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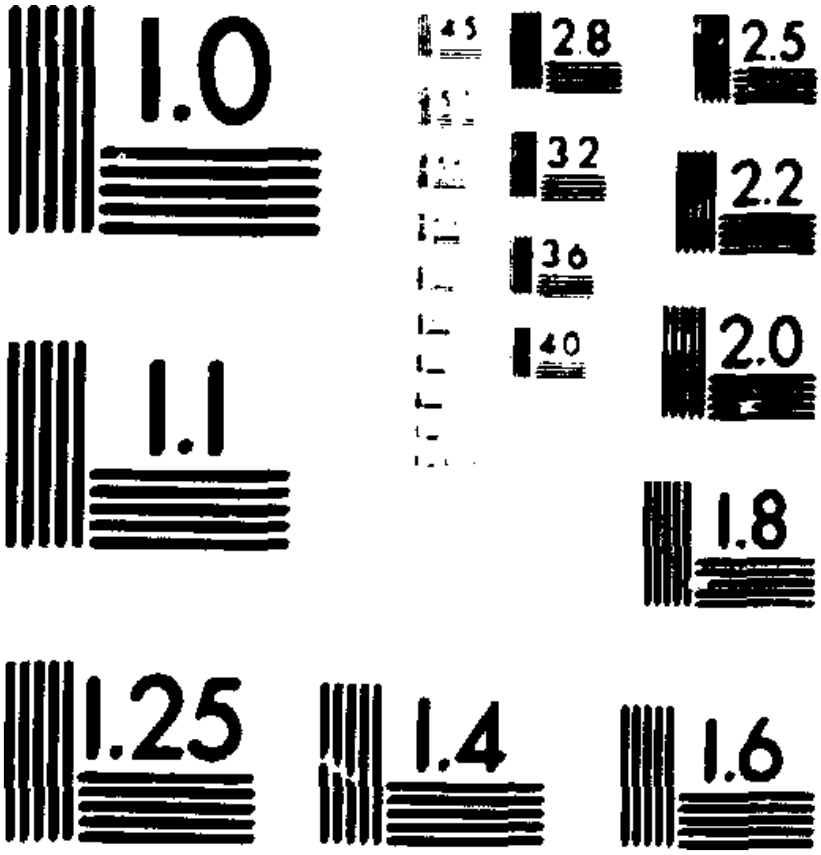

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MATHEMATICAL MODEL OF THE TECHNOLOGY OF THE BAYER ALUMINA MANUFACTURING PROCESS

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3006

ALUTERV-FKI
BUDAPEST
1984

UNITED NATIONS

INDUSTRIAL DEVELOPMENT ORGANIZATION

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ALUTERV-FKI

Budapest

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MATHEMATICAL MODEL OF THE TECHNOLOGY OF THE BAYER ALUMINA MANUFACTURING PROCESS

INTRODUCTION

Demand for aluminium (and consequently its production, too) is the second among the metals, trailing only that for iron but exceeding those of all the classic basic metals like copper, lead, tin, zinc, etc. It is manufactured nearly exclusively by the Hall-Heroult process, i.e. by the electrolysis of alumina in a cryolite melt. On the other hand, some 90 per cent of the basic material of this electrolysis, of the alumina (of which the world production exceeded 30 million tons per annum even during the last recessionary years) is manufactured by one or the other variant of the Bayer process from bauxite. The basis of this process is the digestion of the suitably prepared bauxite in a caustic soda containing liquor and (after separating the components insoluble in the caustic solution) the decomposition of the sodium aluminate liquor in the presence of seed and the subsequent calcination of the crystallized aluminium hydroxide to alumina.

Virtually the only, on a European scale significant mineralogical resource of Hungary is bauxite (not of a high quality but still processable by the Bayer process). Therefore, it is very important to process this ore in the most economic way, at the most favourable technological parameters. This was the reason why the first Hungarian mathematical model of the Bayer process was already elaborated in the mid-60s (when computers were still in their

infancy) in order to help to optimize the operation of the existing alumina plants and the design parameters of the new one, the establishing of which had just been decided.

Because of the complexity and the circuit-character of the Bayer process it is not sufficient to look for the optimum solutions of the unit operations but the whole process (or at least the whole wet section of the process circuit) has to be optimized at the same time, and the optima of all the main process parameters have to be determined by taking into consideration their interrelations. For this purpose it is essential to set up the techno-economical mathematical model of the wet section of the alumina plant.

In the case of designing a new alumina plant the techno-economical model can be divided into four major sections:

a) Calculation of the material flows
b) Calculation of the heat flows
c) Calculation of the investment costs
d) Economic calculations.

These sections can not be sharply divided from each other, the above quadruple structure comes only in its main outlines into display since the calculation of the material flows will require the simultaneous completion of a part of the calorific calculations and both will require some consideration of the investment aspects.

When optimizing the operation of an existing plant the calculation of the investment costs will be replaced by a set of conditions characteristic of the plant in question.

The first two items of the above list - the calculation of the material and heat flows - constitute the technological model, which is the subject of the following description. It has to be mentioned, that the calculation of the heat flows is carried out with a significantly lower accuracy than that of the material flows, first of all as a result of the huge variety of the possible solutions.

1. GENERAL FEATURES OF THE TECHNOLOGICAL MODEL

In order to calculate the material and heat flows the process cycle of the Bayer process had on the one hand to be divided into unit operations (or into their suitable groups) and on the other hand those most important material flows had to be selected, the characteristics of which have to be determined in order to describe unequivocally the process itself. In the course of this a serial number (from 1 to 60) is attached to every important material flow, and ten data are used for the decription of every liquor phase according to the following marking:

N is the total or caustic Na_2O content of the given material according to the actual interpretation, in kg/t alumina,

A is the total Al_2O_3 content of the material, in kg/t alumina,

B is the total mass of the material, in t/t alumina,

V is the total volume of the material, in m^3/t alumina,

W is the heat capacity (or so-called water equivalent) of the material at room temperature, in Mcal/^oC/t alumina,

C is the caustic Na_2O concentration of the material in g/l (only for liquors),

D is the Al_2O_3 concentration of the material in g/l (only for liquors),

M is the molar ratio of the material, in mol caustic Na_2O per mol Al_2O_3 (also only for liquors),

F is the density of the material at room temperature, in t/m^3 and

T is the temperature of the material, in ^oC.

(C, D and M have no meaning for solid materials.)

As it can be observed, the marking system is on the one hand incomplete (since over and above the total mass it gives informations only on two, admittedly the most important two components, the Na_2O and Al_2O_3 contents) and on the other hand redundant, however, it is well proven in practice since it contains every important data. (Only four of the ten data are completely independent, other four can be immediately determined from them in every case, and the remaining two can be calculated by some approaching formulae or by some other method satisfying the accuracy requirements of the mathematical model.)

So according to the marking system of the model A1 means the Al_2O_3 content of the first material stream in kgs at any full cross section of its flow for the time required for the production of 1 t of alumina, C2 is the caustic Na_2O concentration of the second material stream in g/l, F5 is the density of the fifth material stream in t/m^3, etc.

The sequence of calculation of the unit operations is determined by the fact whether the material flows are calculated for 1 t of raw material or 1 t of product. In the first case it is advantageous to start the calculation with the bauxite preparation and digestion, in the second with the precipitation and hydrate filtration. Practical considerations favour the second option. Therefore, the first complex unit operation in the calculation sequence is seeding - precipitaton - hydrate filtration (see Fig.1.),

which can be solved independently after some basic parameters (precipitation time, seeding ratio, concentration and molar ratio of the aluminate liquor, etc.) are given. After calculating the material flows of the precipitation it is expedient to go one step backward in the process cycle to the operation of aluminate liquor cooling. The next complex unit operation to be calculated is that of evaporation - solid caustic dissolving - salt removal, the material flows of which can also be directly determined in the knowledge of the composition of the spent liquor, after fixing the amount of water to be evaporated per tonne of alumina produced.

The other three groups of unit operations of the process cycle, i.e. the bauxite preparation, the digestion and the dilution and red mud settling, and the series of operations of red mud washing connected to the latter can not be calculated directly but only by a series of approximations (iterations) carried out on the basis of the preestimation of three data, suitably of the total Na_2O and Al_2O_3 losses and of a characteristic temperature of the red mud washing system. However, there is no need to calculate the material flows of the bauxite preparation in every iteration step, so the calculation of this unit operation can be left to the end of the calculation sequence.

The material flows of the process cycle have been generally numbered according to the calculation sequence outlined above. The material flows being part of the mathematical model are, arranged in groups, the following (see Fig.1):

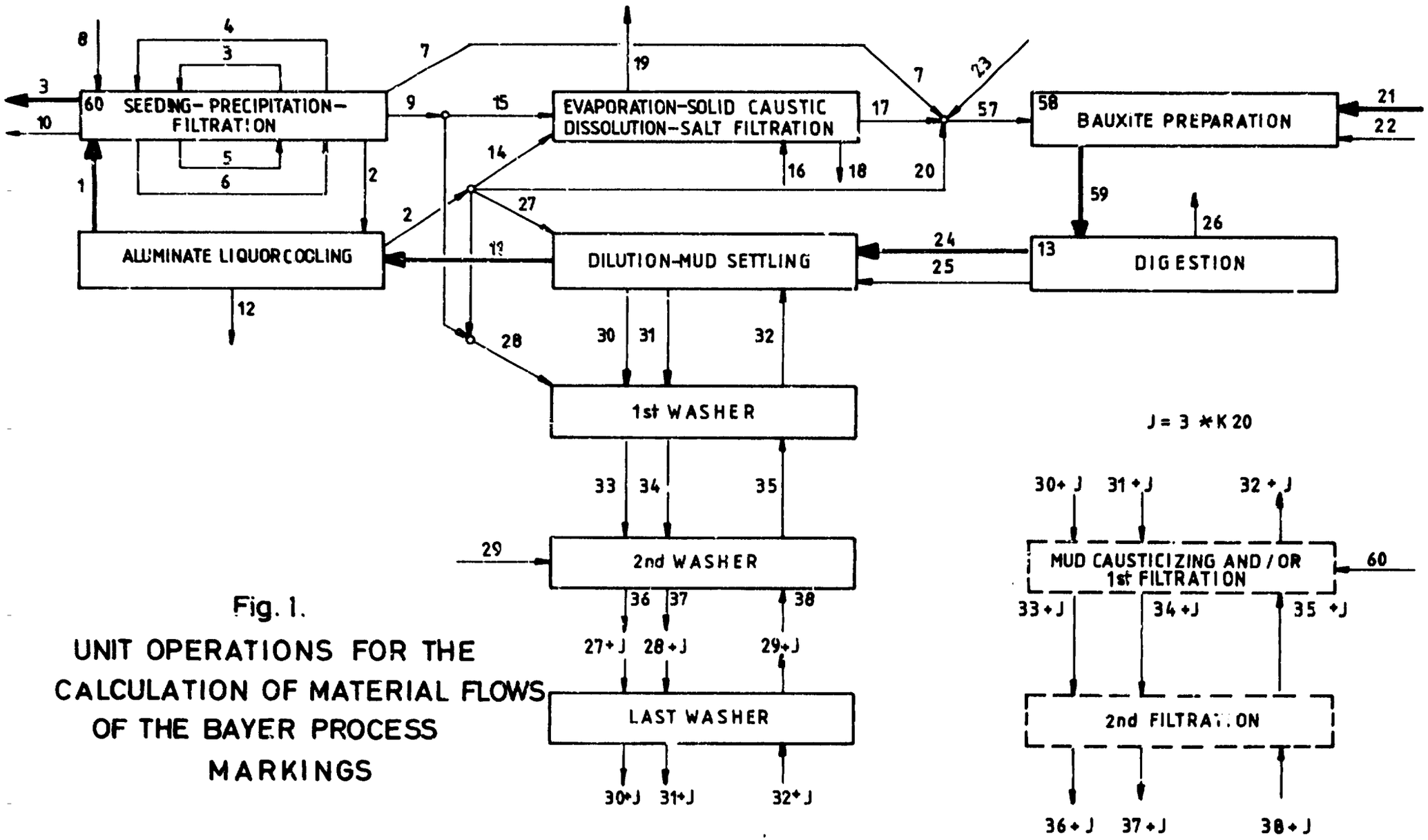

Fig. 1.

UNIT OPERATIONS FOR THE CALCULATION OF MATERIAL FLOWS OF THE BAYER PROCESS MARKINGS

Seeding - precipitation - hydrate filtration:

1. Cooled aluminate liquor (so-called pregnant or green liquor)

2. Spent liquor including the so-called floating hydrate content remaining virtually unavoidably in it during hydrate filtration and/or settling

3. Solid phase of the product hydrate (with the chemical composition of $Al(OH)_3$)

4. Adhesive moisture content of the product hydrate after the first filtration step (with a chemical composition similar to that of the spent liquor, without floating hydrate)

5. Solid phase of the seed hydrate (also with the chemical composition of $Al(OH)_3$)

6. Adhesive moisture content of the seed hydrate (with a chemical composition identical with that of material flow No.4)

7. Alumina hydrate depositions in various places of the precipitation system (this material flow will get to the preparation of the digestion liquor after dissolving it in fresh make-up caustic solution or strong liquor)

8. Pure hydrate wash water

9. Alkaline hydrate wash water originating at the washing of the product hydrate

10. Adhesive moisture content of the product hydrate after washing

(Since the solid phase of the product hydrate does not change during the washing process, there is no need for a new serial number for it.)

60. Total slurry fed into the precipitators (material flows 1 + 5 + 6)

Aluminate liquor cooling:

11. Hot aluminate liquor (i.e. the overflow of the red mud settlers)

12. Condensate of the flash steam evaporated at the aluminate liquor cooling (it has a value different from 0 only in the case of flash cooling)

Evaporation - solid caustic dissolution - salt filtration:

14. The part of the spent liquor to be concentrated by evaporation

15. The part of the alkaline hydrate wash water to be concentrated by evaporation (possibly used for the periodic washing of the evaporator sets, ultimately getting into the strong liquor)

16. Solid make-up caustic with an NaOH content of 97 to 98 per cent

17. Strong liquor after dissolving the solid caustic in it and removing the (mostly carbonate) salts from it

18. Salt (mostly sodium carbonate) removed from the process cycle (including its adhesive liquor content)

19. Water evaporated in the evaporator sets

Digestion:

20. The part of the spent liquor getting into the digestion immediately by bypassing the evaporation

21. Solids content of the bauxite to be processed

22. Adhesive moisture content of the bauxite

23. Make-up caustic fed into the process in a liquid form, as a concentrated NaOH solution

13. Digested slurry in the reaction zone, before flashing

24. Liquor phase of the digested and flashed slurry concentrated during flashing (so-called blow-off liquor)

25. Solid phase of the digested and flashed slurry consisting of the insoluble components of the bauxite and of the desilication product (so-called digestion residue or blow-off mud)

26. Water evaporated during the flashing of the digested slurry

Dilution and red mud settling:

27. The part of the spent liquor fed into the dilution in order to raise the molar ratio of the liquor phase of the diluted slurry

30. Solid phase of the red mud leaving the settlers as an underflow (differing by the amount of $Al(OH)_3$ precipitated as a result of the so-called auto-precipitation and possibly in its Na_2O content from the blow-off mud)

31. Liquor phase of the red mud leaving the settlers

32. Overflow of the first washing stage of the red mud washing system (called also diluting liquor)

Red mud washing:

28. Liquor fed to the first washing stage of the red mud washing system in order to raise the molar ratio of the liquors along the latter (usually the part of hydrate wash

water not concentrated by evaporation and possibly a part of the spent liquor)

29. Liquor fed to an optional stage (most often to the second one) of the red mud washing system in order to raise the molar ratio and to utilize a low-concentration liquor stream of the alumina plant (usually the low-concentration caustic liquor formed during the causticizing of the soda salt removed at the evaporation; however, some alumina plants make up the whole amount or most of their NaOH losses by feeding a causticized soda solution into their mud washing system)

30 + 3n Solid phase of the red mud leaving the nth stage of the red mud washing system as an underflow

31 + 3n Liquor phase of the red mud leaving the nth stage of the red mud washing system

32 + 3n Overflow of the (n+1)th stage of the red mud washing system (in the case of the last washer the pure red mud wash water or so-called make-up water, or the filtrate of any red mud filters)

Red mud filtration (possibly combined with red mud causticizing):

33 + J Solid phase of the filter cake of the first stage of any red mud filtration

34 + J Liquor phase of the filter cake of the first stage of any red mud filtration

35 + J Filtrate of the second stage of any red mud filtration (in case of a single-stage filtration the red mud wash water)

36 + J Solid phase of the filter cake of the second stage of any red mud filtration

37 + J Liquor phase of the filter cake of the second stage of any red mud filtration

38 + J Red mud wash water in the case a two-stage red mud filtration is applied

(J is three times the serial number of the last washing thickener)

Since the number of washing stages is different from plant to plant, no fix serial number could be ordered to the solid and liquor phases of the red mud transported to the disposal area, neither to the red mud wash water; all these depend on the total number of decantation and filtration stages. A maximum total number of 8 countercurrent stages (either 8 decantation stages or 7 decantation plus 1 filtration stages or 6 decantation plus 2 filtration stages) can be handled by the mathematical model presently described.

