# SIMULATION MODULE OF PHYSICS EFFECT OF HYDROGEN ISOTOPIC MIXING IN CRYOGENIC DISTILLATION COLUMN

#### Mircea Bărbuceanu

University of Pitești, Faculty of Sciences, ROMANIA, e-mail: mircea\_barbuceanu@yahoo.com

#### Abstract

In the paper it is described the mathematical model of physics effect of hydrogen isotopic mixing in cryogenic distillation column, the algorithm to the numerical solving and the module of the computer code dedicated to this.

Keywords: hydrogen, isotope, cryogenic, distillation, simulation, mixer.

## 1. Introduction

The efficiently increase of tritium isotopic separation plants by cryogenic distillation require more distillation column than one - a *cascade*. In this structure of separation plants, two or more distillation columns are interconnected by multiple devices (catalytic equilibrators, control devices etc.). Figure 1 show usual structure of a cascade with for cryogenic distillation columns.

As the first effect in the computer simulated is the mixing problem: many liquid or vapor streams with the different isotopic concentrations and thermodynamic properties converge to the same points.

#### 2. Method and samples

The mathematic model consists in four balance equations (of material) in principal:

$$D = D_{1} + D_{2};$$

$$x_{H} = \frac{D_{1}x_{H}^{1} + D_{2}x_{H}^{2}}{D};$$

$$x_{D} = \frac{D_{1}x_{D}^{1} + D_{2}x_{D}^{2}}{D};$$

$$x_{H} = \frac{D_{1}x_{T}^{1} + D_{2}x_{T}^{2}}{D};$$
(1)

where:

 $D_1$  - flow rate of top stream of column 1;



Fig. 1. Ordinary structure of cryogenic distillation plant

 $x_{H}^{1}, x_{D}^{1}, x_{T}^{1}$  - atomic fractions of components *H*, *D*, *T* in *D*<sub>1</sub>;  $D_{2}$  - flow rate of injected stream;  $x_{H}^{2}, x_{D}^{2}, x_{T}^{2}$  - atomic fractions of components *H*, *D*, *T* in *D*<sub>2</sub>;

*D* - flow rate of total stream;

 $x_H, x_D, x_T$  - atomic fractions of components *H*, *D*, *T* in *D*.

Atomic fractions  $x_H^1, x_D^1, x_T^1$  are obtained from material balance equations of top stream components (column 1):

$$\begin{aligned} x_{H}^{1} &= x_{H_{2}}^{1} + \frac{1}{2} \left( x_{HD}^{1} + x_{HT}^{1} \right) \\ x_{D}^{1} &= x_{D_{2}}^{1} + \frac{1}{2} \left( x_{HD}^{1} + x_{DT}^{1} \right) \\ x_{T}^{1} &= x_{T_{2}}^{1} + \frac{1}{2} \left( x_{HT}^{1} + x_{DT}^{1} \right) \end{aligned}$$
(2)

The calculation algorithm is simply and it is showed in figure 2:



Fig. 2. Calculation algorithm for mixing

## 3. Results and Discussions

The experimental input values and the results of mixing simulation are the follows:

DEBITUL SI COMPOZITIA FLUXULUI 1

D1 = 25.00000 moli/h

XH1 = 3.999906000E-0002

XD1 = 9.399644500E-0001

XT1 = 2.003473723E-0002

DEBITUL SI COMPOZITIA FLUXULUI 2

D2 = 4.50000000E + 0001 moli/h

XH2 = 4.00000000E-0003

XD2 = 9.399644500E-0001

XT2 = 1.00000000E-0003

DEBITUL SI COMPOZITIA FLUXULUI FINAL

D = 7.00000000E+0001 moli/h

XH = 1.685680714E-0002

XD = 9.753444464E-0001

XT = 7.798120439E-0003

The final results were in according with the experimental data.

## 4. Conclusions

The module dedicated of mixing problem is valid and may be considered a routine (external) for the simulated code of hydrogen isotopes cryogenic distillation.

### References

[1] Matthew Van Winkle, Distillation, McGraw-Hill Book Company, New York, 1967

[2] Mesahiro K., Yuji M., Kichizo T. - J. of Nuclear Sci. and Tech., 18(7), 1981, p. 525-539

[3] Miller D. G., Paper reviewed for Ind. and Engineering Chemistry (Fundamentals), 1963

- [4] Mittelhauser H. M., Vapor pressure relationship up to the critical point of hydrogen, deuterium and tritium, and their diatomic combination, Cryogenics, 1964, p. 368-373
- [5] Păstrăcioiu Cristian, Metode numerice aplicate în ingineria chimică, Ed. MatrixRom, 2000