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The optimum production of nanoparticles and catalysts in an industrial center by using the mathematical modeling

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ABSTRACT

Regarding the vast applications of nanoparticles and catalysts in industry and medical subjects, determining about their extensive production with attention to the needed investment and economical benefit is some of the anxiety of many countries. Therefore, there are some problems and limitations such as the needed facilities and reserving the environmental standards. With attention to expectations of the present society, determining about these questions need the exact survey: "is investment for producing them mainly reasonable? "which of them should be produced?" Thus, in this article, we present the mathematical modeling of the problem for construction of a productive center. Finally, we can determine about them by solving and analyzing the obtained solutions.

KEYWORDS: suitable production, nanoparticles, catalysts, decision making, LINGO,OR

1. INTRODUCTION

A nanoparticle, is a particle which it's dimension is about 1-100 nm. Nanoparticles contain the combinational nanoparticles such as the 2 layer nuclear structures besides the metallic, insulators and semiconductor types.

Nanotechnology has many applications in electronics, medicinal, pharmacological industries and etc. In fact, the birth of this field is aligned with the famous lecture of "Richard Feynman", the famous professor in physics in California institute of Technology and his famous sentences: "there's plenty of room at the bottom" [1]. Despite after more than 10 years from being sent the first nanomaterials to market and increasing application of this technology in industry, there are low information about it's dangerous effects for environment, health and industries safety [2].

1.1. Nanocatalyst: effect of size reduction

Catalytic technologies are critical to present and future energy, chemical process, and environmental industries. Conversion of crude oil, coal and natural gas to fuels and chemical feedstock, production of a variety of petrochemical and chemical products, and emission control of CO, hydrocarbons, and NO, all rely on catalytic technologies. Catalysts are also essential components of electrodes for fuel cells that use either solid oxide ionic or polymeric proton electrolyte. Drivers for development of advanced catalysts include (i) production of high value products with inexpensive raw materials, (ii) energy-efficient and environmentally-benign chemical conversion processes, (iii) increasingly stringent environmental regulations, and (iv) low-cost catalysts such as with reduction or replacement of precious metals [3].

In catalysis, chemical reactions in solid, gases or liquids are accelerated by introducing a solid phase that ideally contains large enough amounts of the right kind of site for chemical reactants to adsorb, react, and desorbs. Because optimization of the catalyst requires increasing the numbers of sites to expand surface area, the catalytic particle size must be decreased. In contemporary laboratories, active catalysts tend to consist of carefully prepared nanometer-sized particles on supports with nanometer-sized pores or structural features. Modern catalysts typically consist of multiple-component active phases that may include a support tailored to disperse, isolate, or otherwise enhance the structure or properties of individual catalytic particles. One goal of catalysis research is to understand how decreasing the size of catalytic particles alters the intrinsic catalytic performance beyond simply expanding surface area. A corollary goal is learning how to design and prepare catalysts with the most effective size and structure.

The exciting prospect of nanoscience is its potential use in almost any conceivable domain. Every field from medicine and electronics to manufacturing and fashion stand to benefit from advances in nanotechnology. And while nano-scale technology is multifaceted in its application, the use of nanocrystals as catalysts is perhaps the most intriguing. The key concept to understanding nanocrystal catalysis involves the ratio of surface area and

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volume. As an object gets larger, its surface area increases less in relation to its volume. Therefore, smaller objects have more surface area with respect to their volume. This has important implications for chemical reactions. High surface area-to volume ratios are favorable for chemical reactions. Going back to the campfire example, kindling is used to start the fire. The small pieces of wood have a greater surface area with respect to their volume than larger logs. Lighting the kindling therefore results in a quicker combustion. Additionally, if one throws a handful of sawdust onto a burning fire, a giant flare results. This reaction is chemically identical to ordinary wood burning, but it occurs at a much faster rate. The general purpose of catalysts is to increase the speed of a given reaction. This is achieved through kinetic means and does not directly affect the thermodynamic properties of a chemical system. Introducing a catalyst increases the speed of a reaction in one of three ways; it can lower the activation energy for the reaction, act as a facilitator and bring the reactive species together more effectively, or create a higher yield of one species when two or more products are formed. Depending on the application, nanocatalysts can be used in all the ways listed above. Nanomaterials are more effective than conventional catalysts for two reasons. First, their extremely small size (typically 10–80 nm) yields a tremendous surface area-to-volume ratio. Also, when materials are fabricated on the nanoscale, they achieve properties not found within their macroscopic counterparts. Both of these reasons account for the versatility and effectiveness of nanocatalysts [4].