Bauxite preparation:

57. Digestion liquor (also called test tank liquor)

58. Ground bauxite slurry consisting of the solid phase and the adhesive moisture content of the bauxite and of a part of the digestion liquor

59. Adjusted and possibly pre-desilicated bauxite slurry (this is fed into the digestion)

Fig.1 depicts the above material flows and their connections to the various unit operations or groups of unit operations. The main technological line (21: solids content of the bauxite - 59: adjusted slurry - 24: liquor phase of the digested and flashed slurry - 11: hot aluminate liquor - 1: cooled aluminate liquor - 3: solid phase of the product hydrate) is traced by a heavy line. Small

circles represent those technological junctions (which can also be considered as some kinds of unit operations) where liquors are distributed or mixed. The three circles on the left side of Fig.1 can be described by the following two inequalities:

$$X2 \geqslant X14 + X20 + X27 \text{ and}$$
$$X9 \leqslant X15 + X28,$$

where X = N, A or B and

$$X2 + X9 = X14 + X20 + X27 + X15 + X28$$

The small circle on the right side of Fig.1 (which can also be called digestion liquor preparation) can be described by the following equation:

$$X7 + X17 + X20 + X23 = X57$$

The vector with the index O has not been used for the description of a given material flow but for storing some important characteristic parameters of the technology. Similarly, A56, V56, W56 and C56 are also used for different purposes (see later).

The material and heat flows of the Bayer process can be unequivocally determined by fixing some 100 to 200 data. The number of data required for the determining depends on the requirements raised against it: the more technological variants it should be able to describe (see e.g. the causticizing and/or filtration of the red mud) and the more accurate description is expected from it, the more data have to be fixed. A part of these data can not be influenced (e.g. the composition of the raw material, its digestion

and settling characteristics, the temperature of the environment, etc.), however, another part of them can be more or less freely selected between some limits (e.g. digestion temperature, precipitation time, distribution of the alkaline hydrate wash water between evaporation and mud washing, concentration of the caustic liquor originating from the causticizing of soda salt, etc.). The latter data have been divided into two groups on the basis of practical experiences: into those exerting a significant influence on the economics of the alumina production (e.g. the first two of the above mentioned data) and those exerting a much lesser influence on the economics (e.g. the last two of the above data). After a careful selection 21 data have been included into the first group. These have been marked with the letter K and indices ranging from 1 to 21. The other "free" variables and those determined by the raw material or the environment are marked by the letter Y. The following parameters are included into the group of K data:

K1 - is the precipitation time, hours.

K2 - is the caustic Na_2O concentration of the pregnant liquor, gpl.

K3 - is the molar ratio of the pregnant liquor.

K4 - is the amount of solid caustic added to the strong liquor, kg Na_2O/t alumina.

K5 - is the seeding ratio, seed Al_2O_3 kg per alumina content of pregnant liquor, kg.

K6 - is the caustic concentration of the strong liquor, gpl.

K7 - is the amount of water evaporated in the evaporation, t/t alumina.

K8 - is the highest digestion temperature, ^{o}C.

K9 - is the temperature of the last flash (blow-off) tank, ^{o}C.

K10 - is the specific surface area of the seed, based on size analysis and assuming spherical shapes, m^2/g.

K11 - is the clarification temperature, ^{o}C.

K12 - is the final temperature of heat utilization in aluminate liquor cooling, ^{o}C.

K13 - is a factor showing the ratio of the actual digestion discharge molar ratio compared to the equilibrium molar ratio for the given digestion temperature and concentration.

K14 - is the temperature of mud wash water (if mud is causticized, the temperature of causticizing), ^{o}C.

K15 - is the heating surface area per preheater in digestion, m^2.

K16 - is the amount of lime applied for mud causticizing, t/t alumina.

K17 - is the retention time at mud causticizing, h.

K18 - is the number of effects in the evaporation.

K19 - is the number of flash stages at the digestion.

K20 - is the number of red mud washing stages.

K21 - is the capacity of the alumina plant in thousands of tons per annum, based on an 8760 hour per year continuous operation.

Should the mathematical model be combined with an optimizing program, the latter would have to determine the optimum combination of the values of the K data, possibly within some limits. The values of K1 through K17 and K21 can be continuously varied whereas the values of K18, K19 and K20 only in steps of whole units. Any optimizing program has to take this into consideration.

The Y data are listed in an appendix since their list would require too much space at this place.

Before describing the calculation procedures used for the description of the unit operations some repeatedly used equations have to be mentioned in advance. The following equations do not require any explanation:

$$C[g/l] = N\,[kg/t] \,/\, V\,[m^3/t] \qquad (1)$$

$$D[g/l] = A\,[kg/t] \,/\, V\,[m^3/t] \qquad (2)$$

$$M[Mol/mol] = \frac{102}{62}.N[kg/t]/A[kg/t] = \frac{102}{62}.C[g/l]/D[g/l] \qquad (3)$$

$$F[t/m^3] = B[t/t]/V[m^3/t] \qquad (4)$$

The four equations above are valid for every liquor phase, therefore, the number of independent data is less by as much. For solid phases only eqution (4) applies, however, in their case the number of describing data is also less by three.

The following formula has been set up to describe the volume of sodium aluminate liquors by means of linear correlation from the density data of various plant liquors:

$$V[m^3/t]=B[t/t]-0.001135.N[kg/t]-0.00054.A[kg/t] \quad (5)$$

This means that the volume contraction occuring at the mixing of two sodium aluminate liquors of different concentrations or at the dilution of such a liquor with water is not taken into consideration as a result of neglecting the members of the second order of equation (5). However, the relatively minor error due to this neglection has some significant advantages during the calculations since the total volume of two material flows mixed together will be the arithmetical sum of the volume of the two flows.

The heat capacity of the liquors is described by the following approximating formula:

$$W[Mcal/t^{o}C]=B[t/t]-0.000645.N[kg/t]-0.000667.A[kg/t] \quad (6)$$

The variation of the specific heat as a function of the temperature has been neglected in the temperature range below 100 ^{o}C (where it is negligible) and at the digestion the error caused by this has been compensated during the calculation procedure.

The effect of the other components of the liquors have been neglected in both formulae, however, on the one hand their amounts are minor relatively to those of the two main components taken into consideration, and on the other hand they are more or less proportional to the caustic Na_2O content of the liquors and so the coefficients determined by correlation effectively take their averages into consideration.

The densities and specific heats of various solid phases are given as constants among the Y data.

2. DESCRIPTION OF THE MATHEMATICAL MODEL PER UNIT OPERATIONS

The calculations are not described in every minor detail since together with their explanations this would unnecessarily increase the volume of the following description, however, all the important steps of the calculation procedures of every unit operation will be shown and explained. On the basis of these the whole mathematical model can be easily reconstructed.

2.1 Seeding, precipitation, hydrate filtration

As a preliminary step the salt level (or more exactly the ratio of chemically bound Na_2O to caustic Na_2O) of the process cycle has to be estimated. Reference [1] contains an equilibrium curve which can be used for this purpose. After some recalculation the said curve can be approximated by the following formula:

$$MO = 159/c - 0.77 + 0.001 \cdot c \qquad (7)$$

where MO is the saturation ratio of chemically bound Na_2O to caustic Na_2O of a given liquor and

c is the caustic Na_2O concentration of the same liquor in g/l.

The formula is valid between 240 and 350 g/l caustic Na_2O concentrations. This encompasses the whole range of Bayer liquors concentrated or superconcentrated by evaporation and even those further concentrated by dissolving solid NaOH in them.

In the knowledge of the saturation ratio, of the amount of water evaporated per tonne of alumina produced, of the concentration of the strong liquor, of the amount of solid NaOH at disposal for this purpose and of the amount of chemically bound Na_2O to be supersaturated per tonne of alumina produced (which also depends on the method applied for salt removal) the salt level of the process cycle at which the required amount of salt can be removed may be calculated. This ratio of chemically bound Na_2O to caustic Na_2O has been placed into the MO component of the free O vector, so when printing the table of material flows the computer will supply this information, too.

In the knowledge of the estimated salt level of the process liquors the calculation of the precipitation process can be started. The basis of this calculation i · 1 m^3 of cooled aluminate liquor. First the amount of seed has to be added to this, the adhesive liquor content of which will somewhat modify the concentrations of the cooled aluminate liquor. On the other hand, the exact composition of the adhesive liquor will only be known at the end of the calculation of the precipitation process. This problem can be solved by first carrying out the calculation with an adhesive liquor having an estimated composition (e.g. one corresponding to a 50 % precipitation yield) and subsequently repeating it on the basis of the results of the first calculation run. Trial calculations have shown that a single repetition of the calculation supplies satisfactorily accurate results even in the case of relatively extreme initial data.

In the knowledge of the composition of the seed slurry the continuous precipitation process can be calculated from precipitator to precipitator. The differential equation describing the reaction rate of the precipitation set up by Shimosato [2] has been selected from the calculation procedures described in the technical literature for inclusion in the mathematical model. (For some comparison see also [3].) According to [2]

$$-\frac{dA}{d\tau} = K(C_I + r(A_o - A))\frac{(A-A_\infty)^2}{A_\infty^{\,2}} + K'\frac{A-A_\infty}{A_\infty} \qquad (8)$$

where A is the actual,

A_o is the initial and

A_∞ is the equilibrium Al_2O_3 concentration in g/l,

τ is the time in hours,

C_I is the initial seed concentration in gAl_2O_3/dm^3 liquor,

r shows, how many times more active the $Al(OH)_4$ precipitated during the process is compared to be initial seed and

K and K' are rate constants depending on the temperature and the caustic Na_2O concentration of the liquor.

The author has provided partly tabulated, partly graphical data for A_∞, K and K' which completely cover the required area. In order to make them useable for computers empirical formulae have been set up for their description. These are the follwong:

$$\lg A = (0.25+c-0.5c^2).t+0.685+0.35c+0.16c^2 \qquad (9)$$

$$\lg K = 14.068-15.68c+12.82c^2-3.24c^3-33/T \qquad (10)$$

$$\lg K' = (1.18c+0.79).t-11.38\cdot 121.7^{c-2}-0.96 \qquad (11)$$

where c is the caustic Na_2O concentration of the liquor in 100 g/l,
t is the temperature in 100^oC and
T is the temperature in 100 K.

All three equations correctly describe the data of Shimosato between 40 and 68 ^oC (and may be extrapolated to a small extent even outside this range without large errors), the concentration range of equations (9) and (11) is 80 to 190 g/l and that of equation (10) is 80 to 160 g/l caustic Na_2O. Above 160 g/l first the curves belonging to the higher temperatures begin to deviate from the experimental data, at 170 g/l equation (10) still supplies correct data between 40 and 50 ^oC but at 180 g/l only the figure for 40 ^oC seems to be correct.

Equation (8) had two deficiencies: the author has not disclosed, what amounts of contaminants his liquors contained (he has only whitten about "plant liquors") and how active the seed used by him was (or what specific surface area it had). Therefore, the above equations had to be adjusted to the Hungarian plant data. The Ajka Alumina Plant has put to our disposal the experimental data systematically collected in the plant over a time period of four months, which data were approximated by the following reaction rate equation:

$$-\frac{dA}{d\tau} = K.(C_I+A_o-A).(a+b.K10)\frac{(A-A_\infty)^2}{A_\infty^{\ 2}} + K'\frac{A-A_\infty}{A_\infty} \qquad (12)$$

and the caustic Na_2O concentration of the liquor was multiplied by a c coefficient. A computer was used to modify systematically the values of a, b and c until the calculated data closely approximated the plant data (the sum of the

squares of their deviation was minimal). This way an approximation within less than 2 g/l Al_2O_3 could be attained as an average. (For more details see Reference [3].) The optimum values of a, b and c were 0.373; 10.08 and 0.92. The usual values of K10 were between 0.06 and 0.09 m^2/g since the particles were supposed to be spherical, without any pores. The r coefficient in the original Shimosato-equation (8) was left out of equation (12) since there were no significant data at our disposal to make certain whether any interim increase or decrease of the particle size took place during the precipitation process or not and because in the absence of any effective classifying in our plants the grain size distribution of the hydrate leaving the precipitation line has to be the same as that of the hydrate fed into it as seed if a stable, stacionary operation is to be maintained.

The impurity levels of the pregnant liquor have not changed during the four month test period to such an extent that their effect could have been determined. Therefore, their effect could only be taken into consideration on the basis of publication [4] which says that one mol of the main component of the impurities of Bayer plant liquors, sodium carbonate increases the equilibrium Al_2O_3 concentration of aluminate liquors as much as half a mol of caustic Na_2O would do. On the basis of this statement the value of 0.92 got for coefficient c could be broken up in the following way:

$$c = 0.85 + 0.5 \cdot MO \qquad (12a)$$

since the average value of MO was 0.14 mol carbonate-bound Na_2O per mol caustic Na_2O during the test period.

The differential equation corrected in the above way can be used as a difference equation in the case of a continuous precipitation if it is supposed that the slurry held in every precipitator tank is ideally mixed. (Since this is significantly worse than an ideal plug-like flow, it seems to be not too risky to suppose this.) According to this difference equation the amount of alumina hydrate (calculated as Al_2O_3) precipitated under the conditions prevailing in a given precipitator tank during the average retention time is equal to the difference of the Al_2O_3 concentration of the liquor fed into the tank and of that leaving it. Therefore, the calculations are carried out so that the concentrations prevailing in the given precipitator are estimated, the amount of Al_2O_3 precipitated under these conditions is calculated using the difference-form of equation (12) and also equations (9), (10) and (11) and by subtracting this amount from the concentration of the liquor fed into this precipitator the estimate is checked. The calculation is corrected step by step until the difference between the estimated and calculated figures won't be less than a given limit. Subsequently the amount of Al_2O_3 precipitated in the next tank may be similarly calculated. When all the stages of the precipitation system have already been calculated once, the previously mentioned correction of the initial composition of the liquor has to be carried out and the whole calculation has to be repeated step by step once more.

The number of stages of the continuous precipitation line(s) is given among the economically not too significant Y data. By giving a very high value (say, 100) to it the mathematical model will be suitable for the simulation of batch precipitation. Since the differential form of

equation (12) can not be easily integrated because it is too complicated for that, it can be anyway only numerically approximated by using very small steps. By supposing a high number of stages the retention time belonging to one stage can be reduced at will and this way the continuous concentration change characteristic of the batch precipitation can also be approached to taste.

One of the most important parameters of the precipitation, the temperature distribution also had to be put among the Y data. If it were left to the computer to select the optimum temperatures, it would often select such temperatures at which equations (9), (10) and (11) are not defined anymore, and on the other hand the particle size of the hydrate produced at such a temperature would most probably not be acceptable. Therefore, the initial and final temperatures of the precipitation are given among the Y data and a linear temperature drop is supposed between these extremes. The real temperature drop differs only minimally from a linear one (if the size and heat insulation of all the precipitators are the same) since the higher heat losses of the first (hottest) tanks are compensated or overcompensated by the heat set free during the exothermic decomposition of the aluminate liquor which takes mostly place in the first few tanks of the precipitation system.

By the time the precipitation process is calculated over, it will be known how many kg Al_2O_3 can be precipitated of 1 m^3 aluminate liquor. This has to be compared to the amount of precipitated hydrate required (calculated also as Al_2O_3), which contains over and above the required amount of product hydrate (990 to 1020 kg Al_2O_3/t alumina) also the scalings in the precipitators (5 to 20 kg/Al_2O_3/t) and the suspended hydrate content of the spent liquor

leaving the precipitation area. This way the total volume of aluminate liquor required for the production of 1 t of alumina and on the basis of this the amount and composition of the product hydrate, the seed and the spent liquor (including the adhesive liquor content of the first two) can be calculated.

By multiplying the sum of the specific volumes of the aluminate liquor and the wet seed by the precipitation time and taking the invert of this product a figure very characteristic of the precipitation process, the average useful precipitation rate can be calculated. This figure is placed into the DO component of the O vector, expressed as kg Al_2O_3/m^3h.

The amount of alkaline hydrate wash water can be calculated from the adhesive liquor content of the product hydrate by estimating its concentration at the end of the countercurrent washing. This concentration can be estimated on the basis of practical experiences, as a function of the number of countercurrent washing stages, of the concentration of the spent liquor and of the purity required of the product hydrate. It may be in the range of 40 to 60 g/l.

2.2 Aluminate liquor cooling

The aluminate liquor may be cooled in two different ways: by surface or flash cooling. In the first case no water will be evaporated from the aluminate liquor, the amount and concentration of the hot liquor are equal to those of the cooled one. On the other hand, flash cooling involves the evaporation of water, i.e. the mass of the hot aluminate liquor exceeds that of the cooled one by some

5 to 7 %, and its concentration is less by a similar percentage than that of the latter. The first method has a better calorific efficiency and requires lower investment costs, the second has advantageous technological effects as a result of the amount of water evaporated (the red mud can be more efficiently washed with the extra amount of water or the evaporation rate can be reduced and this way steam may be saved). When using the latter method the mathematical model will calculate the amount of flash steam and (since the calculation has begun with the precipitation, i.e. the cooled aluminate liquor) the amount and composition of the hot aluminate liquor.

The ideal recipient of the heat released during the aluminate liquor cooling is the spent liquor since its amount is roughly equal to that of the aluminate liquor and its temperature is less by some 10 to 20 ^{o}C, so it can be heated by the latter in a countercurrent process.

