THE SIMULATION OF MULTIPLE EXTRACTION IN COUNTER CURRENT

T.-M. Sturzu*, and I.-C. Marcu**

abstract: The paper depicts a mathematical algorithm and a TURBO-PASCAL computer programme that permit the effectuation of some calculations for multiple extraction in counter current, using both the Gibbs's triangle (Hunter-Nash method) and the equilibrium diagram (McCabe-Thiele method). The results, which were got on the computer, are in accordance with those obtained by hand execution of the graphical constructions. The depicted algorithm can simplify the hand graphic construction work.

Theoretical Aspects

Multiple extraction in counter current represents the largest used method because, owing to the circulation in counter current of the extractive solvent and of the initial mixture, it is assured a high degree of separation and a reasonable use of the solvent; the method can be made in differential contact equipment [1].

For a ternary mixture with A - the primary solvent, S - the extraction solvent, absolutely immiscible, and B, the useful substance, in the hypothesis that the mixture respects Nernst rule, one can calculate analytically the number of contact steps, applying the equilibrium relation and material balance's conditions for successive contact steps.

Whether the A and B substances are partly immiscible, calculations are graphic effectuated using Gibbs's triangle and *Hunter-Nash method* [2]. Knowing the composition for the mixture that is going to be separated (F point in Fig. 1), its flow, its composition (S), the flow of the solvent and having the equilibrium data, one can get the composition of the final extract (E), joining R point, which expresses the final composition of the refined mixture, with M point that is situated on FS straight line; the position of M point depends on the mixing rapport solvent-to-initial mixture; E point is situated at the intersection of RM straight line with the extract's branch of the saturation isotherm. At the intersection of FE and RS straight lines, there is the operating pole, P.

Through E point, one draws $1 - 1'$ conodum; point 1 from the refined mixture's branch is joined with the operating pole; its intersection with the extract's branch represents $2'$ point; trough this point one draw $2 - 2'$ conodum and so on, until intersection point with the

* Department of Environment Protection, Technical University of Iassy, 73A, D. Mangeron street, 6600 Iassy
** Department of Chemical Technology and Catalysis, Faculty of Chemistry, University of Bucharest, P.O. - Box 12 - 241, Bucharest. E-mail: icmarcu@chem.unibuc.ro

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extract's branch position is situated under R point or at the same place. The optimal value of solvent/initial mixture rapport is determined out of economical principles, taking into account the price of equipment and the damage of solvent [3].

McCabe-Thiele method for the determination of contact step's number for multiple extraction in counter current is, somehow, alike the same method for the fractional distillation. In accordance with this method (Fig. 2), one draws the equilibrium curve $y_B=f(x_B)$ in a rectangular graphic. For the drawing of the operating curve, the points are got with Gibbs triangle's help, drawing through the pole a number of sectional straight lines. Their intersection with the two branches of the saturation isotherm determine the desired values ($y_{B,i}$ and $x_{B,i}$).

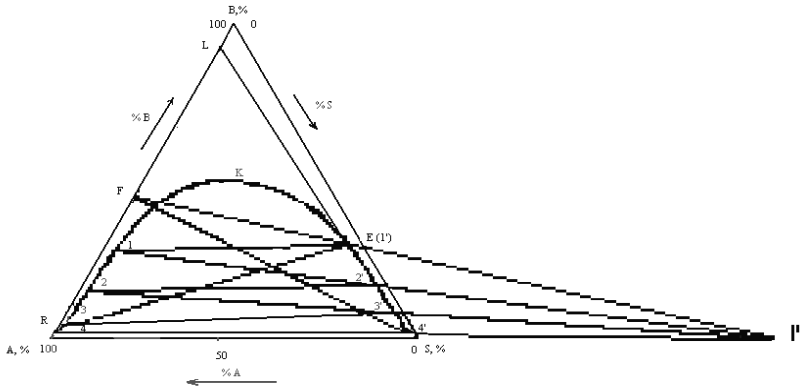

Fig. 1. *The simulation of the calculations for multiple extraction in counter current using Gibbs's triangle.*

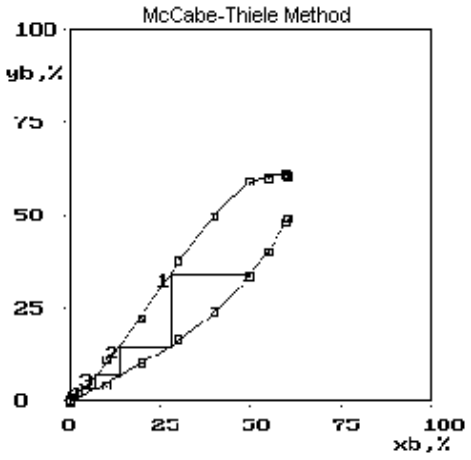

Fig. 2. *The simulation of the calculations for multiple extraction in counter current using McCabe-Thiele method*

The equilibrium curve and the operating one are drawn on the same graphic, and the number of horizontal segments of the graphic construction, in the interval $x_{B,F} - x_{B,R}$, gives the number of theoretical extractive steps.

