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AUTOMATIC DETERMINATION OF THE MINERAL COMPOSITION OF THE PORTLAND CEMENT CLINKER

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Abstract:
This paperwork points out software for the automatic determination of the mineral composition of the cement clinker. Although they have rather similar oxide composition, the mineral structure may be rather different and it influences the quality of the cement. Therefore, the software we suggest allows the fast determination of the mineral composition and any method of improvement, according to the required properties of the Portland cement.
Keywords:
cement, mineral composition, clinker, software.

1. INTRODUCTION

According to the balance diagrams [1], we are able to calculate the basic composition of the clinkers. This calculation is possible if the cement turns solid in case of both termic-dynamic and non termic-dynamic balance.

In case of the complete balance solid state, the product does not turn glassy. In fact, there is no termic-dynamic balance in case of the solid state, and if we consider that possibility, the mineral composition we calculate according to that hypothesis is a potential composition – it is possible only if the chemical composition is not equal to the real mineral composition (of those minerals that make up the composition).

a) Presuming that the clinkers are situated in the termical balance sub-system C_3S-C_2S-C_3A-C_4AF ($M_{Al} > 0,64$), Bogue has determined that we could calculate the mineral elements according to the following formula:

$$\begin{aligned} \%C_4AF &= 3,04\%Fe_2O_3 \\ \%C_3A &= 2,65\%Al_2O_3 - 1,69\%Fe_2O_3 \\ \%C_3S &= 4,07\%CaO - 7,60\%SiO_2 - 6,72\%Al_2O_3 - 1,42\%Fe_2O_3 \\ \%C_2S &= 8,60\%SiO_2 + 5,06\%Al_2O_3 + 1,07\%Fe_2O_3 - 3,05\%CaO \end{aligned} \quad (1)$$

b) For the clinkers in the termic balance sub-system C_3S-C_2A-C_4AF-C_2F ($M_{Al} < 0,64$), the result is based on Bogue's analogical argument. Thus:

$$\begin{aligned} \%C_4AF &= 4,76\%Al_2O_3 \\ \%C_2F &= 1,70\%Fe_2O_3 - 2,65\%Al_2O_3 \\ \%C_3S &= 4,07\%CaO - 7,60\%SiO_2 - 4,48\%Al_2O_3 - 2,84\%Fe_2O_3 \\ \%C_2S &= 8,60\%SiO_2 + 3,36\%Al_2O_3 + 2,14\%Fe_2O_3 - 3,05\%CaO \end{aligned} \quad (2)$$

c) For the intermediary case of the clinkers belonging to the C_3S-C_2A- -C_4AF ($M_{Al}= 0,64$), we have:

$$\begin{aligned} \%C_4AF &= 3,04\%Fe_2O_3 \\ \%C_3S &= 4,07\%CaO - 7,60\%SiO_2 - 5,70\%Fe_2O_3 \\ \%C_2S &= 8,60\%SiO_2 - 4,30\%Fe_2O_3 - 3,05\%CaO \end{aligned} \quad (3)$$

The relations according to Bogue are particular and they use some coefficients specific to the termical balance sub-systems:

$$\begin{aligned} &C_3S\text{-}C_2S\text{-}C_3A\text{-}C_4AF \text{ with } M_{Al} > 0,64 \\ &C_3S\text{ -}C_2A\text{-}C_4AF\text{- }C_2F \text{ with } M_{Al} < 0,64 \\ &C_3S\text{ -}C_2A\text{-}C_4AF \text{ with } M_{Al} = 0,64 \end{aligned} \quad (4)$$

These relations are not valid for other termic balance sub-systems. Considering all these facts,

we have come up with software who determines the composition for each stage of the clinker, for both mineral composition of the dust and the termic balance sub-system. We made the software by generalizing the following example which was based on the weight survey. We are going to describe it in the following.