The end temperature of the aluminate liquor cooling (Y4) is not necessarily equal to the final temperature of heat utilization (K12). The former is prescribed by the precipitation technology, the latter can be somewhat higher as a result of economic considerations since in the case of giving up the amount of heat belonging to the last few centigrades the size of the heat utilizing equipment can be significatly reduced (first of all as a result of the widening temperature gap between the cooled and the heated liquors). This applies first of all to flash cooling at which this temperature gap is significantly reduced by the temperature steps resulting from the finite number of flash stages and by the boiling point elevation of the liquor.

Only that part of the flash steam can be recovered as condensate which has been evaporated in the utilized section of the cooling system since the unutilized cooling is usually carried out by mixing condensers and so this amount of condensate is lost in the cooling towers. Therefore, material flow 12 consists only of the amount of water flash-evaporated in the utilized section of the cooling (this condensate can be used in the plant e.g. for red mud washing) and the amount of flash steam getting into the mixing condensers is equal to B11-B1-B12.

This part of the mathematical model will also calculate the temperature of the preheated spent liquor with the help of the calorific efficiency given among the Y data.

2.3 Evaporation - solid caustic dissolution -salt filtration

In this part of the mathematical model only the liquor flows of the evaporation are calculated. Should only spent liquor be concentrated by evaporation,

$$V14 = K7 \cdot \frac{K6}{K6-C2} \quad m^3/t \qquad (13)$$

of this is required in order to get a strong liquor with a caustic Na_2O concentration of K6 g/l by evaporating K7 t/t of water out of it (when maintaining the previously mentioned approach of the additivity of liquor volumes).

The situation is slightly complicated by the fact that the whole amount or a part of the hydrate wash water is also fed into the evaporators in some alumina plants, partly in order to intensify the salt and organics removal, partly to wash the evaporator sets periodically with it. In the latter

case the wash water will be concentrated by the salts dissolved and the liquors flushed out of the evaporators so that its concentration may attain or approach that ot the spent liquor. Therefore, it may be mixed to the latter (after an optimal desalting) and will ultimately leave the evaporation as strong liquor plus alkaline condensate.

The amount of hydrate wash water used for evaporator washing is more or less proportional to the amount of evaporated water and it amounts to some 5 to 20 % of the latter. This proportionality factor is given among the Y data. Its maximum value may be (K6-C9)/K6, in this case only hydrate wash water is fed into the evaporators. There is also taken care that the amount of alkaline hydrate wash water fed into the evaporation should not exceed the amount forming in the product hydrate filtration (i.e. V15 $\leqslant$ V9).

After all, the calculation of the evaporation is only as much influenced by taking the hydrate wash water into consideration that the amount of water evaporated from the latter has to be subtracted from the total amount of water to be evaporated (i.e. K7).

The solid caustic fed into the process has to be added to the strong liquor formed during the evaporation (it improves the salt removal by its effect of increasing the caustic Na_2O concentration of the latter) and the wet salt has to be subtracted from it. Since the amount and composition of the salt to be removed is a function of the composition of the bauxite processed and depends very little on the freely variable parameters, its characteristics are given among the Y data.

The mathematical model takes the physical Na_2O, Al_2O_3 and other losses of the process at the evaporation into consideration. The data of these can also be found among the Y data. If a negative figure is given for "other losses", the model can also follow the introduction of some nontechnological water (e.g. rainwater, gland water, etc.) into the process.

Since the original caustic Na_2O concentration of the strong liquor (given by K6) suffers some changes during the dissolving of solid caustic, the removal of the salt and the subtracting of physical losses (not to mention the dilution caused by the introduction of some unaccounted water) it is difficult to foresee the concentration of the strong liquor ultimately leaving the evaporation. Since sometimes it is required that this latter concentration be kept to a fixed value, the model has been set up so that K6 can mean the caustic Na_2O concentration of the strong liquor leaving both the evaporator sets or the unit operation. This can be influenced by the value of Y22. (Of course in the latter case the concentration of the strong liquor leaving the evaporator set can not be fixed in advance.)

The heat flows of the evaporation will be dealt with in a subsequent chapter (3.5).

2.4 Digestion

In order to make possible the calculation of the material flows of this unit operation first of all two assumptions have to be made: both the total Na_2O and Al_2O_3 losses of the whole process have to be estimated (for 1 t of alumina produced). The former is marked by

NO, the latter by AO. (These are components of the previously mentioned O vector.) If N16 is subtracted from the estimated value of NO, an estimate for N23 will be arrived at. (The latter is the caustic Na_2O content of the required make-up caustic available in a dissolved form.) Apart from the fact that most of this caustic solution is required for the chemical cleaning of the precipitators and other related equipment from scalings consisting mainly of aluminium hydroxide, it is not advisable to add it to the strong liquor before salt removal even through it would slightly increase the caustic Na_2O concentration of the latter (commercial NaOH solutions usually contain 450 to 500 g/l caustic Na_2O) because it would also reduce the concentration of noncaustic Na_2O in the strong liquor and so the supersaturation of the latter would not increase significantly and might even be reduced in some cases.

If the Al_2O_3 content of the product hydrate is added to the estimated value of AO, the amount of Al_2O_3 to be fed into the process with the bauxite will be obtained. On the basis of this and in the knowledge of the composition of the bauxite to be processed (the data for this are given among the Y data) the components of material flows 21 and 22 can be calculated.

The data of the blow-off mud can be calculated on the basis of the mass and composition of the bauxite. For this it is supposed that all the SiO_2, Fe_2O_3 and TiO_2 content and a defined part of the LOI content and the minor components of the bauxite get into the mud. (Even though a minor part of the SiO_2 content remains temporarily in a dissolved form, much of this will precipitate during the dilution and clarification, therefore, it can be neglected.) The amounts of

the two economically most important components of the blow-off mud, those of the undigested Al_2O_3 and of the Na_2O bound into it are calculated by some approximating formulae. Efforts were made to insert these equations in their possibly most general forms into the mathematical model in order to enable its user to adjust the latter to a new type of bauxite by just modifying some of their coefficients. (These coefficients can be found among the Y data.)

K8 and K13 are the independent variables of the two functions, i.e. the digestion temperature and the coefficient of the digestion molar ratio (it may also be called the "excess liquor coefficient"). The latter shows, how many times the target molar ratio exceeds the equilibrium one calculated for the same temperature and liquor concentration. Neither the liquor concentration nor the retention time have been taken into consideration as independent variables, at least not directly. Usually no significant concentration-dependence can be demonstrated within the range of the usual digestion liquor concentrations for the Al_2O_3 extraction yield, at least not for similar excess liquor coefficients. (For a constant molar ratio higher liquor concentrations usually result in better extraction yields since a higher concentration means a lower equilibrium molar ratio and so a higher excess liquor coefficient, however, this is a result of the latter and not of the former.) The effect of the retention time has been neglected because in the temperature range of modern autoclave-type digestion systems (230 to 250 ^{o}C) the accomodation of the necessary heating surfaces requires so much volume which is more than sufficient to complete the digestion of boehmitic bauxites processed in Hungarian alumina plants. Should the mathematical model be used for direct-steam heated autoclave systems, for tempera-

tures much lower than the above range (say, for 180 °C for boehmitic bauxites), for the digestion of diasporic bauxites even in indirectly heated autoclaves or for tube digestion systems, either the relevant function has to be modified or the Y data have to be determined so that they take into consideration the effect of the retention time. Naturally, in the latter case the model can not be used for automatic optimization of the process parameters, only for a step-by-step approach, since the Y data have to be manually modified from variant to variant. Essentially the same considerations apply for the equation used for the calculation of the amount of Na_2O chemically bound into the blow-off mud.

The equation built into the mathematical model for the calculation of the Al_2O_3 extraction yield is the following:

$$Q = \frac{a}{m} + \frac{b + c \cdot K8 + d \cdot K8^2}{K13 - e} \qquad (14)$$

where Q is undigested part of the Al_2O_3 content of the bauxite in %/100 (essentially the complement of the extraction yield), m is the Al_2O_3/SiO_2 ratio of the bauxite in kg/kg and a, b, c, d and e are coefficients characteristic of a certain bauxite, given among the Y data.

The first part of equation (14) gives the Al_2O_3 losses proportional to the SiO_2 content of the bauxite, whereas its second part has to reflect the hyperbolical character of the isothermic molar ratio vs extraction yield curves. The value of e should be close to 1 since a significant decrease of the extraction yield can be expected when approaching the equilibrium molar ratio.

The following equation is used for the calculation of the amount of Na_2O chemically bound in the blow-off mud:

$$N25 = \frac{A21}{m} \cdot (a + b \cdot K13 + c \cdot K8^2) \qquad (15)$$

where A21/m is - according to the previously used markings - the SiO_2 content of the bauxite in kg/t alumina and a, b and c are coefficients given among the Y data. The equation suggests that the chemical Na_2O losses are to a certain extent proportional to the liquor excess applied and to the digestion temperature (to the latter in a more than linear, rather in a quadratic proportion). The probable reason of the former effect is the often observed fact that the Na_2O content of the sodalite and cancrinite formed during the digestion may slightly change with the amount of excess liquor present and that of the latter the increasing digestion of the TiO_2 content of the bauxite. (Since the TiO_2 content of the bauxite is not part of the mathematical model, its effects have to be ordered to the SiO_2 content. As a given bauxite has a fix ratio of TiO_2 to SiO_2, this can be done without causing any errors. One has only to take care to modify the value of c if this ratio changes.)

When the bauxite-to-blow-off-mud aspect of the digestion has already been calculated through, the calculation of the amount and composition of the liquor flows can be begun. The main task is to determine, how much spent liquor bypassing the evaporation (material flow 20) has to be added to the strong liquor (material flow 17) and to the liquid make-up caustic (material flow 23, also including material flow 7). The composition of material flow 20 is equal to that of material flow 2. Until the amount of the former (e.g. its volume, V20) is not known, the concentration of the

digestion liquor will also be unknown (for the latter parameter a place has been reserved in component CO of the O vector because of its importance). On the other hand, the molar ratio of the digestion (M24) depends on the concentration of the digestion liquor. However, the amount of digestion liquor required (and through this, the only freely variable component of it, material flow 20) is determined by the molar ratio of the digestion. Therefore, three equations have to be set up to determine the values of the above unknowns, V20, CO and M24.

The first of these equations is the Na_2O balance of the digestion liquor preparation:

$$CO.(V17+V20+V23+V*7) = N17+N23+V20.C20 \qquad (16)$$

where two of the unknowns, CO and V20 appear. (V*7 is the volume by which the total volume of the liquor will increase after dissolving it.) Sometimes the diluting effect of the adhesive moisture content of the bauxite (B22) has also to be taken into consideration when determining CO. This is decided by the value given to Y48.

The second equation determines the caustic Na_2O to Al_2O_3 molar ratio of the liquor after digestion:

$$M24.(A21-A25+A17+D20.V20+A7) = \frac{102}{62}.(N17+N23+C20.V20-N25-a) \qquad (17)$$

In this equation M24 and V20 are unknown. a is the amount of caustic Na_2O chemically bound into various salts (mostly into carbonate) during the digestion, in kg/t alumina. Since this is a function of the bauxite composition, it is given among the Y data.

The third equation has been set up between the molar ratio of the liquor after digestion (M24) and the concentration of the digestion liquor:

$$M24 = K13.(0.000052.K8^2 - 0.317 \cdot K8 + 4.866 - 0.135 \cdot \frac{\infty}{K8-52}) \qquad (18a)$$

$$M24 = K13.(0.000052.K8^2 - 0.317 \cdot K8 + 6.42 - 0.4 \cdot \frac{\infty}{K8-52}) \qquad (18b)$$

$$M24 = K13.(0.000052.K8^2 - 0.325.K8 + 6.455 - 0.178.\frac{\infty}{K8-52}) \qquad (18c)$$

Equation (18a) applies for gibbsitic, equation (18b) for boehmitic and equation (18c) for diasporic bauxites. K13 is - as mentioned above - the excess liquor coefficient and the expression in brackets is the equilibrium molar ratio of the liquor as a function of the temperature and the caustic Na_2O concentration. Initially the equilibrium formula for boehmite included in equation (18b) has been set up on the basis of a diagram published by Adamson, Bloore and Carr /5/. This formula very accurately describes the curves of the diagram between 180 and 240 °C and only slightly deviates from the curves given for 160 and 260 °C, respectively. Later, the formula was modified to fit the curve given by the same paper for 140 °C and gibbsite. The formula in equation (18c) was set up by adjusting that of equation (18b) to the test results obtained during the tests carried out with Greek diasporic bauxites of Bauxite Parnasse.

As it can be seen, the molar ratio vs caustic Na_2O concentration function is linear in all three cases. The formula in equation (18b) accurately describes the curves between 50 and 250 g/l caustic Na_2O, i.e. over the whole conceivable concentration range. The formula in equation

(18a) is more or less accurate between 90 and 140 g/l, less accurate at higher concentrations. The formula in equation (18c) is valid between 240 and 260 °C and between 140 and 210 g/l caustic Na_2O concentrations.

The linearity of equations (18a) through (18c) make it possible to solve the simultaneous equations (16), (17) and (18) in an algebraic way (they can be reduced to a single quadratic equation). If another molar ratio furmula of a higher order had to be used, the problem could only be solved by using an iterative algorithm for the solution of the simultaneous equations.

After solving the above simultaneous equations all the material flows entering the digestion process are known, and only one of the material flows leaving the unit operation is still to be determined: the amount of water evaporated during the flash cooling of the digested slurry (material flow No.26). Since it is not practical to carry out the detailed thermal calculations of the digestion at this place of the mathematical model, because the material flows of this unit operation have to be recalculated some 25 times as a result of the iterative approximation of the NO and AO values, it is advisable to use an approximating formula for this purpose. According to this the amount of water evaporated (B26) is

$$Q=a.(1-0.00028.(K8-K9)).\frac{(0.88167+0.0005.(K8+K9)).(K8-K9)}{604.4-0.64\cdot K9} \qquad (19)$$

times the water equivalent of the digested slurry (W13). The latter can be easily calculated from the previously determined material flows. Coefficient <u>a</u> is characteristic for the difference between the theoretical value (flashing

of pure water without heat losses) and the practical one, it may attain in well operated systems 0.95 to 0.96 but is in some cases as low as 0.85. The second factor stands for the difference between a single-step and a multi-step flash system (multi-step systems evaporate less water than single-step ones under similar conditions; the practical systems are of the multi-step type). The numerator of the fraction is the second-order approximation of the difference between the heat contents of water at the boiling temperatures of K8 and K9, respectively. The denominator is a numerical approximation of the heat of evaporation of water at the boiling temperature of K9. The equation gives very accurate results if K8 is between 200 and 250 ^{o}C, K9 is between 110 and 130 ^{o}C and the number of flash stages is higher than three compared to the data found in the VDI tables /6/.

The mass, Na_2O and Al_2O_3 contents of material flow 24 (B24, N24 and A24) can be calculated from the material, Na_2O and Al_2O_3 balances of the unit operation, its other parameters by using equations (1) to (6) in the proper order.

The mass and composition of the digested but still not flash-cooled slurry is very characteristic of the digestion process. These data will also be necessary for the thermal calculations of the digester lines. Therefore, vector 13 which was previously used for other purposes but freed during a reconstruction of the mathematical model is presently used for the description of this material flow. Practical aspects have suggested that B13, V13, W13 and F13 should store data characteristic of the total flow (i.e. including the solid phase, too) but N13, A13, C13, D13 and M13 only those of the liquor phase (e.g. C13 is

the quotient of the caustic Na_2O content and the volume of the liquor phase).

2.5 Dilution - red mud settling

Over and above the digested and flashed slurry the diluted caustic liquor resulting at the red mud washing and possibly the part of the spent liquor not utilized at the evaporation and the digestion are fed into this unit operation, the latter for the purpose of increasing the molar ratio of the diluted slurry in order to reduce the autoprecipitation losses. (One of the Y data decides whether this part of the spent liquor is fed into the dilution or into the first stage of the red mud washing system, or whether it should be distributed between them and if so, to what proportions.)

It should be mentioned here that if the total amount of material flows 14 and 20 exceeds the amount of material flow 2, this means that the molar ratio of the aluminate liquor has been set too low and the latter has to be increased at least to such an extent that the increasing amount of the spent liquor cover the demands of the evaporation and the digestion. On the other hand if the initial estimates for NO and AO are far from their correct values, a temporary deficiency in the amount of spent liquor may arise during the iteration even in the case of otherwise correct variants. Therefore, the requirement of $V2 \geqslant V14 + V20$ can only be raised towards finally iterated variants. Should this requirement not be fulfilled, the whole calculation has to be repeated with an increased M1 with a new iteration target of $V2 = V14 + V20$ because the value of M1 belonging to this equation differs the least from the molar ratio given by K3.

The Na_2O and Al_2O_3 concentrations of the liquor in the settlers have already been determined when calculating the data of material flow 11. The next step is to calculate the so-called autoprecipitation losses which increase the mass and the Al_2O_3 content of the red mud compared to those of the blow-off mud. Two factors determine these losses: the rate of the autoprecipitation reaction of the aluminate liquor and the retention time determined by the total volume of the settler(s).