If A and B substances are absolutely immiscible [2], operating curve becomes a straight line whose slope is:

$$\mathrm{tg}\alpha = \frac{\text{A quantity}}{\text{S quantity}} \tag{1}$$

Distinctive Features of the Simulation for the Solving of Multiple Extraction in Counter Current Problems Using Graphical Methods

The main difficulty of Hunter-Nash method's simulation is the fact that it is rather difficult to elaborate a mathematical method, which is to provide some regressive equation's coefficients in a ternary system.

For eliminating this difficulty, we proposed a model [4], that was applied in industry by other authors [5], named *rectangular-triangular model for liquid-liquid equilibrium in ternary systems*, model which is based on the variable's change:

$$x_A^* = 100 - x_A - x_B / 2 \tag{2}$$

Thus, both in Gibbs triangle and in associated rectangular system, the graphical representations have to be the same. The relation for the extract branch is analogous.

In principle, the simulation of multiple extraction in counter current problems follows the graphical construction depicted in Fig. 1. First of all, one determines the regressive polynomial equation's degree, both for extract's and for refined mixture's branch, that are branches of the saturation isotherm [6]. Then, one determine the polynomial regressive equation's coefficients whose type is:

$$x_B = b_0 + b_1 x_A^* + b_2 x_A^{*2} + b_3 x_A^{*3} \tag{3}$$

where x_A^* are modified equilibrium data in accordance with relation (2). Using this algorithm and relation (2), the form of saturation isotherm is indeed the same in the two systems, thus being possible the analytical treatment of the problems. One also uses analytical geometrical relations [7] that permit the construction depicted in Fig. 1.

McCabe-Thiele method is simpler for the analytical transposition, owing to the use of a rectangular co-ordinates axes system; the simulation realizes the construction depicted in fig. 2, using the algorithm for the determination of a regressive polynomial equation for determining the equations of the two curves [9], and usual analytical geometrical relations that permit a variable drawing of the graphical construction on the display screen, in accordance with the input data. The stages of the algorithm were previously depicted.

The Presentation of the Principal Modules of the Program that Realizes the Simulation

The TURBO-PASCAL program assures the codification of an algorithm that realizes the correlative analysis for equilibrium data, the determination of the regressive equation's

