APPLICATION OF EQUATION-SOLVER EQUATRAN-G FOR SEPARATION PROCESS ENGINEERING

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ABSTRACT

This paper briefly explains the functions of the equation solver called EQUATRAN-G and then evaluates the feasibility and practicality of the software with three actual examples (equilibrium flash calculation, Teiele-Geddes method for distillation and batch distillation) applied in the distillation field of separation process engineering.

INTRODUCTION

The conventional way to calculate the process analysis and design in chemical engineering was to create individual programs by using programming languages such as FORTRAN and BASIC. However, the rapid growth of personal computers and the advent of the packaged software designed for easy mathematical calculations have made it possible to perform such calculations employing only equations without programming.

FUNCTIONS

Equation Solving Functions

EQUATRAN-G enables the numerical calculations of simultaneous linear and non-linear equations, ordinary differential equations including high-order and non-linear types, optimization and least-squares methods such as non-linear equations. Those equations can be entered in any order, and there is no need to modify the equations or transpose them. Calculation procedures are automatically selected and applied. To solve simultaneous non-linear equations, for instance, the iterative method is generally necessary. EQUATRAN-G is able to identify whether the simultaneous equations are linear or non-linear and select a calculation method to solve them. It allows users to specify variable names as well as equations that are used to check the convergence. As for ordinary differential equations, the high-order equations can be written by simply describing one statement that specifies integral calculations, and this is done without having to modify the equations. For optimization calculations, users need to specify only independent and evaluation variables.

EQUATRAN-G can also be used to solve compound-complex problems with a combination of ordinary differential equations and linear/non-linear equations, the simultaneous non-linear equations involved in the calculation of an optimization problems, etc. More complex problems, such as multiple integrals, two-point boundaries value and mini-max problems, parameter identification in dynamic simulation, can be solved with user functions that are described by EQUATRAN-G.

Model Descriptions

EQUATRAN-G features a variety of functions for easy model descriptions as follows:

Array Variables -- One and two-dimensional array variables are used.

Built-in Functions -- Thirty-six different kinds of functions, including logarithmic, trigonometric and exponential functions, etc. are incorporated.

Tables -- When a diagram or a table is given to show the relationships between variables, they are defined by using a TABLE statement and described in equations like a function.

Conditional Equations -- The equations where expressions on the right side change depending on certain conditions can be described.

User Functions and Macros – Modules are available for the description of large-scale models.

Graphing and Report Creating Functions

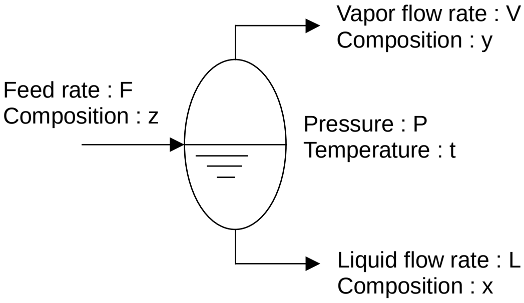
A variety of graphing functions are available for use in the science and technology field, including semi-logarithmic and logarithmic scale graphs, interpolation by spline curves, curve-fitting by linear, quadratic and cubic equations, etc. Graphs are easily created by the AutoSetup function, and data can be clearly and concisely displayed on a graph by employing makeup functions. Reports can be easily created since calculation results are represented in the report-form text where data can be entered in any format.

APPLICATION FOR DISTILLATION

Example 1 Equilibrium Flash Calculation

Problem

The heated ternary liquid mixture of benzene, toluene and xylene with the mole fractions of 0.4, 0.4 and 0.2, respectively are fed continuously into a vapor-liquid separator at the feed rate of F=100 kgmol/h. The temperature of the separator is t=118°C and the pressure is *P*=1140 mmHg. Calculate the composition and the flow rate of the vapor and liquid phases under these conditions assuming that the mixture is an ideal solution.



Equations

Material balance

$$L + V = F \tag{1}$$

$$Lx_i + Vy_i = Fz_i \tag{2}$$

Liquid vapor equilibrium

$$y_i = K_i x_i \tag{3}$$

$$K_i = p_i^\circ / P \tag{4}$$

Vapor pressure(Antoine equation)

$$\log p_i^\circ = A_i - B_i / (t + C_i) \tag{5}$$

Summation of mole fraction

$$\sum (y_i - x_i) = 0 \tag{6}$$

$(i=1,2,\ldots, N)$

Source text

```
/* Equilibrium Flash Calculation */


LOCAL N = 3  /* Number of components */
VAR F = 100   "Feed rate      [kgmol/h]"..
   ,t = 118   "Temperature         [C]"..
   ,P = 1140 "Pressure          [mmHg]"..
   ,L       "Liquid flow rate[kgmol/h]"..
   ,V         "Vapor flow rate [kgmol/h]"..
   ,z(N) = ( 0.4, 0.4, 0.2 ) ..
              "Feed mole fraction    [-]"..
   ,x(N)      "Liquid mole fraction [-]"..
   ,y(N)      "Vapor mole fraction  [-]"..
   ,K(N)      "K value               [-]"..
   ,p(N)      "Vapor pressure     [mmHg]"..
   ,A(N)      "Antoine constants A"..
   ,B(N)      "Antoine constants B"..
   ,C(N)      "Antoine constants C"

/* Material balance */
L + V = F
L*x + V*y = F*z

/* Liquid vapor equilibrium */
y = K*x
K = p/P

/* Antoine equation  p[mmHg], t[C] */
LOG10(p) = A - B/(t+C)

/* Antoine constants (p[mmHg],t[C]) */
    /* Benzene, Toluene and Xylene   */
A = ( 6.90565,  6.95464,  7.00988)
B = ( 1211.03,  1344.80,  1462.27)
C = ( 220.790,  219.482,  215.105)

EQ: SUM(y-x) = 0

RESET L#50 [0,100] BY EQ

OUTPUT L,V,x,y,K
```