Much less theoretical and practical basis is available for the calculation of the reaction rate of the autoprecipitation than in the case of the precipitation. After all, a spontaneous decomposition process and a precipitation process initiated by the already precipitated alumina hydrate as seed are running parallelly, similarly as in the precipitation plant unit, with the difference that the seeding ratio of the precipitation reaction is extremely low and varying from place to place. It is 0 in the top layer of the settler (the alumina hydrate precipitated during the decomposition quickly settles out of this layer) and higher and higher in the lower layers. It is quite impossible to set up a reaction mechanism exactly describing this process under such complicated circumstances, the more so because the accuracy of the measured data is insufficient for this purpose. The concentration difference does not exceed a few g/l on the liquor side or 1 % Al_2O_3 on the solid one and it is impossible to provide a red mud with a constant composition for a test period commensurate with the retention time (i.e. 12 to 24 hours). Therefore, a very much simplified reaction mechanism has been supposed which can be described with the following reaction rate equation:

$$-\frac{dA}{d\tau} = K.\ \frac{(A-A_{\infty})^2}{A_{\infty}^{\ 2}} \qquad (20)$$

where the markings are the same as used in the description of the precipitation.

The already mentioned equilibrium solubility diagram of gibbsite published by Adamson, Bloore and Carr /5/ has been used for determining A_{∞}. Though this diagram shows the solubility curves only between 100 and 140 °C (every 10 °C), on the basis of the relatively uniform spacing of these curves it seams to be justified to extrapolate the equation set up for their description up to 95 °C since settling temperatures are usually between 95 and 100 °C. The equilibrium solutibility diagram published in the said paper can be very accurately described in the relevant temperature and concentration range by the following formula:

$$A_{\infty}=t.(78c+50c^2-20c^3)+8.9c-62.8c^2+32.8c^3 \qquad (21)$$

where A_{∞} is the equilibrium Al_2O_3 concentration in g/l and $\underline{t}$ and $\underline{c}$ have to be given in 100 °C and 100 g/l caustic Na_2O, respectively.

The following aspects have been taken into consideration when determining the reaction rate coefficient:

a) Since the relatively reliable yearly average data available have been given for the whole of the mud settling and washing systems, a common formula should be set up for the calculation of both the settlers and washers.

b) Since the K and K' reaction rate coefficients published by Shimosato (see at the precipitation) have not varied significantly with the caustic Na_2O concentration in the range of lower concentrations (80 to 120 g/l), the concentration dependence of the reaction rate coefficients for

autoprecipitation has been neglected. This may cause relatively large errors in the concentration range used in Hungarian plants at the red mud settling, however, most of the autoprecipitation losses occur not in the settlers but in the first two washing stages according to most practical experiences.

c) Since the reaction rate coefficients of the precipitation roughly double every 10 ^{o}C at caustic Na_2O concentrations not exceeding 160 g/l, an equation of the following type should be used:

$$K = a \cdot 2^{0.1\,t}$$

Though only for the temperature range between 40 and 68 ^{o}C are data available to support this /2/, the temperatures of the two washing stages most exposed to autoprecipitation either fall within this range or come quite close to it.

d) In order to determine the a coefficient of the above formula the yearly average data of the Ajka Alumina Plant for 1965 have been simulated with the help of this mathematical model. The autoprecipitation losses of 1.88 % of the total amount of Al_2O_3 fed into the plant with the bauxite could be reproduced with an a = 0.00106 kg/m^3h coefficient.

On the basis of all those said above the following equation has been incorporated into the mathematical model:

$$K = e^{0.0693 \cdot t - 6.85} \qquad (22)$$

where t has to be substituted in ^{o}C.

As a result of all these the autoprecipitation losses can be calculated in the following way for 1 t of alumina: equation (20) is integrated by neglecting the concentration change caused by the autoprecipitation and the amount of alumina precipitated in a unit volume is multiplied by the available settler volume and divided by the amount of alumina produced during 1 hour.

If the autoprecipitation losses expressed as $Al(OH)_3$ are added to the mass of the blow-off mud, the amount of (dry) red mud leaving the settlers with the underflow slurry can be obtained. The amount of the liquor phase of the underflow depend on the one hand on the settling characteristics of the given red mud and on the other hand on the mud load of the settlers (expressed as kg dry mud/m^2h). The latter can be calculated on the basis of the specific mass [kg/t alumina] of the red mud and of the size of the settler(s). A linear formula has been built into the mathematical model to describe the solids concentration [kg/m^3] vs. mud load [kg/m^2h] function which may obviously be valid only in a relatively narrow mud load range. However, at a given plant capacity only a difference of a few per cent may occur between various realistic technological variants. The two coefficients of the linear function are depending on the characteristics of the bauxite and on other factors (flocculants, etc.), they have to be given among the Y constants, if possible, on the basis of tests carried out on a pilot plant or commercial plant scale.

After having also calculated the amount of caustic Na_2O "adsorbed" on the red mud (for details see the next chapter), the mass and Na_2O and Al_2O_3 contents of every material flow leaving the settler(s) is known, and also

those of the material flows entering the dilution except for the data of material flow 32 (1st washer overflow). The latter can be calculated from the mass, Na_2O and Al_2O_3 balances of the unit operation. Naturally, if the values of NO and AO were estimated with great error margins, these errors would show up just here and completely irrealistic data might be calculated for this material flow during the iterative steps (e.g. negative or very high concentations, a molar ratio less than 1 or even negative, etc.) but this errors will decrease with the proceeding iteration and be completely eliminated by its end.

2.6 Red mud washing

The countercurrent decantation washing of the red mud can be built into the mathematical model as a cyclical procedure, i.e. the washing system can be calculated by proceeding from stage to stage. This is made possible by the fact that the composition of the liquor being in the first washing stage is known by the time the material balance of this stage is calculated since it has already been determined at the calculation of the unit operation of dilution - red mud settling. At the end of the calculation of the 1st washing stage the relevant data of the overflow of the next washing stage can be obtained from the respective material balances, i.e. by the time this stage is calculated, the relevant data will also be known, and so on from stage to stage.

However, for the calculation of the autoprecipitation losses the concentrations are not sufficient, the temperatures of the relevant stages have also to be known. Therefore, a third estimation has to be made at this point: temperature TO of the first washing stage has to be estimated.

After this the calculation will consist of the following steps:

a) The autoprecipitation losses of the given stage are calculated on the basis of the concentrations and the temperature of the liquor being in this stage and of the total volume of the same. The latter may be different from the total volume of the settler(s) (it usually is) but not from the volume of the other stages. This is the case for most alumina plants. If not, a suitably weighted average value should be given among the Y data.

The autoprecipitation losses are calculated by the method described at the red mud settling with the only difference that the following formula is used for the calculation of the equilibrium Al_2O_3 concentration:

$$A_{\infty} = (20c^2+91c).t-4.5c^2-20.5c \qquad (23)$$

which correctly describes up to 120 g/l caustic Na_2O and between 60 and 100 ^{o}C the data published both by Shimosato /2/ and by Adamson, Bloore and Carr /5/. ($\underline{c}$ has again to be substituted in 100 g/l caustic Na_2O and $\underline{t}$ in 100 ^{o}C).

b) On the basis of the autoprecipitation losses the mass and Al_2O_3 content of the red mud entering the stage is corrected in order to obtain the data of that leaving it.

c) Similarly to the procedure applied at the settling the volume of the liquor leaving the stage with the red mud in the underflow is calculated, again by means of a linear formula considered to be relevant for the whole red mud washing

system but different from that used at the settling. The chemical composition of the liquor phase of the underflow is identical with that of the overflow, therefore, the amount of caustic Na_2O and dissolved Al_2O_3 leaving with the underflow can also be calculated.

d) The amount of caustic Na_2O "adsorbed" on the red mud (see later) is added to the caustic Na_2O content of the underflow liquor.

e) The mass and caustic Na_2O and Al_2O_3 contents of the overflow of the next washing stages are determined on the basis of the mass, caustic Na_2O and Al_2O_3 balances of the given washing stage. There is a possibility to introduce various plant liquors into the washing system. The spent liquor left after the demands of the evaporation, digestion and dilution have been satisfied and the alkaline hydrate wash water left over by the evaporation are fed into the 1st washing stage and another diluted caustic soda solution (e.g. that obtained by the causticization of the carbonate salt removed from the strong liquor at the evaporation) can be fed into a selected washing stage the serial number of which has to be given among the Y data. Naturally these have to be taken into consideration in the material balances of the given washing stage.

f) By setting up the heat balance of the washing stage the temperature of the next stage is determined (i.e. the temperature at which the overflow of the next stage has to enter the stage under calculation).

After carrying out the calculation steps from a through f the calculation of the next washing stage may

be begun. Naturally, the temperature of the subsequent stages will not have to be estimated since as a function of the temperature estimated for the first washing stage these can be calculated. In this way the whole washing line can be calculated through stage by stage. If no causticizing and/or red mud filtration follows the washing system, the "next washer overflow" calculated at the last washing stage will be the pure red mud wash water, otherwise the filtrate of the first filtration stage.

The practical observation that the soluble Na_2O losses at the red mud washing are always significantly higher than those calculated on the basis of ideal decantation circumstances and the volumetric flow data of the system justifies the postulation of the adsorption of the Na_2O content of the liquor phase on the red mud or of some other process similar in its effect. Scandrett /7/ tries to explain this phenomenon by supposing that the mixing of the overflow of the next and of the underflow of the previous washing stage is far from ideal, and as a result of this the Na_2O concentration of the liquor phase of the underflow will be significantly higher than that of the overflow. However, the measurements carried out on a commercial scale red mud washing stage of a Hungarian alumina plant could not support this explanation. Adamson and coauthors /5/ explain the above phenomenon by the adsorption effect of the red mud having a large surface area and describe the amount of Na_2O adsorbed on the red mud originating from a ghanaian bauxite by a Freundlich isotherm (i.e. an exponential function having an exponent less than 1) as a function of the Na_2O concentration of the liquor phase. The data of a test series carried out in the laboratory of the Almásfüzitő Alumina Plant on the red mud of a bauxite

originating from Iszkaszentgyörgy could be much better approximated by a Langmuir-type adsorption formula than by a Freundlich-type one, especially after describing the data left and right of a breaking point of the curve at 3 g/l caustic Na_2O with two different functions. The data below 3 g/l caustic Na_2O were best described by the following equation:

$$a = 1.6464 \cdot \frac{c}{1+2c} \qquad (24)$$

where a is the amount of adsorbed caustic Na_2O as % of the dry mud and c is the caustic Na_2O concentration of the liquor in g/l.

For the data above 3 g/l caustic Na_2O concentration the following equation was found to give the closest approximation:

$$a = 0.4328 \cdot \frac{c}{1+0.28c} \qquad (25)$$

It is interesting that the limit of equation (25), 1.546 is nearly exactly twice as high as that of equation (24), 0.823. On the basis of this fact the assumption may be risked that a monomolecular adsorption found below 3 g/l Na_2O, having attained some 80 to 90 % of its limit at this concentration, changes over into a bimolecular one. Of course it is not worth to go into theoretical discussions on the basis of a single test series not reproduced ever since. It is possible that the observed phenomenon has nothing to do with adsorption but is a result of a varying Na_2O content of the sodium aluminium silicate or sodium titanate content of the red mud as a function of the caustic Na_2O concentration of the liquor surrounding it. From the point of view of the industrial practice

the only important thing is the fact that by incorporating equations (24) and(25) into the mathematical model the concentrations measured in commercial plants can be much better approximated. In order to improve the accuracy of the mathematical model it would be important to find out, how various characteristics of a given bauxite or some parameters of its processing (e.g. digestion temperature, grinding, etc.) influence the Na_2O-adsorption of the resulting red mud, however, this would require a very extensive test work.

When formulating the equations built into the mathematical model of the red mud washing the possibility has to be taken into consideration that in the course of the iterative approximation quite irrealistical data may temporarily occur for the caustic Na_2O and Al_2O_3 concentrations of the liquor and also for the temperature of some washing stages. Therefore, equation (20) used for the calculation of autoprecipitation losses has been limited so that on the one hand for unsaturated solutions (when $A < A_\infty$) it should give 0 and on the other hand the losses should never exceed $100/e^n$ kg Al_2O_3/t in the washing stage with the serial number n. Should equation (20) give e.g. 1000 kg Al_2O_3/t alumina for the autoprecipitation losses in the 2nd washing stage, the mathematical model would only take $100/e^2 \sim$ 13.5 kg/t into consideration. These limits are usually sufficiently wide to accomodate the autoprecipitation losses of realistic variants but they prevent the mathematical model from running amok during the iteration process.

Another formula to be limited is equation (24) which is undefined at the caustic Na_2O concentration of c=-0.5 g/l, varies very steeply around this value and gives a positive adsorption at Na_2O concentrations lower than -0.5 g/l. The

latter phenomenon is especially dangerous since the model may arrive at such virtually correct approximations for NO and AO at which the caustic Na_2O concentration of one or the other washing stage remains negative. Therefore, equation (24) has been simplified for caustic Na_2O concentrations less than 0 g/l to the

$$a = 1.6464c \qquad (24a)$$

form which fits jump- and breakless to the curve defined by equation (24), is defined for every value and gives a negative adsorption for a negative caustic Na_2O concentration.

The mud concentration varying linearly with the mud load has also to be limited from below, otherwise if a very high mud load occured temporarily during the iteration, the linear formula could give 0 or negative mud concentrations (i.e. infinitely large or negative volumes for the liquor phase of the underflow). Therefore it is advisable to limit the red mud concentration of the underflow to a minimum of 100 or 150 g/l solids which would not occur in the practice and so not limit any realistic variant.

2.7 Red mud causticizing and/or filtration

These unit operations are only optional parts of the alumina manufacturing according to the Bayer process. They are usually applied only in alumina plants processing a relatively poor quality bauxite for the reduction of the chemical and soluble caustic soda losses. The red mud may also be filtered in order to enable it to be further processed or to make possible its environmentally acceptable disposal. The filtration of the red mud does not

necessarily involve its causticizing (even though according to practical experiences the addition of burnt line significantly improves the filtration characteristics of the mud) but the process of causticizing has to be followed by filtration, otherwise its economic advantages can not be fully utilized.

The calculation procedure of filtration without causticizing is very similar to that of the decantation washing. however, the amount of the liquor phase accompanying the red mud solids is much less, some 0.7 to 1.0 m^3/t instead of the 2 to 4 m^3/t typical for the decantation washers. (The amount of liquor accompanying 1 t of dry mud in the filter cake is given among the Y data).

As a result of the much shorter retention time the amount of autoprecipitation losses can be neglected, and the heat losses may differ from those experienced at the decantation washers. The mud filtration may consist of one or two stages. In the latter case the red mud wash water is added to the mud cake of the first stage in order to dilute it and the resulting slurry is filtered in the second stage. In the former case the wash water (or in the latter one the filtrate of the second stage) is added to the underflow of the last washer to dilute it before the (first) filtration. If there is no sufficient filter capacity available for filtering very much diluted red mud slurries, the amount of wash water used in the filtration system may be limited to a figure given among the Y data. The rest of the wash water is fed into the last decanter-type washing stage in such cases.

Modern roller-discharge rotary drum filters make possible the washing of the mud cake on their surfaces. Simulations have shown that such filters are equivalent from the point of view of washing efficiency to about three countercurrent filter stages without washing. It is indicated among the Y data, whether the filters used in the individual filtration stages may be considered to consist of several countercurrent stages or only of a single one (as e.g. Kelly filters do).

If burnt lime or a slaked lime slurry is added to the red mud, its sodalite or cancrinite structure will be broken up to a varying extent and caustic soda is set free from it. On the other hand, the lime will unite with the Al_2O_3 content of the liquor phase and of the sodalite/cancrinite content of the mud to form a silica-containing tricalcium hydroaluminate, so-called hydrogarnet. The efficiency of the causticizing may be approximated by a still unpublished formula of M.Matula:

$$\eta = \frac{1.5 \cdot M.K14.(1-e^{-0.534 \cdot K17})}{(M+2.5 \cdot S).(70+3.C)} \qquad (26)$$

where S is the SiO_2 content of the red mud in %,

M is the amount of burnt lime (with a 72 % average active CaO content) added to the red mud in % of the dry mud and

C is the actual caustic Na_2O concentration of the liquor phase in g/l.

The formula was based on the result of tests carried out in the research laboratory of the Almásfüzitő Alumina Plant in 1966. It was built into the mathematical model

after some modifications during which M and S have been expressed with other known data and the amount of lime has also been corrected according to its active CaO content given among the Y data.

If a single filtration stage is applied after causticizing, the initial caustic Na_2O concentration can be easily calculated on the basis of the knowledge of the liquor phase of the red mud to be causticized and after calculating the amount of the red mud wash water added for dilution. In the case of a two-stage filtration the liquor added for dilution is not water but the filtrate of the second filtration stage, the caustic Na_2O concentration of which is still unknown. In this case the calculation has to be repeated a few times until the correct concentration is approximated with the required accuracy.

The thermal calculations are also modified in the case of causticizing the red mud. In this case K14 does not mean the temperature of the red mud wash water but that of the causticizing, and only the heat loss of the first filtration stage has to be added to the temperature of the filtrate calculated on the basis of the heat balance of the last washing stage.

2.8 Iteration procedure

When reaching in the course of the calculations the end of the red mud washing (or that of the causticizing and/or filtration, if the process contains these steps, too) it has to be checked whether the estimated NO, AO and TO values of the total Na_2O and Al_2O_3 losses and of

the first washer temperature were correct or not. For this purpose the losses have to be summarized.

The total Na_2O losses consist of the following items:

N10 kg/t leaves the wet section for the calcination with the product hydrate.

N18 kg/t is removed at the evaporation together with the salts.

Y64 kg/t is the sum of the physical losses of the process cycle.