2. THE SO-CALLED SOFTWARE

```
software CompClincher;
uses Crt, Graph, UApp;
const Mc = 56; Ma =102; Ms =60; Mf =160;
Var
  CaO, Al2O3, SiO2,Fe2O3 :  Real;
  SCaO, SAl2O3, SSiO2, SFe2O3 :  String;
  Paragenesis : String;
  M :array[1..4] of real; N:array[1..4,1..4] of Byte ; X:array[1..4] of real;
  B:array[1..4] of real; A:array[1..4,1..4] of real;

procedure Init;
 begin
   Title('Determination of the portland cement clinker for each stage');
   DefineBtn(  0,  10,  55, 620, 393, 0, 0, '', '', Off);
   { define the main menue buttons }
   DefineBtn( 10,  10,  26,  60,  19,  2,  1, 'Info',
    'General information about the software', Off);
   DefineBtn( 11,  75,  26,  60,  19,  2,  1, 'Calculation',
    'Determination of the stage composition ', Off);
   DefineBtn( 12, 570,  26,  60,  19,  2,  5, 'Exit',
    'Stop the software', Off);
   SCaO:='';
   DefineInp(1,100,100,320,30,50,'% CaO ',SCaO);
   SAl2O3:='';
   DefineInp(2,100,130,320,30,50,'% Al2O3 ',SAl2O3);
   SSiO2:='';
   DefineInp(3,100,160,320,30,50,'% SiO2 ',SSiO2);
   SFe2O3:='';
   DefineInp(4,100,190,320,30,50,'% Fe2O3 ',SFe2O3);
   Paragenesis:='';
   DefineInp(5,100,220,320,30,200,'Paregenesis ',Paragenesis);
end;

procedure Info;
 begin
 end;

procedure Calculation;
Var I,J,K,L: Integer; S:String[10]; Code,MM,Poz :Integer; T:Real;
    Sform: array[1..4] of  string[15]; SS:string; Sf: array[1..4] of  string[15];
begin
   Drawinp(1); Drawinp(2); Drawinp(3); Drawinp(4); Drawinp(5);
   Inp(1); Inp(2); Inp(3); Inp(4); Inp(5);
   Val(SCaO,CaO,Code); Val(SAl2O3, Al2O3,Code); Val(SSiO2,SiO2,Code); Val(SFe2O3,Fe2O3,Code);
   for i:=1 to 4  do
    for j:=1 to 4 do
      N[i,j]:=0;
   Insert('-',Paragenesis,length(Paragenesis)+1);
   K:=1;
   for i:=1 to 4 do
    begin
        while (Paragenesis[k]<>'-')  do
        begin
         if Paragenesis[k]='C' then
           begin
            Inc(k);
            if (Paragenesis[k]>='A') and (Paragenesis[k]<='S') or (Paragenesis[k]='-') then
              N[i,1]:=1
             else
              begin
               if (Paragenesis[k+1]>='0') and (Paragenesis[k+1]<='9') then
                 begin
                   S:=Copy(Paragenesis,k,2); Inc(K);
                 end
                 else
                   S:=Copy(Paragenesis,k,1);
               Val(S,N[i,1],Code);
```

```
            Inc(K);
          end;
        end;
      if Paragenesis[k]='A' then
       begin
        Inc(k);
        if (Paragenesis[k]>='A') and (Paragenesis[k]<='S') or (Paragenesis[k]='-') then
          N[i,2]:=1
        else
         begin
          if (Paragenesis[k+1]>='0') and (Paragenesis[k+1]<='9') then
           begin
             S:=Copy(Paragenesis,k,2); Inc(K);
           end
           else
             S:=Copy(Paragenesis,k,1);
          Val(S,N[i,2],Code);
          Inc(K);
         end;
        end;
       if Paragenesis[k]='S' then
       begin
        Inc(k);
