

An Expert System for Solvent Extraction of Rare Earths

Lu Xu,* Yonghui Xiao,[†] and Deqian Li

Changchun Institute of Applied Chemistry, Academia Sinica, Changchun 130022, Jilin, China

Received February 7, 1992

An expert system for solvent extraction of rare earths has been developed using LISP. The goal of this project was to mimic the chemists' inferential abilities to assist in the process of solvent extraction of rare earths. The system includes frequently used extractants, separation of specific rare earths, recommendation of procedures for the separation of mixtures of rare earths using (2-ethylhexyl)phosphonic acid 2-ethylhexyl monoester, selection of parameters for counter-current extraction and methods for evaluation of the technique, and the economics of the processing. The expert system runs on an IBM-PC/XT.

INTRODUCTION

The rare earth family is a group of 17 elements (Sc, Y, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu) which, because they possess unique physicochemical properties, are used widely in the metallurgy and ceramics industries and in the processing of electronic and luminescent materials.

Many methods have been developed for the preparation of the individual rare earth elements, and the most important of these is solvent extraction. A key step in the extraction process is the selection of a suitable solvent, or extractant, and of suitable extraction conditions. The success of this step hinges upon the knowledge and experience of the chemist who is conducting the extraction. Since the publication of the Dendral system,¹ a pioneering effort to develop computer programs which could elucidate the structures of organic compounds, many chemistry-related expert systems have been described,²⁻⁷ but no work on rare earth systems has been reported. Work has been undertaken recently⁸ to design an expert system for planning of the rare earth extraction process, and recent additions to this system include the rules of counter-current extraction, which is a process that is heavily used in plants engaged in the separation of rare earths. The program, which is written in LISP, consists of 4 parts:

1. Separation of individual rare earths and choice among frequently used extractants.
2. Development of recommended procedures for the separation of mixtures of rare earths with (2-ethylhexyl)phosphonic acid 2-ethylhexyl monoester (HEH[EHP]), which in recent years has become one of the most widely used extractants.
3. Optimization of the counter-current extraction process.
4. Evaluation of the technique and the economics of new processes or of plans for rare earth separation facilities.

Knowledge, i.e. rules, was encoded by two methods, production rules and frames, and the whole program runs on an IBM-PC/XT.

I. FREQUENTLY USED EXTRACTANTS FOR INDIVIDUAL RARE EARTH SEPARATION

Solvents used for the extraction of rare earths can be categorized in three groups, determined by the mechanism of their action. These are:

1. Complex acidic extractants, such as HEH[EHP], bis(2-ethylhexyl)phosphoric acid (HDEHP), etc.
2. Complex neutral extractants, such as tributyl phosphate (TBP), trioctylphosphine oxide (TOPO), bis(1-methylheptyl) methylphosphonate (Chinese trade name: P350), etc.
3. Ionic association extractants, such as 1,1,3,3,5,5,7,7,9,9-decamethyldecylamine (Primene JM-T) ($n = 3-5$), R_2CHNH_2 ($R = C_9-C_{11}$), trioctylamine (TOA), etc.

The rules for the use of such extractants for the separation of specific rare earths have been summarized and some examples of these are given here.

A. Extraction of Yttrium.

1. Tributyl phosphate (TBP) is an especially effective extractant for yttrium, and in comparison to other rare earth elements, yttrium is extracted much more efficiently from HCl. Yttrium can also be extracted by TBP from $HClO_4$ with trialkylphosphine oxide.
2. Yttrium can also be effectively extracted from HNO_3 with trialkylphosphine oxide.
3. Yttrium can be extracted only from H_2SO_4 or pyrophosphate with amine extractants.
4. The most commonly used extractants for yttrium are alkylphosphoric acids.
5. Carboxylic acid extractants are often used to extract yttrium.
6. Chelators are used as extractants for yttrium, and thiophenic thenoyltrifluoroacetone (HTTA) is also a very effective extractant for yttrium.
7. Ester, alcohols, and ketones are very poor extractants for yttrium in HCl or HNO_3 .