Y63 kg/t is chemically bound at the digestion (and to a lesser extent at other process steps) into various salts, mainly carbonates.

N[J-2] kg/t is chemically bound in the solid phase of the red mud leaving the process.

N[J-1] kg/t can be found in the liquor phase of the red mud in a dissolved or adsorbed form.

(The square brackets contain the serial number of the respective materials, J is the serial number of the red mud wash water which depends on the number of washing and filtration stages corresponding to Fig.1).

N29 kg/t, the amount of caustic Na_2O fed into the process cycle at one of the red mud washing stages has to be subtracted from the total of the Na_2O losses. So the losses to be replaced with fresh caustic will be

NO'=N10+N18+Y64+Y36+N[J-2]+N[J-1]-N29 kg/t (27)

instead of NO previously estimated.

The total Al_2O_3 losses consist of the following items:

A18 kg/t is removed at the evaporation together with be salts.

Y63 kg/t is the sum of the physical losses of the process cycle.

A[J-2] kg/t is chemically bound in the solid phase of the red mud leaving the process.

A[J-1] kg/t can be found in the liquor phase of the red mud in a dissolved form.

The amount of Al_2O_3 to be fed into the process cycle with the bauxite is over and above the Al_2O_3 content of the product hydrate (A3+A10)

AO'=A18+Y63+A[J-2]+A[J-1] kg/t (28)

instead of AO previously estimated.

On the basis of an estimated TO temperature of the first red mud washing stage a TO' temperature has been calculated from the heat balances of the washing and filtration stages. If red mud causticizing is applied in the process, TO' is that causticizing temperature, at the use of which the temperature of the first

washer would be exactly TO. If not, it is that red mud wash water temperature, at which the result would be the same. It is obvious that the previous estimates would have been correct if the following set of inequalities had been fulfilled:

$$\begin{aligned} &\text{abs } (NO-NO') < a \\ &\text{abs } (AO-AO') < b \\ &\text{abs } (K14-TO) < c \end{aligned} \qquad (29)$$

where a, b and c are the required accuracy limits of the Na_2O and Al_2O_3 balances and of the temperature of the red mud wash water or of the red mud causticizing. Their values are usually set to 0.01 kg/t and 0.01 ^{o}C, respectively. This accuracy seems to be excessive, however, in order to be able to determine corrently the economic consequences of a technological modification, the random errors of the calculation procedure have to be reduced to a minimum.

Should any of the inequalities (29) not be fulfilled, the calculation has to be repeated with a newly estimated set of NO, AO and TO values. The situation is complicated by the fact that the three variables have a cross-influence on each other, e.g. the raising of AO will not only increase AO' but also NO', because more bauxite means more chemical and soluble Na_2O losses and will also slightly modify the value of TO'; the raising of TO will reduce AO' by reducing the autoprecipitation losses, and also NO' because a reduced amount of red mud will reduce the amount of adsorbed and dissolved Na_2O leaving with it; etc.

Therefore, the correct values of NO, AO and TO have to be sought by solving the following simultaneous equations:

$$
\begin{aligned}
&NO'(NO,AO,TO)-NO = 0\\
&AO'(NO,AO,TO)-AO = 0 \qquad\qquad (29a)\\
&TO'(NO,AO,TO)-K14 = 0
\end{aligned}
$$

Since these simultaneous equations can not be solved directly, it has to be supposed that the correct solution is given by the

$$
\begin{aligned}
NO &= NO_o+\Delta NO\\
AO &= AO_o+\Delta AO \qquad\qquad (29b)\\
TO &= TO_o+\Delta TO
\end{aligned}
$$

triplet instead of the NO_o, AO_o and TO_o values of the first attempt. By developing the functions forming the left side of the simultaneous equations (29a) into geometrical progressions according to ΔNO, ΔAO and ΔTO after substituting (29b) into them and by reducing the higher-order members into a single function each,

$$
\begin{aligned}
&NO'(NO_o,AO_o,TO_o)-NO_o+\frac{\partial(NO'-NO)}{\partial NO}\Delta NO+\frac{\partial(NO'-NO)}{\partial AO}\Delta AO+\frac{\partial(NO'-NO)}{\partial TO}\Delta TO+\\
&\qquad +\varphi(\Delta NO,\Delta AO,\Delta TO)=0\\
&AO'(NO_o,AO_o,TO_o)-AO_o+\frac{\partial(AO'-AO)}{\partial NO}\Delta NO+\frac{\partial(AO'-AO)}{\partial AO}\Delta AO+\frac{\partial(AO'-AO)}{\partial TO}\Delta TO+\\
&\qquad +\psi(\Delta NO,\Delta AO,\Delta TO)=0 \qquad\qquad (30)\\
&TO'(NO_o,AO_o,TO_o)-K14+\frac{\partial(TO'-K14)}{\partial NO}\Delta NO+\frac{\partial(TO'-K14)}{\partial AO}\Delta AO+\frac{\partial(TO'-K14)}{\partial TO}\Delta TO+\\
&\qquad +\eta(\Delta NO,\Delta AO,\Delta TO)=0
\end{aligned}
$$

If the initial values are estimated sufficiently close to the correct values, the higher-order members can be neglected and the necessary corrections ΔNO, ΔAO and ΔTO can be determined by solving the resulting simultaneous linear equations.

The values of the partial differential quotients figuring in the simultaneous equations (30) can be approximated by slightly changing the initial data NO_o, AO_o and TO_o of the initially calculated "basic" variant one by one and by calculating the partial difference quotients by comparing the respective data after repeating the calculations three times, first changing NO_o, subsequently AO_o and finally TO_o.

The simultaneous equations (29a) will not be exactly fulfilled for the new material flows calculated with the new set of NO,AO and TO either because of the above neglections. However, if the functions on the left side of simultaneous equations (29a) are continuous, single-valued and monotonous between the values estimated at the first attempt and the correct ones (and care has been taken of this as described in the previous chapters), a better set of values will be obtained for NO,AO and TO. By repeating the whole procedure a few times finally such an approximation will surely be attained which satisfies all the inequalities (29).

Summing up the calculation procedure, a calculation cycle comprises the fourfold completion of the calculations described in Chapter 2.4 through 2.7, the results of the first of which are checked with the help of the simultaneous inequalities (29), and if they do not satisfy them,

the simultaneous equations (30) will be solved after three more calculation runs, and the whole calculation will be repeated with the corrected initial values. When a set of results satisfies the simultaneous inequalities (29), it will be accepted as the correct solution and the subsequent calculations will be begun.

The calculation procedure used is a slightly modified variant of the method described by Zuhrmühl [8].

2.9 Bauxite preparation

The most important data of another three characteristic material flows of the process cycle are calculated in the frame of this chapter: those of the digestion liquor (material flow 57), of the ground slurry (material flow 58) and of the digestion feed (or so-called pre-desilicated slurry, material flow 59).

The mass and the caustic Na_2O and Al_2O_3 contents of the digestion liquor can be obtained by summarizing the relevant data of material flows 7; 17; 20 and 23. Its other characteristics can be calculated by equations (1) through (6).

The amount of the ground slurry is determined on the basis of its required solids concentration in such a may that the quotient of the mass of the dry material content (B21) of the bauxite and of the sum of the volumes of its dry material and adhesive moisture contents and of the volume of the part of the digestion liquor used for grinding should give the dry material concentration stipulated

among the Y data. It has to be mentioned that components N, A, C, D and M of material flow 58 (and also those of material flow 59) contain the respective data of the liquor phase of the slurry whereas components B, V, W and F contain the data of the whole slurry.

The pre-desilicated slurry fed into the digesters is essentially the sum of material flows 21; 22 and 57, but its composition may be slightly modified by the chemical reactions starting already at its relatively low temperature. Pre-desilication is the process in the course of which the clay minerals containing most (or in some cases the whole) of the silica content of the bauxite are partially dissolved in the caustic liquor at temperatures below the atmospheric boiling point and subsequently sodium aluminium silicate (sodalite) will be formed of the relevant components of the liquor which will precipitate onto the solid phase. The efficiency of the pre-desilication is measured by the ratio of Na_2O bound into the bauxite in this process compered to the Na_2O content of the blow-off mud, both calculated for 1 t alumina.

During the processing of some (first of all of gibbsitic or gibbsite-containing) bauxites a "pre-digestion" process may go on parallelly to the pre-desilication, i.e. some of the Al_2O_3 content of the bauxite is dissolved in the digestion liquor. The efficiency of the pre-digestion is measured by the ratio of the amount of Al_2O_3 dissolved in this process compared to the total amount of Al_2O_3 dissolved here and during the digestion itself. The mathematical model will calculate the composition of material flow 59 by taking both processes described above into consideration.

3. THERMAL CALCULATIONS

The task of the next part of the mathematical model is to complete the thermal calculations begun when calculating the material flows of some unit operations (e.g. aluminate liquor cooling, red mud washing) in order to obtain some informative figure for the amount of steam required for the production of 1 t of alumina. No high accuracy was tried to be attained (however, in the case the initial data are given with a proper accuracy, the calculated steam consumption corresponds to that experienced in the plant) but first of all the possibility to be able to estimate correctly the thermal consequences of the variation of the main technological parameters. Therefore, a number of simplifications and neglections were made. Two types of steam were taken into consideration for covering the technological heat requirements: a high-pressure one (20 to 80 bar) for the digestion and a low-pressure one (3 to 6 bar) for the evaporation and if necessary, for other technological purposes. Of course it is possible that steam may be available at three or even four different pressure levels but the effect of using more kinds of steam can also be manually estimated after carrying out the calculations with the two most characteristic ones. The components WO and VO of the O vector are used for storing the specific consumptions of high-pressure and low-pressure steam, respectively.

3.1 Digestion (upper recuperation section)

Modern alumina plants use nearly exclusively continuously operated digestion systems consisting of series-connected autoclaves (a few even more modern ones use

tube digestion) and make far-reaching efforts to utilize the heat content of the digested slurry by flashing the latter in a multiflash system to a pressure approaching the atmospheric one and by heating the slurry to be digested by the vapours released in the multiflash system. After this the preheated slurry is further heated to the digestion temperature, usually by indirect steam (but quite often with a direct one). The indirect heating has been incorporated into the mathematical model, however, by suitably selecting the data the circumstances of a direct steam heating can also be approached.

The slurry to be digested is usually stored at a temperature above 80 ^{o}C (expediently between 90 and 100 ^{o}C) for 8 to 10 hours in Hungarian alumina plants ("pre-desilication", see Chapter 2.9). A slurry with such a high temperature could be hardly further heated by the vapour released in the last flash stage. Therefore, it is expedient to divide the heat recuperation into two sections and to heat the slurry before pre-desilication in the so-called lower recuperation section by the vapour(s) of the last one or two flash stage(s). The vapours of the rest of the flash stages heat the pre-desilicated slurry further in the upper recuperation section. The total number of flash stages is K19, the number of flash stages beloging to the lower recuperation section is given among the Y data (Y88), so the upper recuperation section consists of K19-Y88 stages.

The slurry enters the upper recuperation section at the temperature of T59 and leaves it at TO. (This is not the same temperature that was used in Chapters 2.6 and 2.8. After finishing the iteration this temperature can be erased from the memory of the computer and TO can

be used for other purposes.) At the same time the temperature of the digested slurry drops from T13 to T25. Since material flows 24 and 25 leave the digestion system together, at the same temperature, the T component of one of them (25) can be used to store the temperature of the slurry leaving the upper recuperation section, i.e. the flash tank with the serial number of (K19-Y88), whereas T24 is the temperature of the slurry leaving the last flash stage. The difference (T25-T59) may be called the "temperature gap at the input" of the upper recuperation section whereas the difference (T13-TO) the "temperature gap at the output" of the same. (The markings can be expressively seen in Fig.2. This shows the temperatures of the preheated and flash-cooled slurries as functions of the number of preheating/flashing stages for the whole recuperation range.) At the present phase of the calculation only the values of T13, T24 and T59 are known, the first two of them are equal to K8 and K9, respectively, the third one is given among the Y data.

The average temperature gap adds up of three components: of the average boiling point elevation, of the average temperature drop between two consecutive flash stages and of the average temperature difference between the two sides of the heating surfaces.

The boiling point elevation of sodium aluminate liquors is theoretically (and more or less also practically) independent of their Al_2O_3 concentrations, it only depends on their NaOH concentration and - to a lesser extent - on the concentration of the various sodium salts found in them. On the basis of the data at disposal [11] the following equation has been constructed to describe the boiling point elevation of pure NaOH solutions between 100 and 250 ^{o}C:

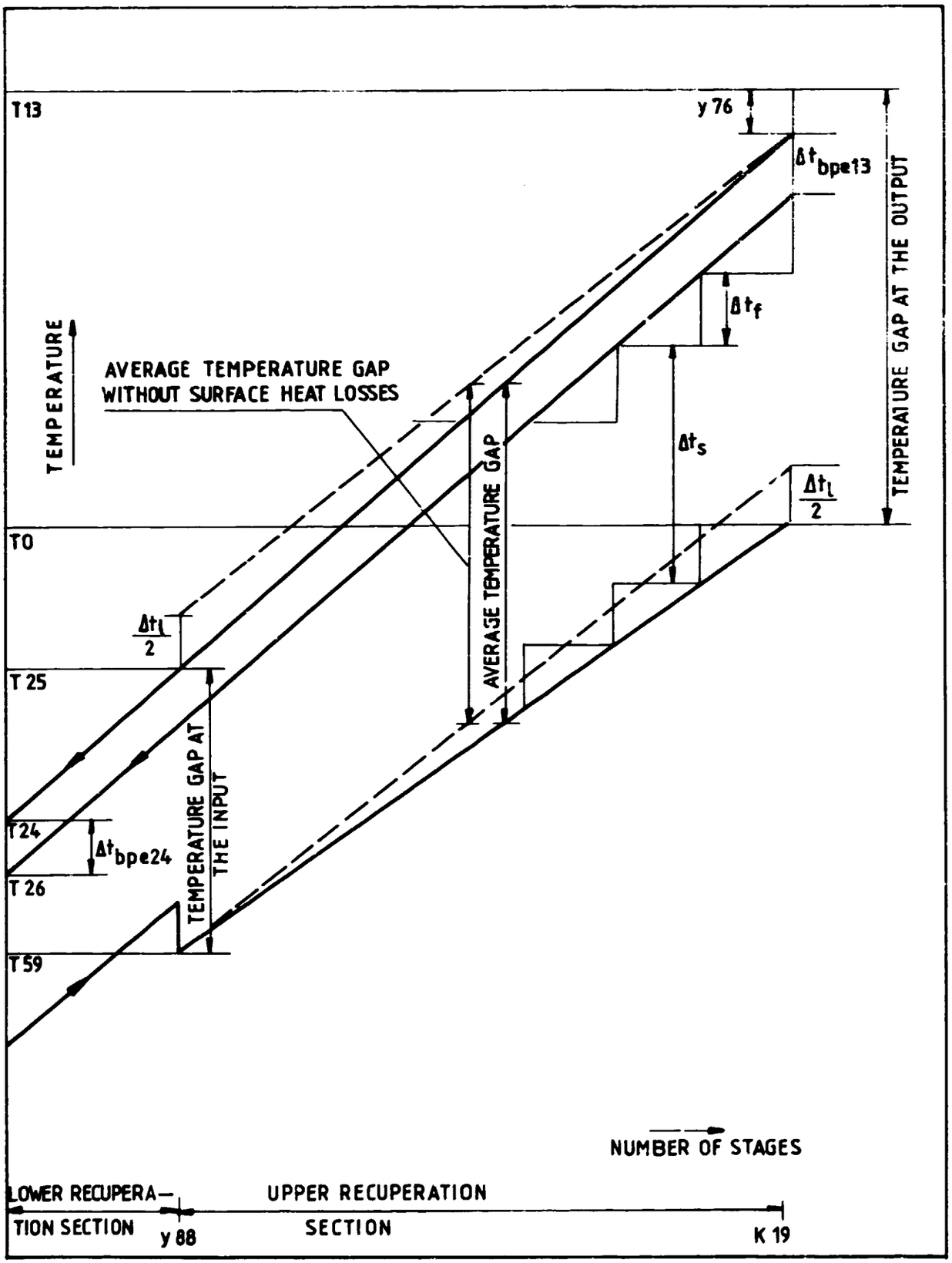

Fig.2. SCHEME OF HEAT RECUPERATION AT DIGESTION

$$\Delta t_{bpe}=t^2.(0.365c-0.076c^2)+t.(1.254c-0.2c^2)+1.068c^2+0.786c \quad (31)$$

where Δt_{bpe} is the boiling point elevation in ^oC,
t is the temperature of the solution in 100 ^oC and
c is its caustic Na_2O concentration in 100 g/l.

Since aluminate liquors are contaminated first of all by Na_2CO_3 and in some cases by Na_2SO_4, and these make three ions per Na_2O whereas NaOH makes four, it is expedien to calculate in the case of liquors containing MO mol chemically bound Na_2O for 1 mol caustic Na_2O with $(1+0.75 \cdot MO).c$ instead of c.

If the boiling point elevation is calculated for both material flows 13 and 24, the difference between them is usually less than 5 or 10 %. This is the result of the fact that the boiling point elevation increases both with the temperature and the liquor concentration. However, the liquor will be concentrated during the flash cooling and the effect of decreasing temperature and increasing concentration more or less compensate each other. Therefore, it is justified to calculate the whole recuperation system with a single (average) boiling point elevation. On the other hand, by subtracting the boiling point elevation of material flow 24 from T24 the T26 temperature of the alkaline condensate leaving the digestion can be calculated.

