The result of investigation can be used for new projects of solid deuterium sources at high flux reactors with heavy water reflectors. A heavy water is a good shield from high energy neutrons and gamma rays. That allows to have a low level of heat load at high flux of thermal neutrons (reactor PIK, Gatchina, reactor ILL, Grenoble). Another possibility is using of solid deuterium sources at neutron spallation sources, where the relation of heat load to neutron flux is better than one for reactors. For example, the solid deuterium source for UCN production is planning to be installed at 1 MW spallation source in Los Alamos (USA).

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COMPUTER SIMULATION OF THE HYDROGEN DISTILLATION AND CECE PROCESS

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I. Introduction

There are a number of reports describing computer simulation procedures for cryogenic distillation [1,2] and CECE process [3,4]. These procedures are based either on the successive iteration method, which does not always present adequate stability in achieving convergence, or on the Newton-Raphson method, which needs large computation efforts for the numerical evaluation of the elements of the Jacobian matrix and calculation of its inverse matrix. Another way of looking at these equilibrium stage processes is proposed [5]. It provides stable and relatively rapid solutions of the basic equations for both above-mentioned processes. For example, approximately 10 seconds are required for computation of a seventy tray catalytic exchange column with six components on an IBM PC 486DX 33.

II. Steady-State Procedure for Cryogenic Distillation Column with a Feedback Stream and Catalytic Equilibrator

The mathematical simulation procedure has been developed for a single cryogenic distillation column with a feedback stream and catalytic equilibrator used for hydrogen isotope separation. The computer programme "Cry_En" has been created on its base. Nonidealities of the hydrogen isotope solutions and heat balance are incorporated. The model column for mathematical simulation is shown in Fig.1. The initial data for the computation:
N – the number of theoretical stages; P – pressure in the top of the column [kPa]; ΔP – pressure drop across the column [kPa]; Bot – flow rate of bottom product [kmol/h]; Top – flow rate of top product [kmol/h]; W = Bot + Top – flow rate of the gas external feed stream [kmol/h];
Aw1, Aw2, Aw3 – composition (atomic fractions of protium, deuterium and tritium) in

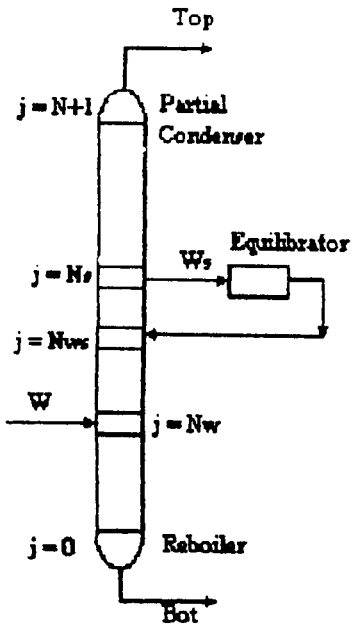
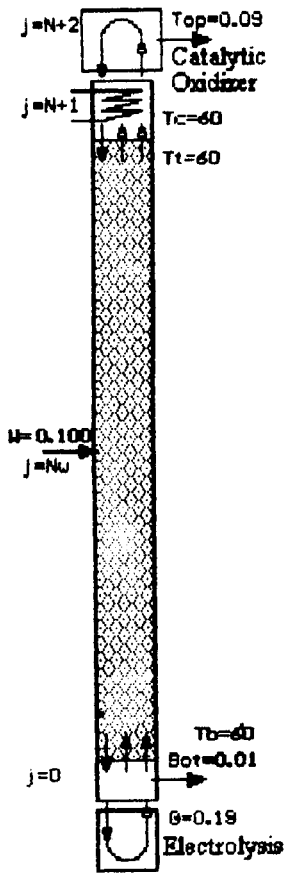


Fig.1. The model column for mathematical simulation



G, W, Bot, Top (kmol/h)
G – flow rate of hydrogen gas
W – feed flow rate
Bot - flow rate of bottom product
Top - flow rate of top product
Temperature
(degrees Centigrade)
Tb – operating temperature at the bottom
Tt – operating temperature at the top
Tc – condenser temperature
N – the number of tray
Nw – feed tray number
N = 60 Nw =20
Atomic fractions of elements in feed water:
aH = 0.899999 aD = 0.1
aT = 0.000001
The pressure at the top
P = 105.3 kPa
The pressure drop across the column ΔP=4 kPa

Fig.2. The model of CECE process with initial data for the case that is close to the case 3 from [4]

the external feed stream; Tw - temperature of the external feed stream [K]; Nw - feed stage number for the external feed stream; Ns - side stream stage number; Ws - flow rate of the gas side stream [kmol/h]; Nws - feed stage number for the equilibrated stream; Tws - temperature of the equilibrated stream [K]; R - reboiler load [kW]; Q - heat subtraction rate per stage [W].