B. Extraction of Lanthanides.

1. Lanthanides (with the exception of Sc and Y, all the rare earths are classified as lanthanides) can be extracted from HNO_3 using TBP, but the process is not efficient and TBP fails to extract lanthanides from HCl. Lanthanides are extracted in a specific order from thiocyanate but in the reverse order from $HClO_4$.
2. Lanthanides can be extracted quantitatively from sulfuric acid or sulfate solution using amine extractants such as Primene JM-T.
3. Alkylphosphoric acids are the extractants most commonly used for the extraction of lanthanides.
4. Carboxylic acid extractants are often used for the extraction of lanthanides.
5. Ethylacetone is a poor chelate extractant for lanthanides. Lanthanides can be extracted with HTTA.

[†] Present address: Tianjin Institutes of Chemical Engineering, Tianjin, People's Republic of China.

Table I. Examples of Ion-Absorbed Rare Earth Minerals

type of ore		amount of oxide (%)							
		Y ₂ O ₃	La ₂ O ₃	Ce ₂ O ₃	Pr ₆ O ₁₁	Nd ₂ O ₃	Sm ₂ O ₃	Eu ₂ O ₃	Gd ₂ O ₃
heavy	ore 1	65	22	<0.1	1.1	3.5	2.3	<0.1	5.7
	ore 2	52	2.3	—	1.2	6.5	4.4	—	7.3
trans	ore 1	46	10.5	3.4	3.2	11.5	3.8	<0.3	5.0
	ore 2	41	11.8	4.0	4.0	14.5	4.5	<0.3	5.1
	ore 3	35	23	0.7	4.3	14.9	3.5	1.1	5.3
light	ore 1	28	26	0.6	5.1	18.5	3.9	1.0	4.7
	ore 2	20	32	1.9	5.8	22.2	4.6	1.4	4.4
	ore 3	10	30	7.1	4.7	30.1	6.3	1.5	4.2
		Tb ₄ O ₇	Dy ₂ O ₃	Ho ₂ O ₃	Er ₂ O ₃	Tm ₂ O ₃	Yb ₂ O ₃	Lu ₂ O ₃	
heavy	ore 1	1.1	7.5	1.6	4.3	0.6	3.3	0.5	
	ore 2	1.7	9.6	1.4	5.4	1.0	5.5	0.9	
trans	ore 1	1.0	6.7	1.2	3.4	0.5	2.9	0.4	
	ore 2	0.95	6.2	0.8	3.5	0.4	2.5	0.4	
	ore 3	0.8	5.1	0.6	2.8	<0.3	1.9	<0.3	
light	ore 1	0.7	4.5	0.4	2.5	<0.3	1.9	<0.3	
	ore 2	0.6	3.0	0.4	1.4	0.3	1.5	<0.3	
	ore 3	0.5	1.8	0.3	0.9	0.1	0.6	<0.3	

C. Extraction and Separation of the Lanthanide Elements.

The following systems are used for different separations:

1. For the purification of yttrium, systems Aliquat 336-HCl-SCN⁻, P350-HNO₃-EDTA, and cycloalkancarboxylic acids with HCl are used.
2. The systems Aliquat 336-HNO₃-LiNO₃, HDEHP-HCl, and HEH[EHP]-HCl, HNO₃ are used to separate yttrium and the lighter rare earths.
3. For separation and purification of the lanthanides, the systems in use are P350-HNO₃, TBP-HCl-SCN⁻, TBP-HNO₃, and HDEHP-HCl.
4. HEH[EHP] can be used to separate heavy rare earths, as is described below.

II. SEPARATION OF MIXTURES OF RARE EARTHS WITH HEH[EHP]

At present, HEH[EHP] is one of the most widely used extractants in rare earth separation. Because of this, the rules governing the use of HEH[EHP] have been put into a separate class.