If the slurry is cooled in a finite number of flash stages, a part of its potential will be lost since even if using heat exchangers with infinitely large heating surfaces the temperature of the heated medium can not approach closer that of the cooled one than the temperature drop falling to one flash stage. Between the temperature limits of T13 and T25 an average temperature drop of

$$\Delta t_f = \frac{T13 - T25}{K19 - Y88} \quad {}^{o}C \tag{32}$$

falls to a flash stage in the upper recuperation section if there are K19-Y88 stages within it.

The third component of the temperature gap is the average temperature difference between the condensation temperature of the flash steam and the temperature of the heated digestion slurry. If such equipment is used for preheating, in which the slurry flows in tubes, the temperature difference will change from point to point along the tubes; if autoclaves complete with heating coils are used for the same purpose (which can be considered to be ideally mixed, i.e. the temperature of the slurry is the same in the whole equipment), the temperature difference will be the same along the whole heating surface. The formulae incorporated into the mathematical model describe the latter case but they can be easily replaced by others describing the former one, if necessary. The member of the temperature gap depending on the heating surface area is according to the heat transfer equation

$$\Delta t_s = \frac{Q.K21}{K15 \cdot n \cdot 8.76 \cdot k} \quad {}^{o}C \tag{33}$$

where Q is the amount of heat transferred in Mcal/t,
K21 is the capacity of the alumina plant in kt/a,
n is the number of simultaneously operating digestion lines and
k is the heat transfer coefficient in $Mcal/m^2h^oC$. The latter is given among the Y data.

The T59-TO heating curve in Fig.2. is not perfectly parallel to the T13-T25 flashing curve but it is usually closer to the horizontal by a few percents. (Anyway, the curves can only be considered to be straight lines as a first approximation.) This is caused on the one hand by the heat losses of the equipment, on the other hand by the dissipation of the amount of heat corresponding to the dilution heat during the evaporative concentration of the flashing liquor. These effects are partly compensated by the fact that the specific heat of the cooled slurry is slightly higher than that of the heated one since on the one hand the specific heat of the slurry recalculated for room temperature also increases during the dissolution of the aluminium hydroxides and on the other hand the correction factor of the specific heat of the slurry depending on the temperature is also higher at a higher temperature than that at a lower one. It has to be mentioned that a further flashing from stage to stage of the alkaline condensate of the flash steam originating from various flash stages was taken into consideration; this enables the heat capacity (water equivalent) of the flashing slurry to be considered constant.

The heat losses are composed of a number of factors. Some steam is lost during the continuous de-aeration of the steam chambers of the equipment and more or less steam passes over from one stage to the next with the slurry and the condensate. Since these factors appear first of all in the first stage of the flashing system and their value is more or less constant from here on (as much steam as has passed over "illegally" from the previous stage to the given one will pass over from here to the next one), they can be taken into consideration

with a Y data depending on the construction features of the given equipment by subtracting it from the T13 starting temperature of the flash cooling. (This data is marked in Fig.2. and in the further equations with Y76). Its value can be 2 to 3 °C under normal conditions.

Over and above these some surface heat losses will also arise, which are much more uniformly distributed along the recuperation section though they are usually higher in the higher temperature stages. An approximating formula has been set up on the basis of the measurements of Måhig and Råcz (12) for the calculation of the surface heat losses of the upper recuperation section expressed in °C as a function of the number of flash stages, of the heating surface area, of temperatures T13 and T59 and of the capacity of the digestion lines taking into consideration an average degree of heat insulation.

There is no reason to strive for a very high accuracy either in this case since this factor comes under normal conditions only to 1 or 2 °C, i.e. as much heat is lost through the (insulated) external surfaces of the equipment as required for the heating of the digestion slurry by 1 to 2 °C. The equation used is as follows:

$$T_1 = \left(\frac{(0.0195 + 0.00014 \cdot K15)\,(K19 - Y88)\,.n.8.76}{K21.W59} + 0.0002\,(K19 - Y88) + 0.0018 \right) . \left(\frac{T13 + T59}{2} - t \right) \quad {}^{o}C \qquad (34)$$

where n is the number of simultaneously operating digestion lines and

t is the temperature of the environment in °C.

The part of the surface heat losses arising on the heat releasing (i.e. cooling, flashing) side reduce the temperature gap (i.e. reduce the heat transfer) but that arising on the heat consuming side (i.e. preheaters) increase the same (i.e. increase the heat transfer). Since these two parts are of the same order of magnitude, their effect may be neglected when calculating the average temperature gap. On the other hand some 50 % of the heat losses have to be taken into consideration when calculating the amount of heat transferred.

Material flow 59 takes over

$$Q = \frac{W59(TO-T59+\Delta t_1/2)}{K19-Y88} \quad \text{Mcal/t} \qquad (35)$$

heat as an average in a single preheating stage. By substituting this into equation (33) the value of Δt_s will be expressed as a function of a single unknown variable, TO.

It follows from those previously described that the average temperature gap is

$$\Delta t_{bpe}+\Delta t_f+\Delta t_s = \frac{(T13-Y76-TO)+(T25-T59)}{2} \qquad (36)$$

If the average value of the boiling point elevation, further on Δt_f from equation (32) and Δt_s on the basis of equations (33) and (35) are all substituted into equation (36), an equation with two unknowns, TO and T25 will be obtained.

If the heat balance of the upper recuperation section:

$$W13.(T13-Y76-T25-\frac{\Delta t_1}{2})=W59(TO-T59+\frac{\Delta t_1}{2}) \qquad (37)$$

is combined with this, or rather a practically equivalent form of it significantly simplify the solving:

$$W13.(T13-Y76-T25)=W59(TO-T59+\Delta t_1) \qquad (37a)$$

the resulting simultaneous equations can be solved for TO:

$$TO=\frac{2.K15.k.(K19-Y88).(T13-Y76-\Delta t_{bpe}-\frac{\Delta t_1}{2}+\frac{T59}{2}.(\frac{W59}{W13}-1))}{2.\frac{W59.K21}{n.8.76}+(1+\frac{W59}{W13}).K15.k.(K19-Y88)+2.K15.k.\frac{W59}{W13}}+$$

$$+\frac{2.T59.(\frac{W59.K21}{n.8.76}+K15.k.\frac{W59}{W13})+\Delta t_1.(2.K15.k.\frac{W59}{W13}-\frac{W59.K21}{n.8.76})}{2.\frac{W59.K21}{n.8.76}+(1+\frac{W59}{W13}).K15.k.(K19-Y88)+2.K15.k.\frac{W59}{W13}} \qquad (38)$$

The third (last) member of the numerator of equation (38) can be neglected in the practice because its value is close to 0 under usual circumstances and it will not reach one thousandth of the total of the first two members even if twice the usual heating surface areas are installed.

It has to be mentioned that the equation can only be considered to be correct between the limits of

$$0.95 < \frac{W59}{W13} < 1.05$$

because if the difference between the heat capacities of the preheated and cooled slurries exceeds these, such large differences will arise between the flash stages that their averaging causes a significant error. However, the accuracy of the approximation can be significantly improved if the member $\frac{W59.K21}{n.8.76}$ found both in the numerator and in the denominator of equation (38) is multiplied by the correction factor $\frac{2.W13}{W59+W13}$. The formula incorporated in the mathematical model includes this correction factor with the further modification that a correction coefficient included among the Y data is ordered to every $\frac{W59}{W13}$ quotient of the formula. This can be used for dual purposes: for the better simulation of plant data and for taking into consideration the effect of direct steam heating. In the latter case the heat capacity of the digestion slurry may increase by 5 to 15 % with the amount of direct steam absorbed, therefore, the $\frac{W59}{W13}$ quotient has to be multplied by a factor between 0.95 and 0.85 if a correct calculation of the recuperation is desired.

When knowing TO, T25 can also be calculated from equation (37).

3.2 Digestion (fresh steam heated section)

When knowing the temperature of the preheated slurry (TO) both the heat (i.e. steam) requirement and the necessary heating surface area may be calculated. The heat requirement is added up of the amount of heat required for preheating the slurry from the temperature TO to the temperature T13, of the heat of dissolution of the aluminium hydroxide and of the heat losses of the digestion equipment. Since the heat losses are proportional to the size

of the digestion equipment, which is on the other hand determined by the necessary heating surface area, the best calculation procedure is to calculate first the heating surface area required by the first two components of the above total and then correct if by the heat losses proportional to it.

For the calculation of the reaction heat of the digestion the data collected by Sato (13) have been taken into consideration. According to these the heat of dissolution is about 90 kcal/kg Al_2O_3 for boehmite and about 140 kcal/kg Al_2O_3 for gibbsite. Since most of the gibbsite present in Hungarian bauxites is dissolved during pre-desilication, the Al_2O_3 undigested during pre-desilication can be considered boehmitic under Hungarian conditions. For other bauxites this might not be the case. Therefore, the calculation method has always to be adapted to the given bauxite.

On the other hand the heat of dissolution is supposed to be distributed similarly to the heat required for heating. This means that if the slurry is heated in a given autoclave by say 40 % of the temperature difference T13-TO, 40 % of the total heat of dissolution is taken into consideration to be required in the same.

In order to be able to combine a continuous cost function with the mathematical model, the heating surface area of the digesters has not been fixed but the number of fresh steam heated autoclaves belonging to a digestion line has been given among the Y data. The required heating surface area is calculated by the model itself and it prints it in the FO component of the O vector. This

solution was necessary because otherwise a slight modification of any data, e.g. of the number of flash stages or even of the precipitation time could have caused a sudden cost increase, because it would have been possible that in a given variant say 3 fresh steam heated autoclaves would have been sufficient but in an other one differing only infinitesimally the model would have required a fourth autoclave for heating the slurry a tenth or even a hundedth of a centigrade. In the present solution the mathematical model takes into consideration a heating surface area only a few tenth or hundredth of a m^2 larger then in the other variant together with only a minor change of the costs and leaves the final decision to the user of the mathematical model, whether this minor change of the required heating surface area is still acceptable or not.

After having determined the total heat requirement the WO specific steam requirement of the digestion can be calculated with the help of the specific heat content (entalpy) of the steam and its condensate and of the thermal efficiency of the heating, all given among the Y data.

3.3 Bauxite preparation, lower recuperation section

The process of bauxite preparation taken into consideration from the point of view of thermal calculations is the following: the bauxite is ground with a part of the digestion liquor in a wet process; the rest of the digestion liquor is added to the ground slurry; the resulting "adjusted" slurry is preheated by the vapours of the last Y88 flash stages of the digestion to such a temperature which ensures that the heat losses of the pre-desilication and the heat requirement of the pre-

digestion are covered and that the temperature of the pre-desilicated slurry still attains the prescribed value of T59 after subtracting the above heat losses and heat requirement. Therefore, the calculation starts at the end of the process. As a first step the heat requirement of the pre-digestion (140 kcal/kg pre-digested Al_2O_3) and the calculated heat losses are added to the heat content of material flow 59 and this way the final temperature of the lower recuperation section (see Fig.2) is determined. Subsequently, the temperature of the adjusted slurry is calculated with the help of the thermal efficiency (90-95 %) given among the Y data. When knowing the said temperature simultaneous equations with two unknowns can be set up for T57 and T58. The first of these equations is the heat balance of the slurry adjustment (i.e. of the mixing of the ground slurry and of the rest of the digestion liquor), the second one the heat balance of the wet grinding. The latter may take into consideration the grinding work transformed into heat, preferably in such a way that heat losses are considered only above that temperature at which the grinding work just compensates them. This temperature may be about 40 to 50 ^{o}C.

3.4 Minor heat consumers and heat sources

Relatively minor heat requirements or heat surpluses may arise at various points of the Bayer process cycle. Those efforts which have been made in order to construct stable thermal flow-sheets for covering the minor heat requirements of the process cycle have not been completely successful. Therefore, only a general thermal scheme has been incorporated into the present mathematical model. This is able to estimate the heat requirements and so enables the model to take the effect of the variation of

various technological and thermal parameters exerted on the total steam consumption into consideration, however, the optimum solution for a given case has to be found manually.

One of the largest heat requirements may arise at the preparation of the digestion liquor. Should the temperatures of material flows 17, 20 and 23 (the latter also containing material flow 7) not be sufficiently high to provide the required temperature T57 of the digestion liquor and also to cover the heat losses of the digestion liquor storage tanks, material flow 17 and/or 20 have to be preheated. The preheating should begin with the cooler one of them, however, should the preheating of this material flow to the temperature of the other one still not be sufficient to cover the heat requirement, it may he preferable to heat them together or parallelly to a common temperature.

The situation at the dilution may be similar. Should the heat contents of material flows 24, 27 and 32 not be sufficient to ensure settling temperature K11 after covering the heat losses of the dilution and red mud settling, material flows 27 and/or 32 have to be preheated.

The third significant heat consumer may be the red mud wash water. Usually the alkaline condensate of the digestion (material flow 26), a part of the alkaline condensate of the evaporation (left over after covering the requirement for hydrate wash water) and the condensate of the flash cooling of the alumina liquor, if any (material flow 12) are used for this purpose. It is preferable to cover the difference between the required amount of red mud wash water and the total amount available from the above three

sources from the warm cooling water of the calciners or the evaporation since these are significatnly hotter than any fresh water. Some weak liquor returned from the mud lakes may also be used for this purpose. (This is usually quite cold but has some dissolved caustic and carbonated Na_2O contents.) Should the prescribed temperature K14 of the red mud wash water (or the wash water temperature given among the Y data in the case of applying mud causticizing) not be attained by mixing the above materials, some of them (preferably the coldest one(s)) have again to be preheated.

In the case of applying a red mud causticizing combined with a two-stage mud filtration it may also be expedient to preheat the filtrate of the second filtration stage (which is preferably led into the causticizing tanks to provide a completely countercurrent system) in order to reduce the steam requirement of the causticizing process.

The items listed above may represent such a significant total heat consumption that it is preferable to cover them by vapours bled from the relevant effects of the evaporators since these are significantly cheaper than the fresh steam. If e.g. 1 t of vapour is bled from the second effect of a four-effect evaporator, this will increase the fresh steam consumption of the same by about 0.6 t, supposed that the total amount of evaporated water remains the same; so it can be said that this vapour costs half as much as the fresh steam. It is given among the Y data, to what temperature a material flow may be preheated by a vapour bled from a certain effect of the evaporators. (Of course, should any circumstance prevent

such a steam saving, the mathematical model can adapt to this: the said Y data have to be given low values, in this case fresh steam will be taken into consideration for preheating.)

A few minor heat consumers like the heat requirement of the preheating of the fresh caustic liquor used for precipitator descaling are preferably taken into consideration with full-value low-pressure steam since the savings to be achieved by using vapours bled from the evaporators for these purposes are not worth the extra efforts required. The steam consumed for the heating of the intermediate tanks of the hydrate filtration is considered to be proportional to the amount of hydrate wash water. The steam to wash water ratio is given among the Y data. Fresh steam was also taken into consideration for suppling that part of the heat requirement of salt causticizing which is necessary for further heating the solution originating from the red mud wash water and for covering the heat losses.

The total vapour bled from the evaporators has to be summarized and the sum checked whether it can be covered by the amount of water to be evaporated for 1 t of alumina. Even if special evaporators are designed for this purpose, not more than 0.33 t of third-effect, or 0.5 t of second-effect or 1 t of first-effect vapour can be utilized per t of total evaporated water. The total amount of water to be bled from commercial evaporators not designed for this purpose may be much less than that. Therefore, a coefficient is given among the Y data to show, how many Mcal heat may be utilized as first-effect vapour per t of evaporated water as a maximum. (Half of this may be utilized as second-effect, a third of this as third-effect vapour,

etc.) should more heat be required of these low-value vapours than allowed, a part (or all) of the requirements will be covered by fresh low-pressure steam.

3.5 Evaporation

A half-empirical formula has been set up for the calculation of the steam consumption of the evaporation which is more or less independent of the effect of vapour bleeding since this has already been previously taken into consideration. According to this, if B19 t of water is evaporated for 1 t of alumina, the amount of heat required for this is

$$Q=B19.(a+b.t)+W14.(c-d.T14)+W15.(e-f.T15) \quad \text{Mcal/t} \qquad (39)$$

where t is the temperature of the strong liquor leaving the evaporator sets given among the Y data in °C and a through f are constants depending on the number of effects of the evaporators and on their operation mode (concurrent, countercurrent or mixed current) also given among the Y data. The temperatures of the pure and alkaline condensates leaving the evaporator (i.e. the possible utilization of their heat content) have to be taken into consideration in the value of a. On the basis of the thermal measurements carried out by ALUTERV in 1959-1960 in the Ajka Alumina Plant the following equation can be used for a four-effect concurrent Vogelbush-type evaporator if the temperature of the pure condensate is 100 °C, that of the alkaline one 95 °C, that of the strong liquor about 70 °C and the temperature of the spent liquor and of the alkaline hydrate wash water are between 70 and 90 °C:

$$Q=B19.(160+0.4\cdot t)+W14.(45.6-0.5\cdot T14)+W15.(45.6-0.5\cdot T15) \qquad (39a)$$

whereas if the latter are between 50 and 70 ^{o}C,

$$Q=B19.(16C+0.4\cdot t)+W14.(28.1-0.25\cdot T14)+W15.(45.6-0.25\cdot T15) \quad (39b)$$

By adding the above Q heat requirement to those summarized in Chapter 34 the total heat requirement to be covered by low-pressure steam can be obtained. By dividing this sum by the heat obtainable from 1 t of low-pressure steam (taking also into consideration that some of the heat content of its condensate may be utilized before returning the latter into the steam plant) the total low-pressure steam consumption (to be stored in the VO component of the O vector) can be calculated.