The steady-state simulation procedure for cryogenic column is composed of the following components:

1) Catalytic Equilibrator model;

2) BeComp procedure allowing to determine profile of concentration of a component when separation factor and flow rates of all streams are given for each stage;

3) Temp procedure which defines the temperature in a stage taking into account vapour and liquid nonidealities when pressure and composition are known;

4) Heat Balance procedure for a more precise definition of flow rates of liquid and vapour streams. The simulation procedure is realised in the following way.

STEP 1. Input of all initial data and determination equilibrium composition in external feed stream.

STEP 2. The definition of the temperature in the feed stage and the calculation of the separation factor for each of six components. These values are given to all stages.

STEP 3. The determination of the flow rates of liquid and vapour streams from the heat balance for the reboiler and material balance for the column.

STEP 4. The concentration profiles within the column are calculated using BeComp for each of six components.

STEP 5. The calculation for each stage, reboiler and condenser:

$$Sj = \sum_{i=1}^{6} X[j,i] \,,$$

where $X[j,i]$ - mole fraction of i-th component in the liquid stream living j-th stage.

STEP 6. If

$$\sum_{j=0}^{N+1} Sj/(N+2) - 1 \leq \varepsilon \,, 0 < \varepsilon \ll 1$$

then go to STEP 8.

STEP 7. The normalisation: $X[j,i] = X[j,i]/Sj$. The calculation of composition after the equilibrator. The calculation for each stage of:
the temperature, new separation factors and new flow rates for liquid and vapour streams. Go to STEP 4.

STEP 8. Convergence is achieved. Output of: calculated composition in the top product and bottom product; composition distribution within the column; temperature profile; composition of the equilibrated stream.

The calculation conditions and the results for two examples are given in Tab.1, Tab.2 and Tab.3. The case 1 shows the possibility of cryogenic column for tritium removal from heavy water used as moderator for nuclear fission reactor. Thus in this case the decontamination factor is equal 424. The case 2 may be considered as the example of the first stage of the heavy water waste contained tritium reprocessing. It is observed from Table 3 that tritium

decontamination factor is equal $2.8 \cdot 10^4$ whereas the deuterium atomic fraction in the Top Product is sufficiently high due to HD.

Table 1

Calculation conditions for two cases

Case	1	2
N	80	80
Nw	40	40
Ns	75	-
Nws	40	-
R, kW	2.0	2.0
Q, W	7.5	5.0
P, kPa	150	150
P, kPa	6.0	5.0
Bot, mol/h	10	200
Top, mol/h	200	200
Ws, mol/h	100	-
Tws, K	25.2	-
Tw, K	25.2	23.5
Aw1, Aw2, Aw3	0.002, 0.99798, 2e-5	0.499999, 0.5, 1e-6
The number of iteration	8 ε =1e−8	8 ε = 1e−8
The time of calc.*	2 m 36 s	2 m 39 s

*The IBM PC 486 DX 33 time

Table 2

Results of calculation in the case 1

Case 1	Feed Composition	Before Equilibrator	After Equilibrator	Bottom Product	Top Product
H_2	4.89e−6	2.63e−7	1.40e−7	2.6e−21	5.08e−8
HD	3.99e−3	6.75e−4	6.75e−4	1.0e−10	4.19e−3
HT	7.28e−8	2.50e−8	3.2e−11	7.6e−12	6.39e−8
D_2	0.9956	0.9993	0.9993	0.9992	0.9958
DT	3.99e−5	7.84e−8	1.03e−7	8.38e−4	3.05e−8
T_2	4.2e−10	1.5e−15	2.8e−15	8.82e−9	2.3e−16
aH	0.0020	3.38e−4	3.38e−4	5.4e−11	0.0021
aD	0.9980	0.9997	0.9997	0.9996	0.9979
aT	2.00e−5	5.17e−8	5.17e−8	4.19e−4	4.72e−8

Table 3

Results of calculations in the case 2

Case 2	Feed Composition	Bottom Product	Top Product
H_2	0.2626407	7.60e−10	0.5252815
HD	0.4747156	0.4747127	0.4747185
HT	9.02e−7	1.805e−6	7.22e−11
D_2	0.2626416	0.5252833	1.420e−8
DT	1.098e−6	2.195e−6	2.47e−17
T_2	1.20e−12	2.41e−12	1.74e−26
aH	0.4999990	0.2373573	0.7626407
aD	0.5000000	0.7626407	0.2373593
aT	1.00e−6	2.00e−6	3.61e−11

III. Simulation Procedure for CECE Process

The mathematical simulation procedure has been developed for multistage water/hydrogen exchange column (CECE process). The algorithm of this procedure is very much alike to the one of the procedure for cryogenic distillation column just considered. But it has its own specific features, such as:

1) presence of three streams (liquid water, water vapour and hydrogen gas);

2) occurrence of exchange reactions and much more complex column configuration;

3) the material balances for the six molecular species (H_2O, HDO, HTO, D_2O, DTO, T_2O) do not hold and that's why the calculation using the procedure BeCompE is carried out not for each of six components, but only for three atomic fractions (aH, aD, aT);

4) the temperature on each of the tray is not calculated but given as initial condition ;

5) presence of the Exchange procedure which allows to define the equilibrium water composition (6 species) in each tray and equilibrium gas composition (6 species) after each catalyst bed and calculates new separation factors both for the water/vapour scrubbing step and for the catalytic exchange step which are used by the BeCompE procedure ;

6) the consideration of the heat balances is not needed.