There are a variety of rare earth deposits from which rare earth elements can successfully be extracted, as a consequence of the higher content of the specific elements and the reduced level of radioactivity. These deposits include primary minerals, placers, and ion-absorbed rare earth minerals. The compositions of different ion-absorbed rare earth minerals are different, but the relative contents of the rare earth oxides appear in a definite and regular pattern which is summarized in Table I. It can be seen from this table that the quantities present of the oxides of the heavy rare earths (Tb, Dy, Ho, Er, Tm, Yb) are proportional to the percentage of Y₂O₃, which varies from 65% to 10%. When the Y₂O₃ content is 52%, the Tb₄O₇ is 1.7%; when the former falls to 10%, the latter also falls, to 0.5%, and the corresponding concentrations of Er₂O₃ are 5.4% and 0.9%, respectively. This trend is reversed in the light rare earth elements. Thus as the Y₂O₃ content falls from 52% to 10%, that of La₂O₃ rises from 2.3% to 30% and that of Sm₂O₃ from 4.4% to 6.3%. Thus the ion-absorbed rare earth minerals may be classified according to their content of Y₂O₃. If the content in an ore of Y₂O₃ is greater than 50%, then the ore is regarded as a heavy rare earth ore, i.e. the proportion of the oxides of the heavy rare earths (Tb, Dy, Ho, Er, Tm, Yb, Lu, and Y) will be higher in such an ore. If, on the other hand, the Y₂O₃ content is below 30%, then the ore is viewed as a light rare earth ore, containing predominantly

La, Ce, Pr, Nd, Sm, and Eu oxides; the content in such an ore of the light rare earth oxides will be higher and that of the heavy rare earth oxides will be lower. If the proportion of Y₂O₃ in an ore is between 30% and 50%, then that ore is called a transition-absorbed rare earth mineral.

If a mixture of rare earths is to be separated using HEH[EHP], the optimum process will depend upon the composition of the mixture. The process, as an example, will be given in part V of this paper.

III. COUNTER-CURRENT EXTRACTION

High purity rare earths are used widely in research and in various industries, such as television manufacturing. The similarity of the properties possessed by each of the rare earths is such that separation of the different elements can be quite difficult. Further, rare earths are very expensive, and thus efficient separation procedures are desirable. For these reasons, it was decided to investigate counter-current extraction as a means of purifying the different rare earths.

Effective extraction and separation is unlikely to be achieved in a single step, and it is necessary to prepare an aqueous solution containing the rare earths and extract this solution repeatedly with an organic solvent. If such multiple extractions are put onto a continuous basis so as to improve the extraction efficiency, the resulting technique is termed counter-current extraction. Counter-current extraction encompasses several processes, the most important of which is fractional extraction, and this process will be considered here.

Fractional extraction falls into two categories, feeding the rare earth species through an aqueous phase and through an organic phase. The following sections describe the former category, i.e. feeding the species through aqueous phase. The principle of mass distribution applies at each stage of a fractional extraction process, as is depicted in Figure 1. Here, A_{ai} and B_{ai} represent the aqueous concentrations of compounds A and B at the i th stage of the procedure and A_{oi} and B_{oi} the corresponding organic phase concentrations, respectively. A is a component which represents the ease with which the material is extracted from the other phase and B denotes the lack of ease of extraction. If a rare earth mixture contains elements A, B, C, D, and so on, it is possible to categorize them into two classes, depending upon the ease with which they transfer from one phase to the other and also the point in the process where their extraction is complete. If A and B are both in a first group and C and D are in a second group,

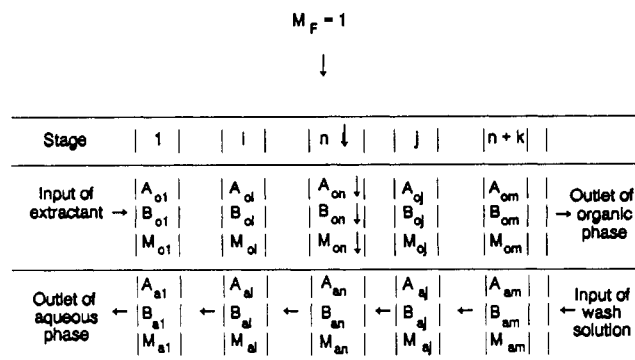


Figure 1. Example of a fractional extraction.