Table 1. Principal modules of the TURBO-PASCAL program

```
Procedure curba(pxmin,pxmax,gr:byte;b,xd:vectx);
 var xmin,xmax,xc,yc,corectie,fsc,pas:real;xg,yg:word;
 begin
 fsc:=2;if cod<10 then corectie:=sin(pi/3) else corectie:=1;
 xmin:=xd[pxmin];xmax:=xd[pxmax];pas:=1/fsc;xc:=xmin-pas;
 repeat
 xc:=xc+pas;yc:=b[1];
 for j:=2 to gr+1 do yc:=yc+b[j]*putp(xc,j-1);
 if yc>=0 then plot(xcen+round(xc*fsc),ycen+round(fsc*corectie*yc));
 until xc>=xmax;
 readkey;
 end;

procedure ecdr1ppd(panta,xd,yd:real;var a0,a1:real);
 begin
 a1:=panta;a0:=yd-a1*xd;
 end;

procedure linieh(x1,y1,x2,y2:real);
 var dx,dy:real;
 begin
 plot(xcen+round(2*x1),ycen+round(2*y1*sin(pi/3)));
 dx:=2*(x2-x1);dy:=2*(y2-y1)*sin(pi/3);
 dr(round(dx),round(dy));
 end;

procedure drfs(var f0,f1:real); {traseaza dreapta fs si returneaza
ecuatia}
 begin
 col(lightcyan); scrish(3,xas,xbs-5,'S');
 scrish(2,xbf/2,xbf,'F');linieh(xbf/2,xbf,xas,xbs);
 ecdr2p(xas,xbs,xbf/2,xbf,f0,f1);readkey;
 end;

function lungseg(x1,y1,x2,y2:real):real;
 var dx,dy,int:real;
 begin
 dx:=abs(x2-x1);dy:=abs((y1-y2)*sin(pi/3));
 int:=sqrt(putp(dx,2)+putp(dy,2));lungseg:=int;
 end;

procedure exls(x1,y1:real;var la,lb:real);
 var xas,a0,a1:real;
 begin
 xas:=100-xss-xbs;xas:=100-xas-xbs/2;
 ecdr2p(xas,xbs,x1,y1,a0,a1);
 pint2d(a0,a1,0,2,la,lb);col(red);
 linieh(la,lb,xas,xbs);scrish(2,la,lb,'L');
 end;

procedure conhn;
var ajuns:boolean;coin,cof,ntr:byte;
begin
 extr[1,1]:=xae;extr[1,2]:=xbe;i:=1;cod:=4;ajuns:=false;
 repeat
 i:=i+1;col(lightmagenta);
 conoda(xae,xbe,xg,yg);linieh(xae,xbe,xg,yg);scrish(1,xg,yg,stru(i-1));
 raf[i-1,1]:=xg;raf[i-1,2]:=yg;if yg<=yr then ajuns:=true;
 if not ajuns then begin
 readkey;ecdr2p(xg,yg,xpol,ypol,a0,a1);
 intdrcb(2,gre,be,a0,a1,xg1,yg1);
 linieh(xg,yg,xg1,yg1);linieh(xg1,yg1,xpol,ypol);
 scrish(1,xg1,yg1,stru(i)+"");
 extr[i,1]:=xg1;extr[i,2]:=yg1;xae:=xg1;xbe:=yg1;readkey;
 end;
 until ajuns;
 ntr:=i-1;
 if codop=1 then begin coin:=42;cof:=80;
 end else begin coin:=1;cof:=45;end;
 writer(14,coin,cof,2,0,1,'Compositions of phases in each step (%):');
 scrisech(1,14,coin,cof);
 if ntr<11 then for i:=2 to ntr do scrisech(i,14,coin,cof)
 else scrisech(ntr,16-ntr,coin,cof);readkey;
end;

procedure scrish(kod:byte;xd,yd:real;sir:string);
var dx:integer;
begin
 if kod=1 then dx:=-4 else if kod=2 then dx:=-8 else dx:=4;
writexy(xcen+round(2*xd)+dx,ycen+8+round(2*yd*sin(pi/3)),0,1,sir);
 end;

procedure mccabe;
var xop,yop,bop:vectx;grop:byte;
 xta,yta,xta1,yta1:real;
begin
 ycen:=30;col(lightmagenta);
 writexy(xcen+50,239,0,1,' McCABE – THIELE METHOD');
 col(lightgray);readkey; plot(xcen,30);dr(200,0);dr(0,200);
 dr(-200,0);dr(0,-200);
 col(yellow);for i:=1 to 5 do begin plot(xcen+(i-1)*50,27);
 writexy(xcen-4+(i-1)*50,20,0,1,stru((i-1)*25));end;
 for i:=1 to 5 do begin plot(xcen-3,30+(i-1)*50);
 writexy(xcen-30,33+(i-1)*50,0,1,stru((i-1)*25));end;
 writexy(xcen+180,10,0,1,'xb,%'); writexy(xcen-35,210,0,1,'yb,%');
 cod:=11;col(lightmagenta);puncte(xb,yb);
 readkey;coeficienti(xb,yb,br,grr);
 curba(1,n,grr,br,xb);
 for i:=1 to n do begin
 xop[i]:=xb[i];ecdr2p(xa[i],xb[i],xpol,ypol,a0,a1);
 intdrcb(2,gre,be,a0,a1,xg,yop[i]);
 end;
 coeficienti(xop,yop,bop,grop);timp(0);
 col(lightcyan);puncte(xop,yop);curba(1,n,grop,bop,xop);
 readkey;i:=0;
 xta:=xbf;yta:=calculy(grop,xta,bop);col(red);
 repeat
 i:=i+1;timp(0);
 intdrcb(1,grr,br,yta,0,xta1,yta1);
 plot(xcen+round(2*xta),ycen+round(2*yta));
 dr(round(2*(xta1-xta)),0);
 writexy(xcen-8+round(2*xta1),ycen+round(2*yta1),0,1,stru(i));
 if yta1>xbr then begin
 xta:=xta1;yta:=calculy(grop,xta,bop);
 plot(xcen+round(2*xta1),ycen+round(2*yta1));
 dr(0,round(2*(yta-yta1)));
 end; readkey;
 until (yta1<=xbr) or (yta<0.75*xbr);
end;

{ P R I N C I P A L C O M P O U N D I N S T R U C T I O N }
'm':BEGIN
 initgraph(gd,gm,pdriver);cleardevice;
 cod:=3;coeficienti(xa,xb,br,grr);cod:=4;coeficienti(ya,yb,be,gre);
 ecdr2p(xas,xbs,xbf/2,xbf,b0,b1);
 xm:=xas-(xas-xbf/2)*ksol/(1+ksol);ym:=f0+f1*xm;
 ym:=xbs+(xbf-xbs)*ksol/(1+ksol);
 intdrcb(1,grr,br,xbr,0,xr,yr);ecdr2p(xr,yr,xm,ym,c0,c1);
 intdrcb(2,gre,be,c0,c1,xae,xbe);ecdr2p(xbf/2,xbf,xae,xbe,a0,a1);
 ecdr2p(xr,yr,xas,xbs,b0,b1);pint2d(a0,a1,b0,b1,xpol,ypol);
 if xpol>0 then codop:=1 else codop:=2;
 if codop=1 then begin
 xcen:=40;ycen:=270; end else begin
 xcen:=390;ycen:=270;
 end;
 if codop=1 then writer(2,20,80,1,3,2,'HUNTER-NASH METHOD') else
 writer(2,1,60,1,3,2,'HUNTER-NASH METHOD');triunghi(cod);
 col(blue);puncte(xa,xb);col(red);puncte(ya,yb);
 col(lightblue);curba(1,n,grr,br,xa);col(lightred);curba(n,1,gre,be,ya);
 col(black);rect(xcen+203,ycen-8,40,8,9);drfs(f0,f1);
 scrish(1,xm,ym,'M'); key:=readkey;ecdr2p(xr,yr,xm,ym,b0,b1);
 scrish(2,xr,yr,'R');linieh(xr,yr,xm,ym);readkey;
 linieh(xm,ym,xae,xbe);scrish(3,xae,xbe,'E');readkey;
 linieh(xr,yr,xas,xbs);key:=readkey;linieh(xr,yr,xpol,ypol);readkey;
 linieh(xbf/2,xbf,xae,xbe);readkey;linieh(xae,xbe,xpol,ypol);
 scrish(1,xpol,ypol,'P');readkey;conhn;
 mccabe;col(lightcyan);timp(0);readkey;
END;
```

