The Mathematical Modeling of a Chemical Production Prediction for a Chemical Companie and the Impact of the Results Polutants on the Environment

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Chemical companies have the object of activity the production of chemicals that have a harmful effect on the environment and increase the pollution. To quantify the pollution generated by a chemical company is useful the knowledge of the production prediction of chemical and the assessment of ecologic impact that it causes on the environment. In this paper, we present the methodology of elaborating a chemical production prediction, using linear mathematical models and the effects on the environment in case of the the pollutants resulting from the production process.

Keywords: chemicals, environment, pollution, ecologic impact

For developing the production prediction for a chemical is required following completion of steps [1], as shown in figure 1.

Data colection regarding the time evolution of the production level of that chemical; for chemicals of great importance that data can be obtained from statistical yearbooks, monographs and encyclopedias and for other products from specialized magazines (chemical engineering, with technical-economic nature, etc.);

Data validation are necessary especially when data coming from different sources using different units of measure and often have different degrees of confidence; it is about the elimination of the values that appear as single, entirely different from the others;

Identification the type of the production development - acyclic or cyclic - and choosing the most appropriate mathematical model for the character of that evolution - linear, exponential, logistic etc.

The working tool is the graphical representation of data regarding the production development level in time, but a great role in this stage has the experience and intuition of the person that examines of the problem.

Solving the mathematical model, respectively setting numerical values of the mathematical coefficients of the model is made taking into account the available data on the evolution of the production level, or analytically (for cases of simple models such as the growth linear, exponential or logistic) or using methods of numerical calculation for more complicated models such as the polynomial models and logistics.

An important consideration for the process of developing of prognosis in general, but very important in this stage is the minimum number of values for the production level that can give plausibility for the prediction: for *m* coefficients of mathematical model is required minimum *(m + 1)* level of the production values; practically not used less than five values, usually over seven values;

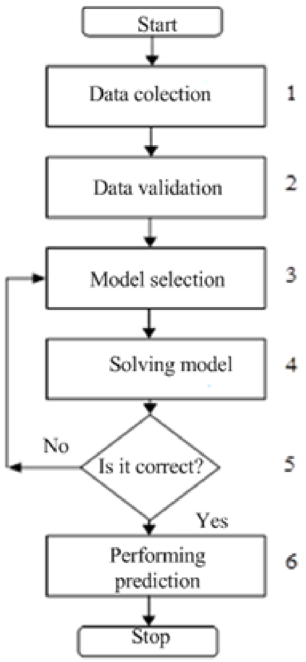

Fig. 1 Flowchart regarding development prediction stages

Verifying the correctness of the model

Statistical calculation methods (analytical or numerical) used to solve the chosen mathematical model, almost always make it possible to obtain numerical values of its coefficients. It is however necessary to check how the model describes the evolution of the level of production or in other words the accuracy or adequacy of the model. It is about, in principle, by comparing data calculated by mathematical model comparing data at different times with the initial data from which was started at the same points in time; This comparison can be done using statistical tools - reliable tests, standard deviation, coefficient of variation - but usually is sufficient to examine the percentage deviation of calculated values from baseline data, for any moment:

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$$\frac{calculated\ value - value\ date}{value\ date} * 100 \epsilon [-10; 10] \quad (1)$$

It can be considered that the model chosen is correct and can move on to making the prediction. Otherwise it is necessary to repeat the step 3 and select other mathematical model. It is worth mentioning that in adoption the decision on the correctness of the model should be considered the differences tendency between the date values and calculated values.

Making the prediction is to calculate values of the production levels attributing in the next period, the suitable values of the independent variable. Such calculated production levels only reflect the trends in the previous period from which were derived the initial data. Of course, that in any prediction, these calculated values are likely not absolutely certain becouse as to them it will manifest the influence of a number of factors not take into consideration in the prior period (with random or incidental influence) and other unknown future factors,. The time for which the prediction is made , can not exceed, according to the expertise, 1/3 up to 1/2 of the period covered by the initial data.