Table II. Selected Parameters for Counter-Current Extraction

	<i>k</i>					
	0.5	0.58	0.6	0.7	0.8	0.9
<i>W</i>	4.80	4.17	3.92	3.30	2.83	2.46
<i>S_o</i>	4.91	4.28	4.03	3.41	2.94	2.57
<i>E_M</i>	0.846	0.828	0.819	0.793	0.767	0.743
<i>E'_M</i>	1.023	1.026	1.028	1.033	1.039	1.044
<i>n</i>	21.8	24.8	25.8	31.6	40.7	57
<i>m</i>	7.79	7.56	7.98	8.30	8.65	9.03
<i>n + m</i>	29.6	32.4	33.8	39.9	49.4	66.0
<i>R</i>	145.3	138.7	136.2	136.0	145.2	169.6

Table III. Scheme of Product

no.	oxide	% content	no.	oxide	% content
1	Y ₂ O	99.9	8	Eu ₂ O	99.99
2	La ₂ O ₃	99	9	Eu ₂ O ₃	>99.95
3	La ₂ O ₃	99.99	10	Gd ₂ O	>99
4	CeO ₂	>85	11	Tb ₄ O ₇	>99.95
5	Pr ₆ O ₁₁	≥99	12	Dy ₂ O ₃	>99
6	Nd ₂ O ₃	≥99	13	concentrated heavy REO	
7	Sm ₂ O ₃	≥99			

Table IV. Mixed Rare Earth Oxides

oxide	% content	oxide	% content
Y ₂ O ₂	12.29	Tb ₄ O ₇	0.70
La ₂ O ₃	27.85	Dy ₂ O ₃	3.19
CeO ₂	1.61	Ho ₂ O ₃	0.58
Pr ₆ O ₁₁	7.24	Er ₂ O ₃	1.63
Nd ₂ O ₃	25.91	Tm ₂ O ₃	<0.3
Sm ₂ O ₃	5.10	Yb ₂ O ₃	1.46
Eu ₂ O ₃	0.81	Lu ₂ O ₃	<0.3
Gd ₂ O ₃	4.30		

Table V. Major Chemical Materials

name	specification	name	specification
mixed REO	REO > 92%	mixed alcohols	technical pure
HCl	technical pure	kerosene	technical pure
H ₂ SO ₄	technical pure	HEH[EHP] resin	technical pure
NH ₄ OH	technical pure	N235	technical pure
HEH[EHP]	technical pure	H ₂ O ₂	chemical pure
naphthenic acid (defatted)	technical pure	Zn powder	chemical pure (200 mesh)

then the first group can be said to have an "ease of extraction" component *A*, while the second has a "difficulty of extraction" component, *B*. The flow rate of the (*A* + *B*) component in the aqueous phase leaving the extractor is M_{ai} while the flow rate of the same component in the organic phase leaving the extractor is M_{oi} , where *M* represents a mixture of *A* and *B*. Finally, M_f is the flow rate of the rare earths in aqueous solution.

The most important steps in the optimization of counter-current extraction are as follows:⁹

1. Identification of the best extraction system and determination of the separation coefficients β and β' . An extraction system appropriate to the problem at hand must be selected. Then the ratio of organic phase to aqueous phase, degree of saponification, concentrations of solute, washing solution, and acidity, as well as the separation factor, are determined in a single stage experiment.