        if (Paragenesis[k]>='A') and (Paragenesis[k]<='S') or (Paragenesis[k]='-') then
          N[i,3]:=1
        else
         begin
          if (Paragenesis[k+1]>='0') and (Paragenesis[k+1]<='9') then
           begin
             S:=Copy(Paragenesis,k,2); Inc(K);
           end
           else
             S:=Copy(Paragenesis,k,1);
          Val(S,N[i,3],Code);
          Inc(K);
         end;
        end;
    if Paragenesis[k]='F' then
        begin
        Inc(k);
        if (Paragenesis[k]>='A') and (Paragenesis[k]<='S') or (Paragenesis[k]='-') then
          N[i,4]:=1
        else
         begin
          if (Paragenesis[k+1]>='0') and (Paragenesis[k+1]<='9') then
           begin
             S:=Copy(Paragenesis,k,2); Inc(K);
           end
           else
             S:=Copy(Paragenesis,k,1);
          Val(S,N[i,4],Code);
          Inc(K);
         end;
        end;
      end;
      Inc(k);
  end;
 for I:=1 to 4 do
    M[I]:=N[I,1]*Mc+N[I,2]*Ma+N[I,3]*Ms+N[I,4]*Mf;
 B[1]:= CaO/Mc;
 B[2]:= Al2O3/Ma;
 B[3]:= SiO2 /Ms;
 B[4]:= Fe2O3 /Mf;
 for I:=1 to 4 do
     begin
       A[i,1]:=N[1,i]/M[1]; A[i,2]:=N[2,i]/M[2]; A[i,3]:=N[3,i]/M[3]; A[i,4]:=N[4,i]/M[4];
     end;
 Mm:=4;
 for k:=1 to mm do
 begin
  if a[k,k]=0 then
   begin
    j:=k+1;
    while (j<=mm) and ( a[j,k]=0) do j:=j+1;
    if j<=mm then
```

```
     begin
      for l:=k to mm do
      begin
        t:=a[k,l]; a[k,l]:=a[j,l]; a[j,l]:=t;
      end;
      t:=b[k];
      b[k]:=b[j];
      b[j]:=t;
    end
    else
     begin
      Outtextxy(100,500,'The system cannot be solved by Gauss' method');
      Halt;
    end;
  end;
  for i:=k+1 to mm do
   begin
      for j:=k+1 to  mm do
      a[i,j]:=a[i,j]- a[k,j]*a[i,k]/a[k,k]; b[i]:=b[i]-b[k]*a[i,k]/a[k,k];
   end;
end;
x[mm]:=b[mm]/a[mm,mm];
for k:=mm-1 downto 1 do
 begin
  t:=0;
  for j:=k+1 to mm do t:=t+a[k,j]*x[j] ;
  x[k]:=(b[k]-t) /a[k,k];
 end;
j:=0;
k:=1;
poz:=1;
for i:=1 to length(Paragenesis) do
  if Paragenesis[i] <>'-' then   Inc(j)
   else
     begin
      Sform[k]:=copy(Paragenesis,poz,j);
      poz:=i+1;
      Inc(K);
      j:=0;
     end;
Str(x[1]:6:3,Sf[1]);
Str(x[2]:6:3,Sf[2]);
Str(x[3]:6:3,Sf[3]);
Str(x[4]:6:3,Sf[4]);
SS:='';
DefineInp(10,90,260,350,30,0,'The stage composition of the clinker is:',SS);
DrawInp(10);
SS:=SF[1];
DefineInp(6,100,300,320,30,100,'% '+Sform[1]+'  ',SS);
DrawInp(6);
SS:=SF[2];
DefineInp(7,100,330,320,30,100,'% '+Sform[2]+'  ',SS);
DrawInp(7);
SS:=SF[3];
DefineInp(8,100,360,320,30,100,'% '+Sform[3]+'  ',SS);
DrawInp(8);
SS:=SF[4];
DefineInp(9,100,390,320,30,100,'% '+Sform[4]+'  ',SS);
DrawInp(9);
 WaitEsc;
end;

procedure Run;
  begin
   { Start main menu }
   MainSel := 10;
   repeat
    ClearClient;
    HMenu(10, 12, MainSel);
    case MainSel of
      10: Info;
      11: Calculation;
    end;
   until MainSel = 12;
 end;
```

```
procedure Done;
 begin
  EndGraph;
  DoneButtons;
 end;

begin
 Init;
 Run;
 Done;
end.
```