Experimental part

Below we present the methodology in developing a chemical production prediction using linear models.

The model of the linear growth is in relation (2) and approximates on small intervals of time any development. In case of long periods of time, the increase is less able to correctly describe the evolution of the production of a chemical.

Based on the output of the *n* values of the level production N_1, N_2,..., N_n is aimed to correlate them to a linear relation in the form of the equation:

$$N(t) = a + bt; t = 1,...,n, \quad (2)$$

to than extrapolate the development to the next period for further *r* values: t = n + 1, n + 2, ..., n + r.

In order to determine the values of coefficients *a* and *b* is used *the minimization method of the sum of squares of differences* between data values N_1, N_2 ,..., N_n, and those calculated N(l),N(2),...,N(n):

$$min\Psi = \sum_{t=1}^{n}\left[N_t - (a+bt)\right]^2, \quad (3)$$

Analyzing derivatives with respect to *a* and *b* and canceling them, will obtain:

$$\begin{cases} \frac{\partial\psi}{\partial a} = 0 = -2\sum_{t=1}^{n}(M_t - a - bt) \\ \frac{\partial\psi}{\partial b} = 0 = -2\sum_{t=1}^{n}(N_t - a - bt)\cdot t \end{cases}, \quad (4)$$

or after transformations:

$$\begin{cases} na + b\sum_{t=1}^{n} t = \sum_{t=1}^{n} N_t \\ a\sum_{t=1}^{n} t + b\sum_{t=1}^{n} t^2 = \sum_{t=1}^{n} N_t\cdot t \end{cases}, \quad (5)$$

Because:

$$\sum_{t=1}^{n} t = \frac{n(n+1)}{2}, \quad (6)$$

we can write:

$$\begin{cases} na + \frac{b}{2}n(n+1) = \sum_{t=1}^{n} N_t \\ \frac{a}{2}n(n+1) + b\sum_{t=1}^{n} t^2 = \sum_{t=1}^{n} N_t\cdot t \end{cases}, \quad (7)$$

and solving, we will obtain:

$$b = \frac{2(n+1)\sum_{t=1}^{n} N_t - 4\sum_{t=1}^{n} N_t\cdot t}{n(n+1)^2 - 4\sum_{t=1}^{n} t^2}, \quad (8)$$

$$a = \frac{2}{n(n+1)}\left(\sum_{t=1}^{n} N_t\cdot t - b\sum_{t=1}^{n} t^2\right), \quad (9)$$

To perform manual calculations is useful the systematization of that data as in table 1, before applying relations (8) and (9). This ensures the verifiability of calculations and by examining the last column can decide on the correctness of the model.

Table 1

THE SISTEMATIZATION OF THE DATA

t	N_t	t N_t	t^2	N(t)	(N(t) – N_t)100/ N_t
1 2 ... n					
Sums					

Regarding the research on the effects and impacts of pollutants resulting from the production process of chemical to the environment, we choose for example the determination of SO_2 pollutant impacts on the environment, resulting from the processing of oil.

The effect is the result of an action. It describes an event that has the objective consequence of an action. The impact is subjective transposition of this event on a scale of values. It is the result of comparing two states: a state resulting from the action and a reference state.

The impact involve the action from a target system. The considered source system is a human activity. The target system is a component of the ecosystem (human beings, fauna, flora, air, water, soil). We can define the impact like a change in condition of the target system under the action of the source system. The impact analysis first requires to define the target initial state, will then see the change of this situation. Constant changes, represent the impact itself. Overall, direct impacts on the target system generates a sequence of side impacts.

In conclusion can be summarized:

Effect (E) = phenomenon observed in the target element level;

Impact (I (E)) = Status of reference after effect (O (E)).

For example, the amount of pollutant like SO_2 resulting from the processing of oil, which is emitted in the surrounding environment is an effect. The air pollution induced of this is an impact, and SO_2 is an impact factor (fig. 2).