The average separation factors β in the extraction section and β' in the washing section may be calculated by the equations

$$\beta = E_A/E_B \quad \beta' = E'_A/E'_B$$

where E_A , E_B , E'_A , and E'_B are the average extraction ratios of component *A* and *B* in the extraction and washing sections, respectively.

2. Identification of the separation target. This step consists mainly of determining the ease and lack of ease of extraction of the components *A* and *B*, the purities of *A* and *B*, the percentage purification, and the percentage yield of *A* and *B*.

Let f_B be the mole fraction of component *B*, and $f_A = 1 - f_B$ the mole fraction of component *A*. If the purity of *A* is desired to reach P_{An+m} (the purity of component *A* in the product from the outlet of organic phase) with a yield of Y_A , then the purifying ratio of *A* is

$$a = \frac{P_{An+m}/(1 - P_{An+m})}{f_A/f_B}$$

and the purifying ratio of *B* is

$$b = \frac{a - Y_A}{a(1 - Y_A)}$$

The purities of *B* and *A* are

$$P_B = \frac{bf_B}{f_A + bf_B} \quad P_A = 1 - P_B$$

3. Determination of the optimum ratio of extraction and the quantities of extraction and wash. The overall extraction ratio in the extraction section, $E_M = (A_o + B_o)/(A + B)$, the overall wash ratio in the wash section, $E'_M = (A'_o + B'_o)/(A' + B')$, the maximum quantity *S* (g/min) of (*A* + *B*) extracted, and the maximum wash quantity (*W*) are calculated using the equations

$$S = W + f'_A \quad W = 1/(\beta^k - 1)$$

$$E_M = S/(W + 1) \quad E'_M = S/W$$

where f'_A is the mole fraction of *A* in the outlet of organic phase, *k* is an empirical parameter.

4. Determination of the numbers of stages, *n* and *m*. The extraction stage number, *n*, and the wash stage number, *m*, are computed with the following functions

$$n = \log(b)/\log(\beta/E_M) \quad m + 1 = \log(a)/\log(\beta'/E'_M)$$

5. Determination of the flow rate. The flow rate is defined as $V_f V_A V_w$, where V_f signifies the flow rate of the aqueous phase, V_A is that of the extractant, and V_w represents the flow rate of the wash solution (all