4. OUTPUT OF THE CALCULATION RESULTS

A printing program has been prepared for the mathematical model, which prints all the vectors from 0 to 60 on a line-printer, each vector into a separate line, with all ten compoments. In order to make sure that the initial data are always unequivocally ordered to the material flows, the printing program always reprints the Y and K data together with the calculation results. A set of data and a table of material flows calculated from it are attached to the description of the mathematical model.

5. UTILIZATION OF THE MATHEMATICAL MODEL

The mathematical model of the Bayer process described above can be utilized in a number of ways. These can be divided into three groups:

1.) Checking of the material flows of existing alumina plants.

2.) Calculation of the material flows and estimated steam requirements of new or reconstructed alumina plants being designed, i.e. the supply of data for process and mechanical engineering.

3.) Supply of technological data for manual or computerized economic calculations.

1. Checking of the material flows of existing alumina plants

There are two main utilization possibilities within this group: the modelling of well-known (e.g. domestic) and of lesser-known (e.g. foreign) alumina plants.

In the first case all the necessary initial data of the calculation are at the disposal of the user of the mathematical model. Should the material flows or other technological parameters (e.g. concentrations, etc.) calculated by this significantly differ from those measured in the plant, conclusions can be drawn on the technological mistakes committed. E.g. when modelling the operation of a Hungarian plant it was found that nearly 3 m^3 of unaccounted ("false") water was introduced into the process for every tonne of alumina produced. This significantly increases the heat consumption of the process and reduces the efficiency of the red mud washing.

The characteristic technological parameters of foreign alumina plants can also be more or less reconstructed by the mathematical model by varying the Y and K data until the results of the modelling approach the data published in the technical literature or disclosed by the plant. In order to facilitate this work a frame program has been constructed to the mathematical model which simultaneously varies three of the Y and/or K data until three of the calculated data (any components of vectors O through 60) attain some prescribed values. This frame program operates rather similarly to the procedure described in Chapter 2.8.

2. Supply of engineering data

When fixing the initial parameters (Y and K data) the mathematical model will calculate the amount and composition of every significant material flow of the main unit operations of the Bayer process cycle of alumina manufacturing. These results serve as the basis of every engineering phase both in the case of designing a new alumina plant or expanding an existing one. The use of the mathematical model significantly accelerates the technological (chemical, process) engineering and supplies much more accurate data both for the mechanical engineering and the economic calculations as any manual calculation would do. Since its setting up about twenty years ago this mathematical model was used for such purposes for at least twenty different projects, for the calculation of many hundreds of variants.

Since the output system described in Chapter 4 supplies the calculation results in a very much compressed form which can not be easily interpreted by uninitiated people, some interpreting programs have also

been set up to transform the calculation results into proper material and heat balances. However, it is very difficult to prepare such interpreting programs so that they fit to every possible technical solution , therefore, they are quite rarely used.

3. Economic calculations

The economic calculations which may be carried out with the help of the mathematical model can be divided into three main groups, though these groups can not be sharply separated from each other.

The first group consists of the economic comparison of such technological variants which have no effect on the capital costs of a plant or at least these may be neglected. Such an alternative may be to add the spent liquor intended for increasing the caustic Na_2O to Al_2O_3 molar ratio in the red mud settlers and washers in order to reduce the autoprecipitation losses to the dilution of the blow-off slurry or into the first red mud washing stage. If all the other technological parameters are fixed, this question can be decided by comparing the bauxite, caustic soda and steam consumption of the two alternatives. (The better solution in most cases is to add it to the first washer.)

Another parameter which can be optimized by only comparing the consumption figures is the optimum temperature of the red mud wash water. (In the case of the Ajka Alumina Plant a temperature of 77 ^{o}C was found to be optimal.)

The second group comprises those calculations in which the variants compared also differ in their capital costs, but these differences are confined to one or two plant units. Such a calculation may be the determination of the optimum number of red mud washing stages, of digestion flash stages, of evaporator effects, or even the decision between a flash system and plate heat exchangers at the alumina liquor cooling. (On the basis of such calculations a 7-stage mud washing system, a 9-stage flash system, a 5-effect evaporator and surface cooling of the aluminate liquor were selected.)

The third group consists of those calculations at which the alternatives involve different capital costs at most plant units. E.g. the variations of the precipitation time, of the evaporation rate, of the temperature and molar ratio of the digestion, of the concentration and molar ratio of the aluminate liquor have primary or secondary effects on the capital costs of nearly every plant unit, so their optimum values can only be determined by taking into consideration the changes caused by their variation all over the plant.

On the other hand, the parameters belonging to the third group have a very strong cross-influence on each other. Therefore, their optima can only be determined by varying most or all of them simultaneously.

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APPENDIX

LIST OF THE Y DATA OF THE MATHEMATICAL MODEL

Y1 - is the average outdoor temperature, ^{o}C.

Y2 - is the average indoor temperature, ^{o}C. Y1 and Y2 are used when calculating the heat losses of digesters, filters, settlers, precipitation tanks, etc.

Y3 - is the Al_2O_3 content of the washed product hydrate, kg/t alumina. It depends on dust control, L.O.I., type of calcination, etc. It is usually in the range of 990 to 1005 in the case of modern kilns, and in the range of 1005 to 1020 in the case of older ones.

Y4 - is the temperature of the cooled aluminate liquor fed into the precipitation, ^{o}C.

Y5 - is the temperature of the first tank in the continuous precipitation line, ^{o}C.

Y6 - is the temperature of the last tank in the continuous precipitation line, ^{o}C.

Y7 - is the temperature of the filtered spent liquor or that of the tray thickener overflow, ^{o}C.

Y8 - is the temperature of the filtered product hydrate, ^{o}C.

Y9 - is the temperature of the pure hydrate wash water, ^{o}C.

Y10 - is the temperature of the alkaline hydrate wash water, ^{o}C.

Y11 - is a parameter used for calculating the amount of scalings in precipitation and hydrate classification, given as kg Al_2O_3 per ton of alumina and hour of precipitation time.

Y12 - is the water content of the wet product hydrate in the first filtration stage or that of the compacted solids in the primary thickener underflow before injection with water, $\frac{\text{kg water}}{\text{kg wet hydrate}}$.

Y13 - is same figure for seed, $\frac{\text{kg water}}{\text{kg wet hydrate}}$.

Y14 - is the temperature drop of the aluminate liquor between the red mud settlers and the aluminate liquor cooling, ^{o}C.

Y15 - is the temperature of the washed product hydrate, ^{o}C.

Y16 - is the hydrate content of the spent liquor (filtrate or tray thickener overflow) expressed as the ratio of Al_2O_3 in suspended hydrate [gpl] per caustic Na_2O concentration [gpl] in the liquor.

Y17 - is the amount of Na_2O bound in sodium carbonate which has to be supersaturated in the strong liquor in order to maintain a stable salt level, kg/t alumina.

Y18 - is the Na_2O content of product hydrate, kg/t alumina.

Y19 - is the free water content of the washed and filtered product hydrate, $\frac{\text{kg water}}{\text{kg wet hydrate}}$.

Y20 - is the caustic Na_2O concentration of the alkaline hydrate wash water, gpl.

Y21 - is the amount of alkaline hydrate wash water fed to the evaporation, m^3/t evaporated water. (The rest goes to the first red mud washing stage; if a negative figure is given, the alkaline wash water is mixed to the spent liquor, and average concentrations will be calculated.)

Y22 - shows, whether the strong liquor concentration given in K6 applies before or after solid caustic dissolving and salt removal (in the first case it is 0, in the latter it is 1).

Y23 - is coefficient b of reaction rate equation (12) of the precipitation.

Y24 - is coefficient a of equation (12).

Y25 - is the first coefficient of equation (12a).

Y26 - is the second coefficient of equation (12a).

Y27 - is the amount of the filtered carbonate salt including the adhesive strong liquor, t/t alumina.

Y28 - is the volume of the filtered carbonate salt including the adhesive strong liquor, m^3/t alumina.

Y29 - is the Al_2O_3 content of the filtered carbonate salt including the Al_2O_3 content of the adhesive strong liquor, kg/t alumina.

Y30 - is the caustic Na_2O content of the filtered carbonate salt including the caustic Na_2O content of the adhesive strong liquor, kg/t alumina.

Y31 - is a correction factor of the caustic Na_2O concentration in the precipitation used for the calculation of the reaction rate constants in equations (10) and (11).

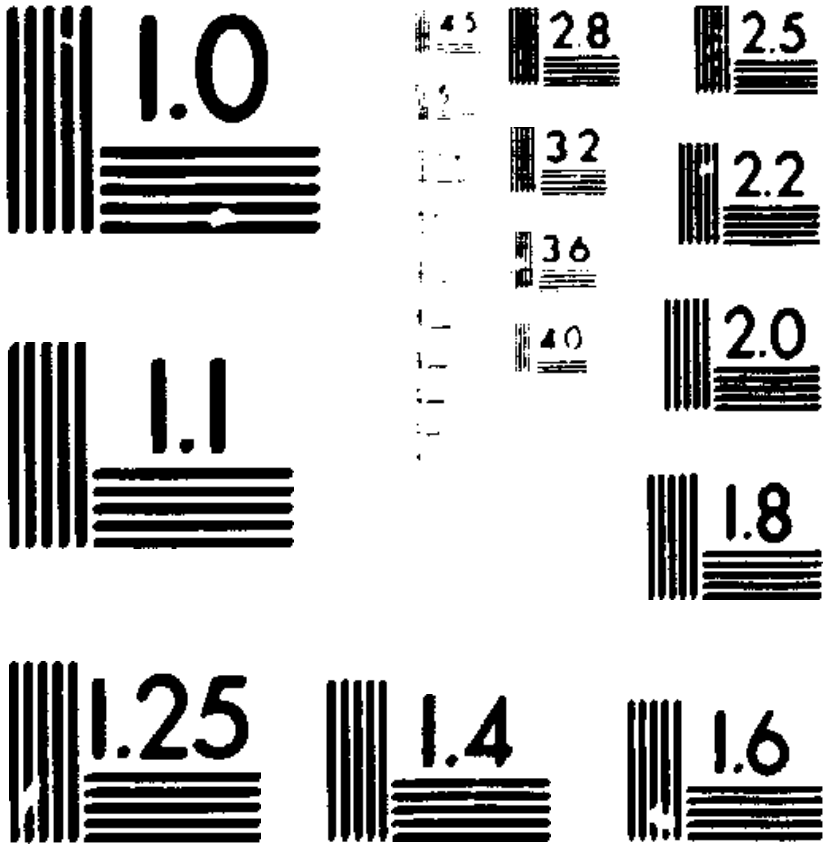
Y32 - is coefficient a of equation (14). It means the Al_2O_3/SiO_2 ratio to be attained in the blow-off mud when applying an infinitely high digestion molar ratio. If there is only a single test result available, the Al_2O_3/SiO_2 ratio of this test will be used for Y32 and 0 is written into Y34, Y39 and Y40.

Y33 - is the Al_2O_3/SiO_2 ratio of the bauxite to be processed, kg/kg.

Y34 - is coefficient b of equation (14).

Y35 - is one of the components of coefficient a of equation (15) serving for the calculation of the Na_2O content of the red mud (the one proportional to the SiO_2 content) (see also Y57, Y71 and Y75).

Y36 - is the amount of Na_2O bound into various salts during digestion (and to a lesser extent during the other steps of the process), kg/t alumina.



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Y37 - is the amount of caustic Na_2O recovered by salt causticizing and fed into the red mud washing system, kg/t alumina.

Y38 - is the concentration of the liquid make-up caustic, gpl Na_2O.

Y39 - is coefficient d of equation (14).

Y40 - is coefficient c of equation (14).

Y41 - is coefficient e of equation (14).

Y42 - is the total Al_2O_3 content of the bauxite to be processed, kg/t dry bauxite. Lime addition can be taken into consideration by proportionally reducing the Al_2O_3 content.

Y43 - is the density of bauxite solids, t/m^3.

Y44 - is the adhesive moisture content of the bauxite relative to its dry material content, t/t. Various amounts of water introduced into the process between bauxite grinding and digestion can be taken into consideration in this figure.

Y45 - is the amount of blow-off mud formed when attaining a theoretical extraction yield, t/t dry bauxite.

Y46 - is the density of the blow-off mud, t/m^3.

Y47 - is the ratio of the Na_2O contents of the blow-off and settler muds. This coefficient enables the user of the mathematical model to take into considera-

tion the well-known phenomenon that a part of the sodium titanate formed during the digestion may release its Na_2O content to a more diluted liquor.

Y48 - is a constant which decides if the adhesive moisture content of the bauxite is taken into consideration when calculating the equilibrium digestion molar ratio (if yes, Y48 = 1; if not, Y48 = 0).

Y49 - is a correction coefficient for calculating the amount of flash steam released in the digestion system (coefficient a of equation (19)). By reducing this figure the effect of the introduction of some water into the digestion (e.g. of direct steam and/or gland water) can be simulated.

Y50 - is the first coefficient of equation (22) used for calculating the autoprecipitation in settling and washing.

Y51 - is the height of the red mud settlers, m.

Y52 - is the constant of equation (22).

Y53 - is the height of the red mud washers, m.

Y54 - is the thermal efficiency of the heat interchange at the aluminate liquor cooling, %/100.

Y55 - is the temperature of the causticized salt slurry or any other diluted plant liquor fed into the red mud washing system (material flow 29), ^{o}C.

Y56 - is the heat loss coefficient of the red mud settlers and washers calculated for a unit settling area, $Mcal/m^2h^oC$.

Y57 - is the other component of coefficient a of equation (15).

Y58 - is the total settling area of the red mud settlers, m^2.

Y59 - is the total settling area of the red mud washers, m^2 per washing stage. If the various washing stages have different settling areas, an average figure has to be given, weighted according to the aspects of heat losses and autoprecipitation.

Y60 - is the heat loss coefficient for mud filtration, $^oC/^oC$.

Y61 - is the temperature of the red mud wash water if the mud is causticized, ^oC. (If not, this temperature is given in K14).

Y62 - is the correction coefficient of equation (26) used for calculating the efficiency of mud causticizing.

Y63 - is the sum of physical Al_2O_3 losses, kg/t alumina.

Y64 - is the sum of physical Na_2O losses, kg/t alumina.

Y65 - is the total amount of physical losses, t/t alumina. (If a negative figure is given, the effect

of the introduction of some unaccounted water into the process can be simulated. This amount of water will show up in the material balance of the evaporation.)

Y66 - is a distribution coefficient for the part of the spent liquor used neither in the evaporation nor in the digestion between dilution and the first mud washing stage. (If 0, all spent liquor is fed into the first mud washing stage; if 1, it is fed into the dilution; by giving a figure between 0 and 1 the spent liquor can also be distributed between this two units in any proportion required.)

Y67 - is the caustic Na_2O concentration of the causticized salt solution or any other plant liquor fed into the red mud washing system, gpl.

Y68 - is a coefficient showing what part of the soluble Na_2O content of the red mud is returned from the mud pond, kg/kg.

Y69 - is the maximum amount of filtrate which may pass through the mud filters, m^3/t alumina. If 0 or a high figure is given, no restriction will be taken into consideration and the total amount of available wash water will pass through the filters. If a restriction is applied, the excess amount of red mud wash water will bypass the filters and enter the last decantation stage.

Y70 - if this figure is 0, it means that plate heat exchangers are used for aluminate liquor cooling; if it is 1, a flash system is used; figures between 0 and 1 make the modelling of mixed systems possible.

Y71 - is coefficient b of equation (15).

Y72 - is the number of the simultaneously operating digester lines.

Y73 - is the heat transfer coefficient of the live steam heated preheaters or digesters, $Mcal/m^2h^oC$.

Y74 - is the heat transfer coefficient of the flash steam heated preheaters, $Mcal/m^2h^oC$.

Y75 - is coefficient c of equation (15).

Y76 - is the constant heat loss mentioned at the description of the digestion, expressed in ^oC.

Y77 - is the temperature of the slurry fed into the digester lines (i.e. the final temperature of of the predesilication, if any), ^oC.

Y78 - is the constant of the linear function describing the relationship between mud load and mud compaction in settlers mentioned in Chapter 2.5, t mud/m^3 underflow.

Y79 - is the load-coefficient of the same linear function, h/m.

Y80 - is the same for washers as Y78 and is for settlers.

Y81 - is the same for washers as Y79 is for settlers.

Y82 - is the number of stages in the continuous precipitation line(s).

Y83 - is the correction coefficient mentioned in connection with equation (38).

Y84 - is the saturation temperature of the high pressure steam, ^{o}C.

Y85 - is the heat content of the high pressure steam, Mcal/t.

Y86 - is the heat content of the condensate of the high pressure steam, Mcal/t.

Y87 - is the thermal efficiency of the high pressure steam heating, %/100.

Y88 - is the number of flash stages heating the slurry before digestion.

Y89 - is the number of digesters per digestion line heated with high pressure steam.

Y90 - is the number of unheated digesters per digestion line.