Environmental impact is a function of anthropogenic actions on the environment and their consequences: the impact on the environment at time t = f (action (intensity, duration); the consequence of action (environmental impact, duration)). Illustrations of these two types of actions is shown in tables 2, 3.

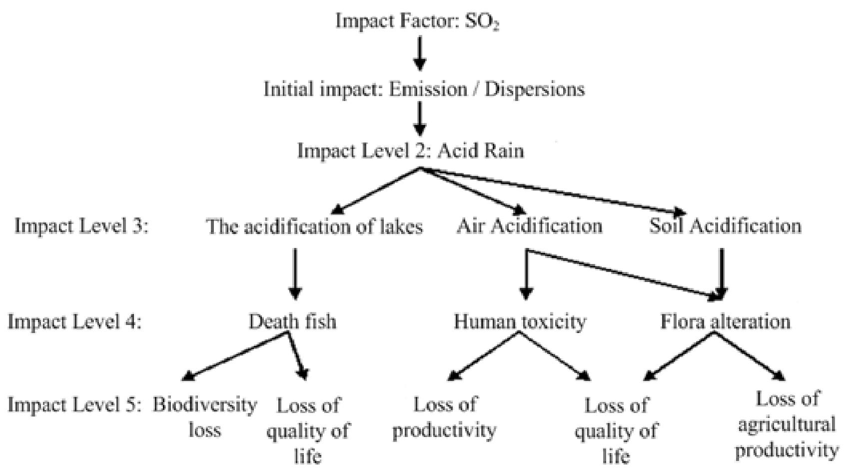

Fig.2. Viewing environmental impact

Table 2
ENVIRONMENTAL IMPACT ACCORDING TO ANTHROPOGENIC ACTIONS AND THEIR CONSEQUENCES ON THE ENVIRONMENTAL

Action	Consequences
Oil processing (quality and quantity)	The exhaustion of natural resources
Emission of gaseous and liquid effluents and the loss of energy in the environment (quantity and quality)	The effect on the physical environment (changes in concentration) The effect on the living environment (ecotoxicity) The effect on ecosystems (moving ecological balance)

Table 3
ENVIRONMENTAL ASSESSMENT METHODS

Measured item	Possible targets
An environmental system: It's either an environmental system in relation to a variety of anthropogenic systems A_i	Evaluation of the system E at time t; - Monitoring the evolution of E; - Assess the overall impact of all systems A_i have on E.
An impact or risk of impact: Let A an anthropogenic system in relationship with several environmental systems E_i	- Reducing the impact or risk impact on E_i; - Comparison of impact or impact risk due to A have on E_i.
An risk of accidents: Let A a system or anthropogenic relationship with more environmental systems E_i Risk of impact or impact:	- Reduce the risk of accidents due to A
- Let A system in relation to one anthropogenic system environment E, on which an action occurs.	Evaluation of an action involves knowing and measuring the following parameters: - Efficay: the results obtained correspond to the objectives set? - Efficiency: given the means employed, the results are satisfactory? - Relevance: to achieve its objective, the means provided are relevant?

Conclusions

Predicting the evolution of chemical production is very important for assessing the environmental impact.

In the environmental analysis, we have to consider the potential impact. It is characterized by a combination of three parameters:

- source action (nature and intensity);
- exposure and availability of the target systems;
- the sensitivity of target systems.

If we consider a pollutant being emitted into the environment, the potential impact will depend on:

- the amount and the concentration of the emitted substance;
- mobility and dispersion tendency of the substance;
- persistence in the environment that depends on its degrabilitatea;
- transformation into other products in the environment;
- harmful effect on humans, animals, plants and on other ecosystems.

Environmental assessment methods differ depending on the intended objectives, that are presented in table 3.

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Manuscript received: 26.04.2016

INCEPAND CU ANUL 2017 REVISTA DE CHIMIE
va fi editata pe suport magnetic
avand urmatorul ISSN:

Revista de Chimie (Bucuresti), CD-ROM. English ed.)

ISSN 2537-5733

ISSN-L 1582-9049