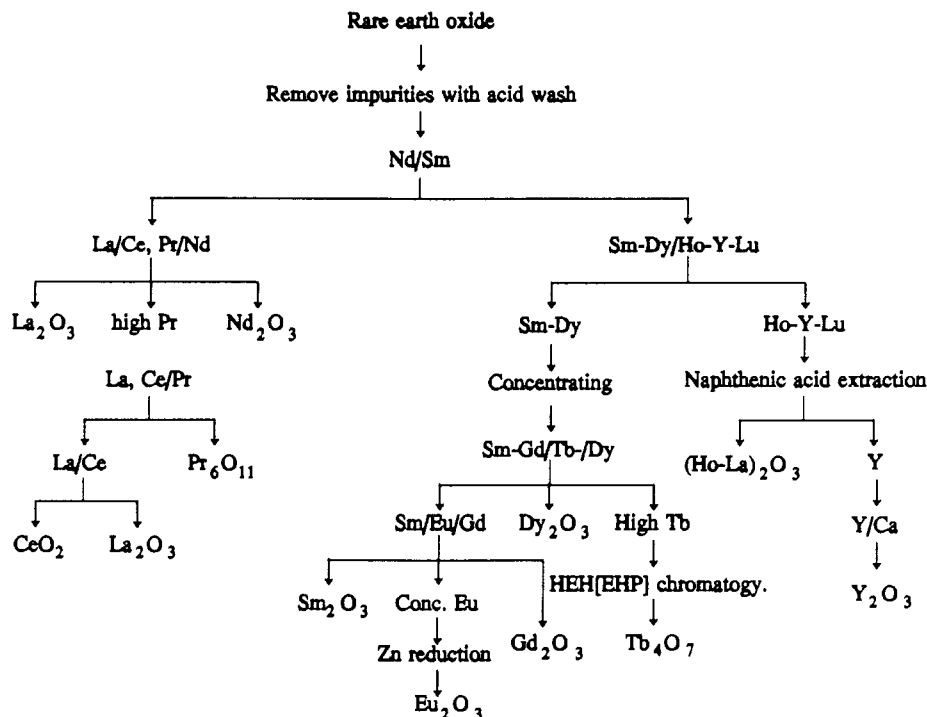


Figure 2. Optimum recommended process.

Table VI. Example of the Components of a Heavy Rare Earth Ore

oxide	% content	oxide	% content
Y ₂ O ₃	65	Tb ₄ O ₇	1.1
La ₂ O ₃	2.2	Dy ₂ O ₃	7.5
Ce ₂ O ₃	<0.1	Ho ₂ O ₃	1.6
Pr ₆ O ₁₁	1.1	Er ₂ O ₃	4.3
Nd ₂ O ₃	3.5	Tm ₂ O ₃	0.6
Sm ₂ O ₃	2.3	Yb ₂ O ₃	3.3
Eu ₂ O ₃	<0.1	Lu ₂ O ₃	3.5
Gd ₂ O ₃	5.7		

flowrates are in milliliters per minute):

$$V_f = M_f / C_f$$

$$V_a = S / C_a$$

$$V_w = 3W / C_H \text{ (assume that 3 M HCl can wash 1 M Re}^{3+}\text{)}$$

where C_f and C_s represent the concentrations (M) of mixed rare earths in aqueous phase and in organic phase, respectively; C_H denotes concentration of the HCl washing solution (M); M_f is the feeding rate of rare earth species. When M_f is 1 mmol/min, then

$$V_f : V_a : V_w = 1 : V_s / V_f : V_w / V_f$$

As an example, the oxide Gd₂O₃ is used as a host substance in a transition emission complex compound and for such purposes; its purity must be higher than 99.99%. This oxide is produced in a yield of over 90% from raw material containing about 99.0% Gd₂O₃ and with the major impurities Eu₂O₃ and Sm₂O₃. With this target, the parameters shown in Table II are computed using the above five steps. In this calculation, k is an empirical parameter used for the optimum calculation of the maximum wash quantity, W .

IV. ECONOMIC AND TECHNICAL EVALUATION IN THE PREPARATION OF RARE EARTHS

The technical and economic evaluation of various processes for the isolation of rare earths is usually conducted in two

phases. The first, technical evaluation, depends upon data such as ore type, ore content of rare earth oxides, chemical engineering materials, analytical instruments and methods, and selection of equipment. The second, economic evaluation, is concerned with estimates of the necessary investment, financial appraisal, uncertainty analysis, and capital cost, as well as environmental protection, large-scale material treatment methods, and so on. Economic evaluation is beyond the scope of this paper, which will be limited to technical evaluation.

If the technical evaluation is done by a human, the main steps are as follows:

1. First, a scheme for the products of rare earth oxides should be made out by the factory producing rare earths, which includes what oxides are to be prepared and the annual yield (tons/year).
2. Based on the scheme, a process will be recommended by an expert on rare earth extraction.
3. Based on steps 1 and 2, the raw material of oxides, the materials for processing, analytical methods and instruments for material, intermediate and end products, and the equipment required will be selected and adapted.