Y91 - is the heat loss coefficient of the predesilication, $^{o}C/^{o}C$.

Y92 - is the thermal efficiency of the slurry heating before digestion (in the predesilication unit, if any), %/100.

Y93 - is the predesilication efficiency defined as the amount of Na_2O bound into the predesilicated bauxite before digestion compared to that present in the blow-off mud, %/100.

Y94 - is a coefficient showing the change in bauxite mass when Na_2O is bound into it during predesilication, t/kg Na_2O.

Y95 - is the Al_2O_3 extraction yield during predesilication, %/100.

Y96 - is the solids concentration of the ground bauxite slurry, t/m^3.

Y97 - is the active CaO content of the burnt lime used at the red mud causticizing, %/100.

Y98 - is the adhesive liquor content of the mud filtered in a first red mud filtration stage (if any), m^3/t solids.

Y99 - is the same for the mud filtered in a second stage (if any), m^3/t.

Y100 - is the heat loss coefficient of the bauxite grinding, Mcal/t dry bauxite and ^oC, where the temperature difference is calculated between the temperature of the ground slurry and the temperature given in Y101.

Y - is that grinding temperature at which it is supposed that grinding work compensates for heat losses, ^{o}C.

Y102 - is the temperature of the liquid make-up caustic after using it for precipitator cleaning, ^{o}C.

Y103 - is the heat loss coefficient of the test tank liquor storage, $^{o}C/^{o}C$.

Y104 - is the temperature of the strong liquor leaving the evaporator set, ^{o}C.

Y105 - is the balance of the heat of dissolution and the heat loss at the solid caustic dissolution, Mcal/t solid NaOH.

Y106 to Y110 - are temperatures which show up to what temperature any steam bled from the evaporators can be used for heating. Y106 is the temperature characteristic of the last-but-first effect, Y107 that of the last-but-second one, etc. There is space to accomodate the data for 6-effect evaporator sets.

Y111 - is the temperature of the hottest water being available without preheating costs (in most cases warm water from evaporator condensers or the coolers of the calciners), ^{o}C.

Y112 - is the percentage of alkaline condensate left after subtracting various losses, t/t.

Y113 - is the coefficient showing how much alkaline condensate can be theoretically obtained in the evaporation out of one ton of evaporated water, t/t.

Y114 - is the temperature of the alkaline evaporator condensate, ^{o}C.

Y115 - is a coefficient showing what part of the heat content of the alkaline condensate can be utilized, $^{o}C/^{o}C$.

Y116 - is a coefficient showing how much heat is lost at the salt filtration, centrifuging, settling, etc., $^{o}C/^{o}C$.

Y117 - is coefficient a of equation (39).

Y118 - is coefficient b of equation (39).

Y119 - is coefficients c and e of equation (39) if coefficients d and f are 0.

Y120 - is the heat utilization efficiency of the heat content of the condensate of the high pressure digestion steam, %/100.

Y121 - is the heat content of the low pressure steam, Mcal/t.

Y122 - is the heat content of the condensate of the low pressure steam in the evaporation, Mcal/t.

Y123 - is the saturation temperature of the low pressure steam, ^{o}C.

Y124 - is the temperature of the condensate recyled from the alumina plant to the steam or power plant, ^{o}C.

Y125 - is the heat required for dissolving precipitator scalings, Mcal/kg Al_2O_3.

Y126 - is the heat utilization factor of pure evaporator condensate, %/100.

Y127 - is the amount of steam required a the product hydrate filtration for periodical reheating compared to the amount of hydrate wash water, t low pressure steam/t pure hydrate wash water.

Y128 - is the heat loss coefficient at the dilution, $^{o}C/^{o}C$.

Y129 - is the thermal efficiency of the low pressure steam heating in the evaporation, %/100.

Y130 - is the maximum temperature of the liquor (wash water or filtrate of the second filtration stage) added to the red mud causticizing, ^{o}C. (If the heat requirement of the mud causticizing can be covered by heating the liquor in question to the maximum allowed temperature, this can be suitably solved by using steam bled from the evaporators; if not, the extra heat required has to be provided by live steam heating.)

Y131 - is the heat loss coefficient of red mud causticizing, $^{o}C/^{o}C$ h.

Y132 - is the maximum amount of heat utilizable from evaporator bleeding, Mcal/t evaporated water.

Y133 - is a correction coefficient of Na_2O adsorbtion (equation (24) or (25)) for causticized red mud.

Y134 - is the heat loss coefficient at salt causticizing, $^{o}C/^{o}C$.

Y135 - is a figure representing unaccounted water introduced into precipitation, t/t alumina.

Y136 - is the serial number of the red mud washing stage into which the causticized salt slurry is fed.

Y137 - is the complementary number of the mud washing stage into which the liquor from red mud causticizing is fed. (If 0, it is fed into the last washing stage; if 1, into the last but one; etc.)

Y138 - is the total volume of one stage of the continuous precipitation, m^3.

Y139 - is the estimated total of Al_2O_3 losses, kg/t alumina (starting figure of the iteration).

Y140 - is the number of theoretical counter-current washing stages equivalent to the first red mud filtration stage.

Y141 - is the number of theoretical counter-current washing stages equivalent to the second red mud filtration stage.

Y142 - is the key number for selecting the red mud filtration and/or causticizing technology:

if Y142 = 0, no filtration, no red mud causticizing,
if Y142 = 1, one filtration stage, no red mud causticizing,
if Y142 = 2, two filtration stages, no red mud causticizing,
if Y142 = 3, one filtration stage followed by red mud causticizing and a second filtration stage,
if Y142 = 4, red mud causticizing followed by one filtration stage,
if Y142 = 5, red mud causticizing followed by two filtration stages.

Y143 - is the key number for selecting the appropriate equilibrium solubility formula:

if Y143 = 1, the solubility formula for gibbsite,
if Y143 = 2, the solubility formula for boehmite,
if Y143 = 3, the solubility formula for diaspore.

Y144 to Y150 - are coefficients used for special purposes.

RAYON MATERIAL FLOWS

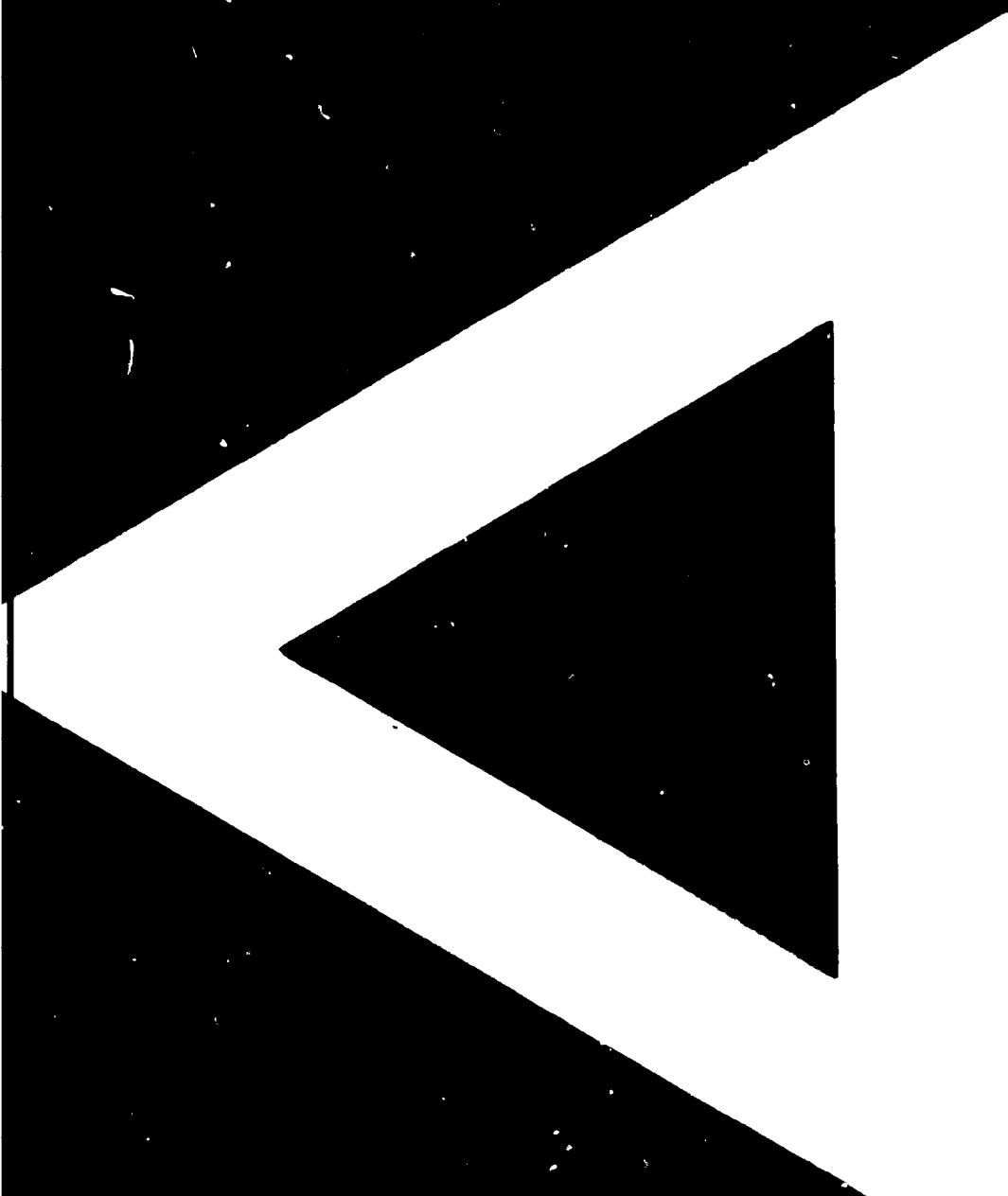
J		A	H	V	W	C	D	P	F	T
1	28.11	205.00	0.0	2.520	1.897	272.98	955.54	8.914	344.491	147.198
2	2317.53	2311.52	17.592	14.812	15.949	140.01	139.58	1.650	1.290	62.000
3	1471.21	472.35	17.146	13.994	15.226	140.86	69.48	3.335	1.225	48.000
4	0.0	1405.58	1.534	0.438	0.300	0.0	0.0	0.0	2.420	48.000
5	45.83	26.66	0.341	0.318	0.346	140.20	70.72	3.401	1.232	48.000
6	0.0	4023.04	0.155	2.543	1.231	0.0	0.0	0.0	2.420	60.000
7	209.36	130.58	2.273	1.848	2.014	140.20	70.72	3.401	1.232	60.000
8	0.0	11.18	0.017	0.007	0.013	0.0	0.0	0.0	2.420	50.000
9	0.0	0.0	1.554	1.554	1.554	0.0	0.0	0.0	1.000	95.000
10	41.83	20.66	1.723	1.657	1.603	25.00	12.09	3.401	1.040	60.000
11	5.00	2.42	0.222	0.214	0.217	23.34	11.29	3.401	1.037	55.000
12	2317.63	2311.52	17.592	14.812	15.949	140.00	139.58	1.650	1.290	97.000
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	82.000
14	1552.04	1453.78	11.495	7.408	8.743	280.44	274.71	1.500	1.620	245.000
15	1703.24	879.83	15.511	12.060	13.774	140.86	69.48	3.335	1.225	82.831
16	41.83	20.66	1.723	1.657	1.603	25.00	12.09	3.401	1.040	60.000
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.120	20.000
18	1818.67	695.17	9.413	6.508	7.643	279.46	137.55	3.342	1.440	100.750
19	3.00	1.50	0.020	0.012	0.004	0.0	0.0	0.0	1.000	105.000
20	0.0	0.0	7.000	7.000	7.000	0.0	0.0	0.0	1.000	82.000
21	33.30	16.42	0.240	0.236	0.257	140.06	69.48	3.335	1.225	82.831
22	0.0	1213.00	1.219	0.569	0.364	0.0	0.0	0.0	3.200	20.000
23	0.0	0.0	0.132	0.132	0.182	0.0	0.0	0.0	1.000	20.000
24	68.11	0.0	0.270	0.176	0.219	500.00	0.0	0.0	1.567	20.000
25	1852.69	1453.78	10.924	8.005	8.420	265.25	279.73	1.560	1.564	125.000
26	67.39	181.95	0.440	0.296	0.189	0.0	0.0	0.0	3.200	195.501
27	0.0	0.0	0.120	0.128	0.120	0.0	0.0	0.0	1.000	111.126
28	0.0	0.0	0.0	0.0	0.0	140.86	69.48	3.335	1.225	82.831
29	154.66	76.29	1.345	1.098	1.195	140.86	69.48	3.335	1.225	82.831
30	20.00	0.0	1.023	1.000	1.010	20.00	0.0	0.0	1.023	60.000
31	67.39	183.88	0.440	0.297	0.190	0.0	0.0	0.0	3.197	100.000
32	656.70	626.52	5.752	4.446	4.927	140.00	139.58	1.668	1.294	100.000
33	801.64	679.78	13.423	11.874	12.452	67.51	57.25	1.940	1.130	84.111
34	67.39	187.05	0.454	0.299	0.191	0.0	0.0	0.0	3.192	84.111
35	315.85	255.96	5.070	4.171	4.645	70.65	57.25	2.030	1.134	84.111
36	306.13	282.51	10.378	9.803	10.019	31.23	24.74	2.077	1.059	76.770
37	67.39	192.41	0.462	0.302	0.192	0.0	0.0	0.0	3.183	76.770
38	154.14	111.53	4.788	4.508	4.614	34.19	24.74	2.273	1.062	76.770
39	144.42	103.44	10.103	9.444	9.943	14.67	10.51	2.297	1.027	73.339
40	67.39	190.63	0.464	0.305	0.193	0.0	0.0	0.0	3.176	73.339
41	78.02	47.69	4.672	4.538	4.590	17.32	10.51	2.712	1.030	73.334
42	69.90	45.61	9.995	9.476	9.921	6.98	4.44	2.587	1.012	71.848
43	67.39	198.99	0.472	0.306	0.194	0.0	0.0	0.0	3.173	71.848
44	41.72	20.21	4.021	4.555	4.501	9.16	4.44	3.346	1.015	71.848
45	32.00	18.70	9.448	9.448	9.415	3.23	1.89	2.815	1.005	71.303
46	67.39	198.99	0.472	0.306	0.194	0.0	0.0	0.0	3.173	71.303
47	9.72	1.51	0.810	0.797	0.802	3.23	1.89	10.613	1.016	71.303
48	0.00	-0.00	0.136	0.136	0.136	0.00	-0.00	0.0	1.000	80.001
49	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
51	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
52	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
53	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
54	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
55	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
56	0.0	17.04	0.0	333.913	329.726	3.23	0.0	0.0	0.0	0.0
57	1940.08	922.73	9.996	6.927	8.129	280.08	133.21	3.459	1.443	28.135
58	1749.74	832.23	11.017	6.998	7.878	272.15	129.44	3.459	1.574	28.358
59	1892.63	922.73	11.493	7.702	8.673	265.82	129.58	3.375	1.558	90.000
60	2207.52	2142.09	27.023	18.801	19.194	140.70	131.76	1.757	1.437	59.833

Y DATA

	1	2	3	4	5	6
0	20.000000	20.000000	1008.00000	62.000000	60.000000	50.000000
10	0.260000	0.150000	0.200000	3.000000	55.000000	0.010000
20	1.000000	0.0	10.000000	0.373000	0.851690	0.500000
30	0.920000	1.350000	9.000000	0.0	0.500000	20.000000
40	0.0	666.669722	3.200000	0.100000	0.520000	3.200000
50	6.000000	6.000000	6.000000	0.950000	80.000000	0.005000
60	80.000000	0.0	3.000000	3.000000	0.0	0.0
70	0.0	4.000000	0.500000	0.530000	0.0	3.000000
80	0.0	16.000000	0.812000	261.000000	741.800049	245.000006
90	0.390000	0.950000	0.700000	0.000880	0.0	0.200000
100	45.000000	70.000000	0.620000	105.000000	0.0	70.000000
110	35.000000	0.950000	0.700000	82.000000	0.970000	0.050000
120	665.000000	159.300003	158.100006	158.100006	1.000000	0.900000
130	0.0	0.0	1.000000	0.100000	0.500000	1.000000
140	0.0	1.000000	3.000000	0.340000	0.100000	3.000000

X DATA

0	100.000000	140.000000	1.650000	0.0	2.000000	280.000000
10	169.000000	62.000000	1.088200	80.000000	90.500000	0.0

ZENGZHOU ALUMIN. PLANT

7	8	9	10	
48.000000	48.000000	95.000000	60.000000	
22.000000	5.000000	0.120000	25.000000	
0.020000	0.012500	1.500000	3.000000	
20.000000	500.000000	0.0	0.0	
1.000000	1.000000	0.061600	0.069500	
0.0	1200.00000	300.000000	0.100000	
20.000000	0.0	0.0	0.0	
90.000000	0.200000	0.0	0.200000	
1.000000	1.000000	2.000000	3.000000	
0.0	0.820000	0.0	0.200000	
90.000000	110.000000	130.000000	150.000000	
97.000000	0.400000	10.600000	0.900000	
0.100000	0.010000	1.000000	0.0	
0.0	2800.00000	250.000000	1.000000	
0.010000	20.000000	1.000000	1.000000	
7.800200	245.000000	125.000000	0.070000	
0.0	3.000000	3.000000	4.000000	375.00