A model column composed of N trays and (N-1) catalyst beds is illustrated in Fig.2.

The computer code "KIO" has been created on the base of the considered procedure. The case 3 in Reference 4 required more than 1000 iterations for the Successive iteration method ("Nonconvergence" - see Table 2 in Ref.4) and only 4 iterations for the Newton-Raphson method. The case that is very close to this case (see Fig. 2) requires 4 iterations and 8 second for its calculation by code "KIO" on the IBM PC 486DX 33. The results are given in Table 4. Hence we can see that presented method is as good as the Newton-Raphson one in this instance.

The case 4 given in Table 5 is interesting from the point of view of the heavy water waste contained tritium processing. Thus in this case (Table 6) we obtain heavy water as the bottom product that can be used for fission nuclear reactors and the raw material as the top product for further reprocessing with the aim to derive the heavy water containing a small tritium amount. The case 5 demonstrates good possibilities of CECE process for the heavy water waste processing.

Table 4

Results of calculations in the case 3 [4]

Case 3 [4]	Feed Composition	Bottom Product	Top Product
H_2O	0.8102534	0.0245763	0.9658506
HDO	0.1794894	0.2609214	0.0338435
HTO	1.793e−6	3.054e−6	7.29e−10
D_2O	0.0102552	0.7144823	0.00030586
DTO	2.07e−7	1.694e−5	1.34e−11
T_2O	1.06e−12	1.01e−10	1.47e−19
aH	0.8999990	0.1550385	0.9827724
aD	0.1000000	0.8449515	0.0172276
aT	1.00e−6	1.000e−5	3.71e−10

Table 5

Calculation conditions for two cases

Case	4	5
N	70	90
Nw	22	45
P, kPa	110	110
P, kPa	10.0	10.0
Bot, mol/h	30	50
Top, mol/h	15	50
G, mol/h	220	220
Tb, C	78	85
Tt, C	78	84
Tc, C	20	20
aD, aT	0.8, $1.00e-7$	0.5, $1.00e-5$
The number of iteration	3. $\varepsilon = 1e{-}8$	7 $\varepsilon = 1e-8$
The time of calc.	6 s	20 s

Table 6

Result of calculations in the cases 4 and 5

KIO	Case 4			Case 5		
	Feed	Bottom	Top	Feed	Bottom	Top
H_2O	0.0407	5.40e−6	0.3561	0.2517	2.33e-6	0.9990
HDO	0.3186	4.57e−3	0.4786	0.4967	9.53e−4	9.93e−4
HTO	3.95e−8	6.79e−10	1.41e−10	9.88e−6	1.89e−8	3.68e−11
D_2O	0.6407	0.9954	0.1653	0.2517	0.9990	2.53e−7
DTO	1.61e−7	2.99e−7	9.88e−11	1.01e−5	4.00e−5	1.90e−14
T_2O	1.01e−14	2.26e−14	1.48e−20	1.02e−10	4.02e−10	3.58e−22
aH	0.2000	2.29e−3	0.5954	0.5000	4.77e−4	0.9995
aD	0.8000	0.9977	0.4046	0.5000	0.9995	4.97e−4
aT	1.00e−7	1.50e−7	1.20e−10	1.00e−5	2.00e−5	1.84e−11

IV. Conclusions

The mathematical simulation procedure and computer code "Cry_En" for a single cryogenic column used for hydrogen isotope separation have been developed. The code allows to carry out the calculation in a wide range of conditions and has good convergence characteristics though needs further enhance (to make shorter a computation time).

The simulation procedure and computer code "KIO" for a multistage water/hydrogen exchange column has been developed. The static behaviour of a similar column can be studied in detail. The procedure is applicable in cases with any deuterium concentration and has good convergence characteristics.

Both steady-state procedures do not use Newton-Raphson method. This is due to the fact that the convergence characteristics of the plate separation factors are much less sensitive to the type of the iterative method than plate temperatures (or concentrations). That's why large computation efforts are not needed and computer storage requirement is small.

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TWOFOLD PURPOSE DETRITIATION PLANT

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I. Introduction

At present, two plants operate for the protium and tritium extraction from heavy water and it's concentration at the research reactor (at Laue-Langevin Institute, Grenoble, France [1]) and at the nuclear power stations (at Darlington, Canada [2]). The final purpose of this plants is the maintenance of tritium and protium concentrations on the certain level (< 70 GBq/kg of D_2O and 99.8% D_2O). The construction of similar plant was begun for the reactor PIK in PNPI.

In order to use the operating detritiation plants for the reprocessing of tritiated heavy and light water wastes, a new technology should be develop. It allows to create the detritiation plant of twofold purpose. The description of the PNPI full scale experimental base for the development of new technologies is given.