1.2. Applications of nanocatalysts

In era of nanotechnology where size of every object is going to smaller and smaller with their enhanced properties; catalysts of nano size are also used in several chemical processes and beneficial for human being. In this section we are trying to collect all literature data on application of nanocatalyst reported within the last few years [4].

1.3. Operational research technique

Operational Research (OR) is the use of advanced analytical techniques to improve decision making. It is sometimes known as Operations Research, Management Science or Industrial Engineering. People with skills in OR hold jobs in decision support, business analytics, marketing analysis and logistics planning – as well as jobs with OR in the title. It is often considered to be a sub-field of mathematics. The mathematical modeling method and the solving techniques are explained in many references by that and we can point to [5], for example.

2.The research method

In this study, our needed information is gathered by verifying the sources, proofs and the view of the experts. For modeling the problem, “the OR methods” and for solving it, “the LINGO software” were used.

2.1.Problem definition

In constructing a problem center for nanoparticles and catalysts, the optimization of the mean of the corrosion resistance of the productive materials and also getting into the highest benefit is needed.

Also, there are some limitations in this center for producing 6 group containing: semiconductors, nanoparticles, polymeric nanoparticles, ceramic, metallic, catalysts and nanocatalysts, which are:

1-the special space is limited for constructions of this center, which the production of each of these groups need a special space.

2-the laboratory instruments is limited because these ones are produced mainly from the other countries.

3- there are some defined capital for constructing this center.

4- each of the above materials need a special time for production in the programming period.

In fact, the problem is decision making about the production or nonproduction of each of 6 above groups and the production content of any of them, so that the resistance aim of the production materials towards the corrosion and the economical benefit aim in the maximum utility (with the priority that is 0.7 and 0.3 respectively) are obtained. The information of this problem are prepared according the below table by verifying the sources, proofs and the view of the related experts.

Table 1. data of the problem

	Metallic nanoparticles	**ceramic nanoparticles**	**polymeric nanoparticles**	**semiconductor nanoparticles**	**catalysts**	**nanocatalysts**	**restriction**
Needed facilities	1	1.5	3	2.2	2	3	<=10
Needed investment	1.5	1.6	1.8	1.9	1	2	<=8
Needed time	2	1.3	1.5	1.1	1	1.1	<=12
Needed space	9	7	6	4	8	16	<=40
Reserving the standards	1	2	3	4	5	6	>=3
resistance aim	0.15	0.5	0.75	0.25	1	2	-
economical aim	0.4	0.6	0.7	0.8	1	2	-

2.2. The modeling of the problem

The model of this problem is atypical nonlinear which also have the zero and one variables. The variables and the objective functions are described as:

Xi: the group production amount i^{th} (i=0,…,1) in the programming period
Yi: production or nonproduction i^{th} (i=0,…,1) with o and 1 values
F1: the produced materials resistance objective function towards corrosion
F2: production economical benefit objective function
F: the objectives combinational function F1 and F2 with the important priority 0.3 and 0.7, respectively

On the basis of table 1, function F1 and F2 are explained as below:
F1=((0.15*X1+0.5*X2+0.75*X3+0.25*X4+X5+2*X6)/(X1+X2+X3+X4+X5+X6))
F2=(0.4*X1+0.6*X2+0.7*X3+0.8*X4+X5+2*X6)

