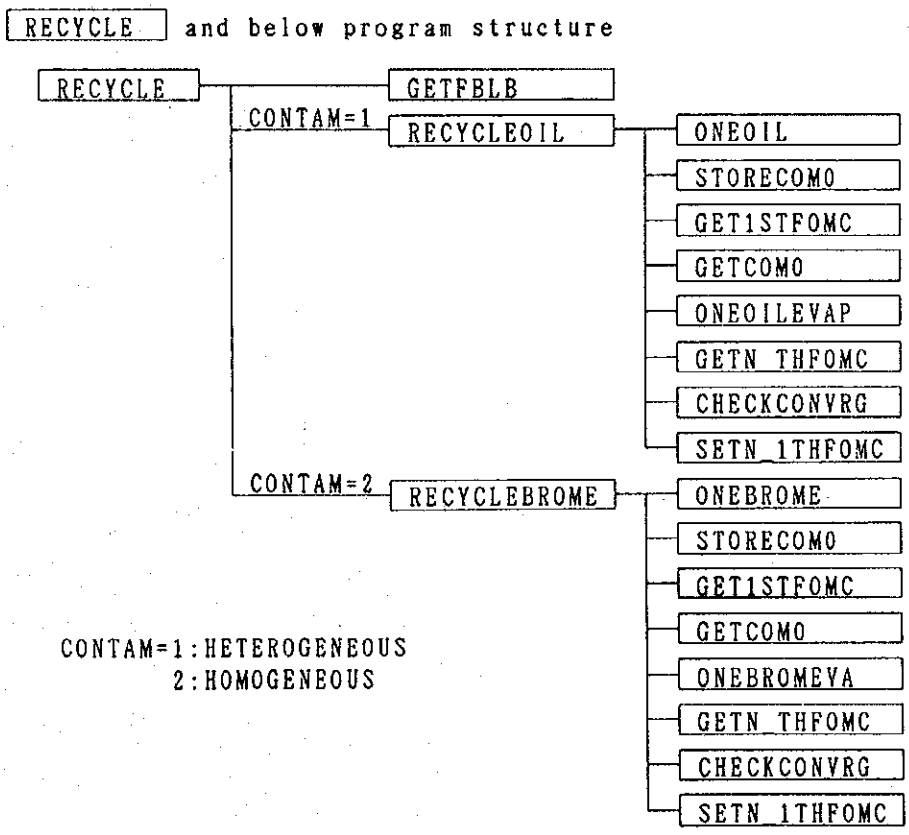


Fig. 4 RECYCLE and below Program Structure