Our system has been constructed to mimic these steps. As an example, the composition of a typical rare earth product is shown in Table III. This table does not contain the annual yield of oxides, which is measured in tons. The raw material of mixed oxides that is to be used to produce the compounds in Table III is shown in Table IV. The optimum process derived from the information in Tables III and IV is shown in Figure 2. Here, a triple outlet scheme has been selected because it leads to a process which can be simplified. The materials required for the processing cited in Figure 2 are listed in Table V, and the analytical methods used include extraction chromatography, weight analysis, spectrophotometry, and capacity analysis for the total content of the rare earths and other elements such as Si, Pb, Fe, and so on in the intermediate and end products. Inductively coupled plasma atomic emission spectroscopy is used to determine microim-

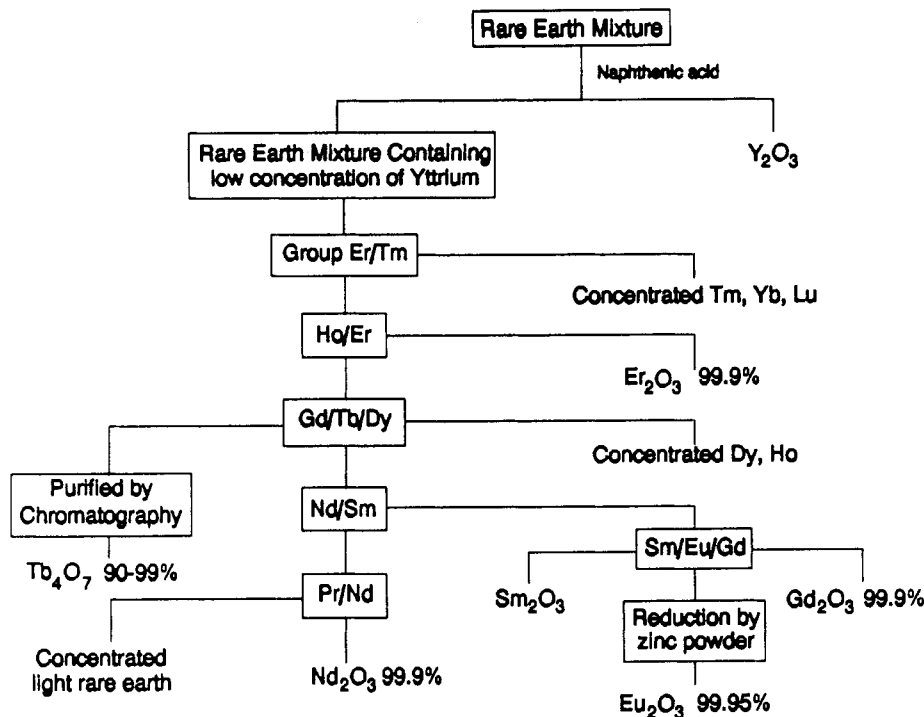


Figure 3. Components of a heavy rare earth ore and flowchart for its separation.

purities, and X-ray fluorescence spectroscopy is used to determine the content of individual rare earths in the raw material and intermediate products.

The equipment required consists of an extraction trough, a ceramic chemical reactor, pumps, a source of ammonia, a chromatographic column, and instruments for determining the content of rare earths. With these data and parameters, i.e. the chemical raw materials, the analytical instruments, and the specifications, types and amounts of major production equipment, the technical evaluation and the economic evaluation are performed as described above. Finally, a comprehensive summary of the technical and economic evaluation is prepared.

V. KNOWLEDGE EXPRESSION AND INFERENCE STRATEGY

In the construction of expert systems, the two most commonly used methods of encoding knowledge are "production rules" and "frames". In this work, both of these methods have been used. Production rules take the form: If x , then y is true. For example:

If the content of Y_2O_3 is 50%

THEN the ore is a heavy rare earth ore

The left-hand side (x) may contain any number of clauses combined by Boolean algebra operators. A "frame" describes the hierarchical dependencies between objects. In a frame, the upper level (or parent) object passes attributes to the objects beneath it in the hierarchy (children). In other words, children inherit attributes from their parents. Frames take the form

```

(<FRAME>(<SLOT1>(<FACET1>(<VALUE1>)
                                (<VALUE2>)
                                .
                                .
                                .
                                (<FACET2>(<VALUE1>...))
                                (<SLOT2>(<FACET1>(<VALUE1>)...))...))
                                .
                                .
                                .
  