With attention to this matter that the problem has 2 objectives, is classified in the problem group MODM. There are different methods for solving these problems, that the weights method (Wj) is used here (weights for f1 and F2 functions are 0.7 and 0.3 respectively). Thus, this combinational objective function and the problem model are explained as below [6]:
F= (0.7F1+0.3F2)= ((0.105*X1+0.35*X2+0.525*X3+0.175*X4+0.7*X5+1.4*X6)/
(X1+X2+X3+X4+X5+X6))+(0.12*X1+0.18*X2+0.21*X3+0.24*X4+0.3*X5+0.6*X6)

The model:

```
Max (F)=((0.105*X1+0.35*X2+0.525*X3+0.175*X4+0.7*X5+1.4*X6)/
( X1+X2+X3+X4+X5+X6))+(0.12*X1+0.18*X2+0.21*X3+0.24*X4+0.3*X5+0.6*X6);
Y1+ 1.5*Y2+3* Y3+2.2* Y4+2*Y5+3*Y6<=10;
1.5*Y1+ 1.6*Y2+1.8* Y3+1.9* Y4+Y5+2*Y6<=8;
X1<=1000*Y1;
X2<=1000*Y2;
X3<=1000*Y3;
X4<=1000*Y4;
X5<=1000*Y5;
X6<=1000*Y6;
9*Y1+ 7*Y2+6* Y3+4* Y4+8*Y5+16*Y6<=40;
2*X1<=12;
1.3*X2<=12;
1.5*X3<=12;
1.1*X4<=12;
X5<=12;
1.1*X6<=12;
( X1+2*X2+3*X3+4*X4+5*X5+6*X6)/ ( X1+X2+X3+X4+X5+X6)>=3;
Xi>=0      i=1,..,6;
Yi= 0,1    i=1,..,6;
```

2.3. Solving the problem

After solving by LINGO, the following results are gained (table 2). We can calculate the amount of these functions by replacing the variables amounts in the functions F1 and F2, which are 0.956 and 47.6 respectively.

Table 2. output of LINGO software

```
Local optimal solution found at iteration:          52
  Objective value:                          15.09447


       Variable           Value        Reduced Cost
             X1        0.000000            0.000000
             X2        9.230769            0.000000
             X3        0.000000            0.000000
             X4        10.90909            0.000000
```

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        X5       12.00000          0.000000
        X6       10.90909          0.000000
        Y1       0.000000         -106.8927
        Y2       1.000000          0.000000
        Y3       0.000000         -206.6486
        Y4       1.000000          0.000000
        Y5       1.000000          0.000000
        Y6       1.000000          0.000000

      Row    Slack or Surplus     Dual Price
        1      15.09447          1.000000
        2      1.300000          0.000000
        3      1.500000          0.000000
        4     0.000000          0.1068927
        5      990.7692          0.000000
        6     0.000000          0.2066486
        7      989.0909          0.000000
        8      988.0000          0.000000
        9      989.0909          0.000000
        10       5.000000          0.000000
        11       12.00000          0.000000
        12      0.000000          0.1327566
        13       12.00000          0.000000
        14      0.000000          0.2077443
        15      0.000000          0.3007135
        16      0.000000          0.5608848
        17       1.356725          0.000000
```

3. Conclusion

OR technique is the best method for solving the production problem of nanoparticles and catalysts. The verification and analysis of the obtained solutions shows that with attention to the conditions and limitations of the problem, production of Metallic nanoparticles and polymeric nanoparticles (X1, X3) is not suggested. But, the production of the rest of groups is suggested with obtained amount in solution (table 3). Also, we can see that the most resistance toward corrosion (0.956 unit) is obtained for products. However, the maximum benefit (40.6) is gained.

Table 3. optimal solution

group	Metallic nanoparticles (X1)	ceramic nanoparticles (X2)	polymeric nanoparticles (X3)	semiconductor nanoparticles (X4)	Catalysts (X5)	Nanocatalysts (X6)
value	0	9.230769	0	10.90909	12.00000	10.90909

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