3. CALCULATION EXAMPLE

Considering a quaternary mix with the composition 66,7% CaO; 21,4% SiO_2; 6,9% Al_2O_3; 5% Fe_2O_3 and knowing that this mixture belongs to the paragenesis C_3S-C_2S-C_3A-C_4AF – in case it reaches a balance – we have to establish the stage composition of the clinker.

During the crystallizing processes, the weight of the mixture is constant. When we perform the weight survey for each of the four oxides, we have:

$$\begin{cases} m_{CaO_{iniţial}} = m_{CaOdinC_3S} + m_{CaOdinC_2S} + m_{CaOdinC_3A} + m_{CaOdinC_4AF} \\ m_{SiO_{2iniţial}} = m_{SiO_2dinC_3S} + m_{SiO_2dinC_2S} \\ m_{Al_2O_{3iniţial}} = m_{Al_2O_3dinC_3A} + m_{Al_2O_3dinC_4AF} \\ m_{Fe_2O_{3iniţial}} = m_{Fe_2O_3dinC_4AF} \end{cases} \quad (5)$$

Considering that:

$$\begin{aligned} M_{C_3S} &= 3\cdot 56 + 60 = 228 \\ M_{C_2S} &= 2\cdot 56 + 60 = 172 \\ M_{C_3A} &= 3\cdot 56 + 102 = 270 \\ M_{C_4AF} &= 4\cdot 56 + 102 + 160 = 486 \end{aligned} \quad (6)$$

And that: x = $\%C_3S$; y = $\%C_2S$; z = $\%C_3A$ şi u = $\%C_4AF$, we have:

$$66{,}7 = x\frac{3\cdot 56}{228} + y\frac{2\cdot 56}{172} + z\frac{3\cdot 56}{270} + u\frac{4\cdot 56}{486} \quad (7)$$

$$21{,}4 = x\frac{60}{228} + y\frac{60}{172}$$

$$\left.\begin{aligned} 6{,}9 &= z\frac{102}{270} + u\frac{102}{486} \\ 5 &= u\frac{160}{486} \qquad \Rightarrow u \end{aligned}\right\} \Rightarrow z \quad (8)$$

$$x + y + z + u = 100$$

After the calculation, we have:

$$\begin{aligned} u &= 15{,}19\ \%C_4AF \\ z &= 9{,}83\ \%C_3A \end{aligned} \quad (9)$$

If we replace the „u" and the „z" from the first equation, we have:

$$\begin{cases} x + y = 74{,}98 \\ \frac{60}{228}x + \frac{60}{172}y = 21{,}4 \end{cases}$$ and we calculate:

$$\begin{aligned} x &= 55{,}56\ \%C_3S; \\ y &= 19{,}42\ \%C_2S \end{aligned} \quad (10)$$

The software runs if we take the following steps:

Step 1. – *Open dialogue window* made of:

- the name of the software: "Determining the composition of the portland cement clinker for each stage";
- the menu bar with the buttons: "Info", "Calculation" şi "Exit";

- the windows for introducing the primary data: %CaO, %Al2O3, %SiO2, %Fe2O3 and Paragenesis;

Step 2. – *Introduce data* – with the help of the keyboard;

Step 3. – *Data processing* – it begins when we press the "Calculation" key, by selecting the right key from the menu bar. The algorithm is based on the example we have already discussed about, and it turns it into a general rule. Thus, it should:

a) – identify the paragenesis we have used and make another matrix N[i,j], i = 1 ... 4, j = 1 ... 4, where the coefficients of the oxides correspond to the mineral elements;

b) – calculate the molecular weight of each stage:

$$M[i] = N[i,1]*Mc + N[i,2]*Ma + N[i,3]*Ms + N[i,4]*Mf\ ,\ i = 1 \dots 4 \quad (11)$$

c) – calculate the free elements (%oxide/ oxides' molecular weight) and the coefficients of the unknown quantities of the equation system:

$$B[i] = x[1]*A[i,1] + x[2]*A[i,2] + x[3]*A[i,3] + x[4]*A[i,4]\ ,\ i = 1 \dots 4 \quad (12)$$

where:

$$A[i,1] = N[1,i]/M[1];\ A[i,2] = N[2,i]/M[2];\ A[i,3] = N[3,i]/M[3];\ A[i,4] = N[4,i]/M[4]; \quad (13)$$

d) – solving the equation system by Gauss' method;

e) – posting the results;

Step 4. – *Closing the working window* by pressing the "Exit" key or introducing new data and performing a new calculation.

5. CONCLUSIONS

The method and the software we have discussed about in this paperwork allow us to determine the mineral composition of the Portland cement clinker faster. According to the properties of the cement we would like, we can get some useful information about the composition we need for the clinker. Therefore, we can get a finite good of a higher constant quality.

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