Results

```
/* Equilibrium Flash Calculation */


<<   Calculation Results   >>
L       =  56.35664 : Liquid flow rate[kgmol/h]
V       =  43.64336 : Vapor flow rate [kgmol/h]
x       =             : Liquid mole fraction   [-]
  1) 0.2889993   2) 0.4344453   3) 0.2765554
y       =             : Vapor mole fraction   [-]
  1) 0.5433351   2) 0.3555209   3) 0.101144
K       =             : K Value                  [-]
  1) 1.880057   2) 0.8183329   3) 0.3657279
```

Example 2 Teiele-Geddes Method for Distillation

Problem

Calculate the vapor composition, liquid composition and temperature at each stage of the distillation column for separation of pentane and hexane. Constant molar overflow is assumed at each stage. The structure of the distillation column and the operating conditions are listed below.

Structure of distillation column

- Total number of stages N = 10
- Feed stage $N_f = 7$

(The top is the first stage.)

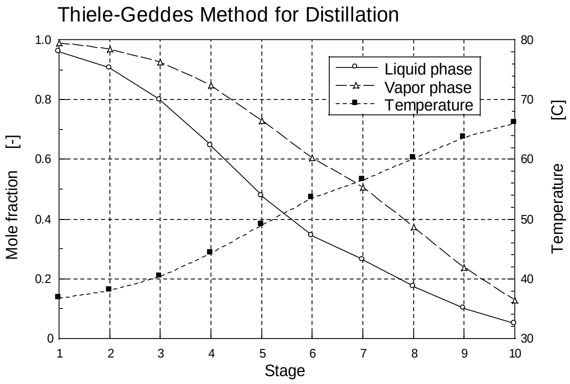
Operating conditions

- Reflux ratio $R = 3$ [-]
- Distillate flow rate $D = 4.8$ [kgmol/h]
- Feed flow rate $F = 10.0$ [kgmol/h]
- Feed mole fraction of pentane $z_f = 0.5$ [-]
- q-value (Liquid ratio of feed) $q = 0.1$ [-]
- Operating pressure $P_{total} = 760$ [mmHg]

Source text

Omitted

Results



Example 3 Batch Distillation

Problem

This is a case of stripping the methanol from a solution containing 22.3 mol% of methanol in the water by the batch distillation column. Calculate the changes in the distillate composition of the column with five ideal stages. (The condenser and reboiler are regarded as one stage.) It is assumed that constant molar overflow is expected within the column and the initial condition is supposed to be the distillation that starts after a sufficiently long time of total reflux operation. The condenser is a total condenser.

Operation Conditions

Reflux ratio	$R = 3$
Flow rate of distillate	$D = 2$ [kgmol/h]
Feed mole fraction of methanol	
	$x_F = 0.2$ [-]

Liquid Holdup

Condenser	$U_1 = 2$ [kgmol]
Each stage	$U_j = 0.1$ [kgmol]
Reboiler	$U_N = 20$ [kgmol]

Equations

Material balance

$$U_1 \frac{dx_{1\,i}}{dt} = -(D+L)x_{1\,i} + Vy_{2\,i} \qquad (1)$$

$$U_j \frac{dx_{j\,i}}{dt} = Lx_{j-1\,i} - \left(Vy_{j\,i} + Lx_{j\,i}\right) + Vy_{j+1\,i}$$

$$(j = 2,3,\cdots,N-1) \qquad (2)$$

$$U_N \frac{dx_{N\,i}}{dt} = Lx_{N-1\,i} - Vy_{N\,i} + Dx_{N\,i} \qquad (3)$$

Total material balance

$$V = D + L \qquad (4)$$

$$\frac{dU_N}{dt} = -D \qquad (5)$$

$$R = \frac{L}{D} \qquad (6)$$

Summation of mole fraction

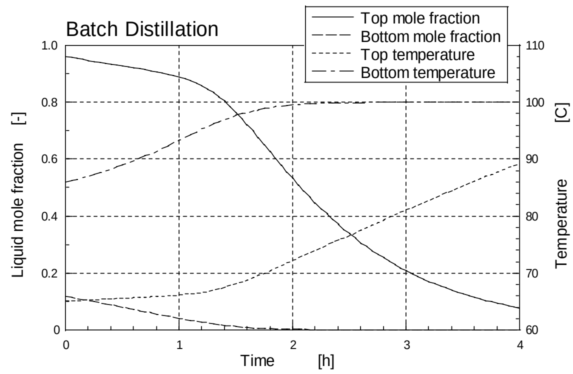
$$\sum_i x_{j\,i} = 1 \qquad (7)$$

$$\sum_i y_{j\,i} = 1 \qquad (8)$$

Source text

Omitted

Results



CONCLUSION

Compared with conventional programming languages, EQUATRAN-G is easy to use, can modify the mathematical models more easily because of the use of equations and can enhance productivity. EQUATRAN-G can also be applied in a variety of areas ranging from balance calculations (e.g., equilibrium flash calculations) to dynamic simulations (e.g., batch distillation calculations).