coefficients for the two branches of the saturation isotherm in rectangular system associated to the Gibbs triangle, respectively the regressive equations for the two curves in the case of McCabe-Thiele method. One realizes then the graphical constructions depicted in Fig. 1 and 2, being displayed only the essential data that had been implicitly calculated, especially the composition of the two phases (extract and refined mixture) for each contact step.

For determining the point of intersection of a straight line with a curve we used the *halving interval method*, because we couldn't know exactly the polynomial regressive equation's degree, and owing to the possibility of using regressive equations that are different from the polynomial ones [9]. Though the effort of calculation is higher, this method is safer owing to its better possibility of adaptation at different types of regressions.

For realizing the two depicted graphical constructions we used the program which permits their display and shows the compositions for each extractive step. The principal modules of the programme are presented in Table 1.

Results and their Interpretation

Having as an aim the validation of calculating algorithm and of the proposal programme we take into account the extraction of acetone out of an initial mixture acetone-water with 50% (weight) acetone, using as an extractive solvent pure chlorbenzene. We worked with 100 g initial mixture. Equilibrium data for the ternary system acetone-water-chlorbenzene were those from the specialized literature [8]. One imposed that the refined mixture must contain max. 2% acetone. We made then the hand construction of the graphics and the simulation at the computer. Using *Hunter-Nash method*, for the branches of the saturation isotherm there have been obtained, in rectangular system of co-ordinates associated to Gibbs's triangle, the regressive equation's coefficients. Using a similar algorithm, we got the regressive equations for equilibrium and operating curves for *McCabe-Thiele method.*

Using the program we can reproduce the graphical construction depicted in Figs. 1 and 2, for any correct input data; for stimulation there were used usual analytical geometrical relations. For the considered example, we got 4 contact steps and the compositions of the two phases (extract and refined mixture) for each extractive step. They are depicted in Table 2.

Table 2. The obtained results for the phase composition in each extractive step

No. of step	RAFINED MIXTURE			EXTRACT		
	% water	% acetone	% chlorbenzene	% water	% acetone	% chlorbenzene
1.	72.98	26.67	0.35	1.01	32.58	66.41
2.	86.87	13.10	0.03	0.31	14.36	85.32
3.	94.31	5.57	0.12	0.33	5.99	93.69
4.	98.01	1.78	0.21	0.39	1.85	97.76

Comparable results were obtained both experimentally and by hand drawing of graphical constructions. We note that the time for the graphics elaboration is about two hours, while at the computer the results are obtained in only a few seconds, and also that at less values of

the concentrations, hand graphical constructions are considerably influenced by the executor's ability, being subjective and generating errors.

Conclusions

a) The paper depicts a mathematical algorithm and a TURBO-PASCAL computer programme that permit the effectuation of some calculations for multiple extraction in counter current, using both the Gibbs's triangle (Hunter-Nash method) and the equilibrium diagram (McCabe-Thiele method).

b) The results that were got on the computer are in accordance with those obtained by hand execution of the graphic constructions.

c) The depicted algorithm can simplify the hand graphic construction work.

d) The elaborated programme can be used both in industry and in researching units for calculations and in instructional units as a didactic facility.

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