```

A frame may contain any number of slots, each slot may contain any number of facets, and each facet may contain any number of values. For example, a frame for an extractant is illustrated here:

Frame name: name of extractant

Slot 1: AKO'(extractant category)

Slot 2: NICKNAME

Slot 3: TYPE (value: extractant)

Slot 4: MOLECULAR FORMULA

Slot 5: MOLECULAR WEIGHT

Slot 6: AVAILABLE-IN-INDUSTRY

Slot 7: SOURCE

Slot 8: PRICE

:) physicochemical properties of extractant

:) behavior of extraction for rare earths

The system contains about 200 rules bearing on the parameters discussed above. Some data were stored in the knowledge base, and if an inquiry is made of the system, it will make an inference based on the rules in the knowledge base and provide the answer. Forward- and reverse-chaining are used, and both inferences are adopted simultaneously. In other words, the inference engine may approach the problem from either the top or the bottom, beginning with either facts or conclusions. For example, in the HEH[EHP] separation system, if we know the contents of the mixed rare earths (see Table VI), i.e., we begin with a series of facts which are known to be true, and want to determine what process should be adapted, i.e., what conclusions can be reached, the program, at first, will search the name of that mixed rare earths. Once the name is found, all the rules supporting the separation of that mixture will be scanned repetitively from the slots (i.e. from the knowledge base) until no new facts can be concluded.

An example of a frame is

```
(HWREM (TYPE
      (VALUE(MIXERNAME)))
  (SUPPORTED-RULE
    (VALUE(34)))
  (SEP-RULE
    (VALUE(1)))
```

In this example, HWREM (= heavy rare earth ore) is the frame name and the three slots are TYPE, whose value in this case is MIXERNAME; SUPPORTED-RULE, which has a value of 34, i.e. HWREM is supported by rule 34; and SEP-RULE, an available rule, whose value is 1.

The content of rule 34 is

```
(34(AND(>=(DISTR'Y)50)
      (>=(DISTR'HWRE)17)
      (IN(DISTR'HWRE)7 12)
      (IN (DISTR'LWRE)5 20))
  (IS'MIXERNAME'HWREM)
```

and its meaning is

(34 (if the content of Y_2O_3 is greater than 17%
heavy rare earth oxides is greater than 17%
and that of medium rare earth oxides (Sm, Eu, Gd)
is between 7% and 12%,
and that of light rare earth oxides is between 5% and
20%;
then the rare earth mixture is HWREW)

The content of rule 1 is

```
(1(IS' MIXERNAME'HWREM)
  (IS'METHOD'NAPHTHENIC_ACID_SOLVENT_EXTRACTION)
  (IS'SEPARATE_BETWEEN'(Y.La)))
  (BECAUSE THE DISTRIBUTION OF  $Y_2O_3$  IS GREATER
```

and its meaning is:

(1 if MIXERNAME for rare earth mixture is HWREM
then naphthenic acid is used to separate Y from the
other lanthanides
because the content of Y_2O_3 in the mixture is greater)

According to Table VI, the process is depicted in Figure 3 is the optimum process for the mixture described in the figure.

The content of yttrium is higher and its atomic weight is smaller than those of the other rare earths, and consequently, the mole percent of yttrium is larger than that of the other rare earths. Accordingly, naphthenic acid is used to extract the yttrium in the first step and HEH[EHP] is used to extract the other rare earths.

CONCLUSION

During the 4-year period beginning in 1987, a comprehensive information system of rare earths has been built in this laboratory.¹⁰ It does not contain databases but can support studies of the relationships between data and applications of artificial intelligence, such as the expert system described here. This system has been completed and released, but it is desirable to improve the power of the system continuously.

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