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Optimization of the pyrolysis of ethane using fuzzy programming

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Abstract

The aim of this paper is to apply fuzzy/possibilistic optimization focus in the context of the pyrolysis of ethane. The methodology is based on the fact that minimal/maximal values of these parameters are target values along the year rather than fixed real numbers. The fuzzy model is obtained taking into account the behaviour of the ethane conversion, steam/hydrocarbon ratio, inlet pressure and inlet temperature. The results demonstrated that the degree of optimism, $\alpha = 1$, describes better the real behaviour of the process with an equilibrium approach dimensionless parameter (EA) below 0.65 and a minimum total cost of US$ 2.55.

Keywords: Possibilistic; Degree of optimism; Fuzzy coefficients; Furnace; Ethane; Pyrolysis; Optimization

1. Introduction

The ethylene process was used commercially before 1920. Ethylene has become one of largest volume chemicals in the world [1]. So far, several optimization techniques have been published, however, few optimization studies of the ethylene process have been made. The first study was made for [2] where the pyrolysis furnace was studied using a simulator using mass and energy balance equations for simplified systems, i.e., systems with simplified kinetics, only two or three species of importance, etc. Unfortunately, the assumptions used in these earlier works do not adequately apply to many specific reaction systems. In fact, several process optimization studies [3,4] have shown that optimal values of several of the independent variables lie on or near the upper or lower boundaries of the independent variables. However, in the ethylene process is particularly difficult when a gradual addition of the constraint and unconstrained variables is included in the pyrolysis furnace. In this case, the design data, objective function and constraints are stated in vague and linguistic terms. It appears that it is more reasonable to have a transition state from absolute permission to absolute non-permission. This implies that the constraint is to be stated involving vague and imprecise information. In the literature several applications of the fuzzy logic in optimization have been reported [5–9].

The fuzzy mathematical programming in the first category was initially developed by Bellman and Zadeh [5]. It treats decision-making problem under fuzzy goals and constraints. The fuzzy goals and constraints represent the flexibility of the target values of objective functions and the elasticity of constraints. From this point of view, this type of fuzzy mathematical programming is called the flexible programming. The second category in fuzzy mathematical programming treats ambiguous coefficients of objective functions and constraints but does not treat fuzzy goals and constraints. Dubois and Prade [10] treated systems of linear equations with ambiguous coefficients suggesting the possible application to fuzzy mathematical programming for the first time. A remarkable development is done by Kuzmin [11]. He introduced four inequality indices between fuzzy numbers based on the possibility theory into mathematical programming problems with fuzzy coefficients. Since the fuzzy coefficients can be regarded as possibility distributions on coefficient values, this type of fuzzy mathematical programming is usually called the possibilistic programming.

In fact, using possibilistic optimization approach, a solution can be achieved that provides a maximum degree of overall satisfaction [12–14]. To determine an optimal solution, decision problems may be formulated as a fuzzy decision model, particularly when the available data are known exactly though varying

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within a tolerance limit. The coefficients of some constraints may be fuzzy numbers and the original fuzzy problem is transferred into a crisp satisfactory model [15]. The purpose of this study was to develop a fuzzy model with economics of the pyrolysis furnace in an ethylene process using ethane feed. The plant size is 300,000 TPY of ethylene. A further objective is to study the sensibility of the model when the degree of optimist changes.

2. Ethane pyrolysis

The ethane is pyrolyzed during the ethylene production using a furnace [1]. The feed enters the furnace convection and it is preheated to 833–972 K by the flue gases before being further heated in the radiation section. Dilution steam, added to inhibit coke formation, is also preheated in the convection section before being mixed with the feed. The ethane–steam mixture is divided among parallel coils in the firebox. The mixture enters the radiation section at 414–552 kPa where the ethane is pyrolyzed to the primary products of hydrogen, methane and ethylene, along with a mixture of smaller amounts of C_3 to C_5 hydrocarbons. The effluent leaves the furnace at 350–450 kPa and 833–972 K. The furnace effluent is cooled in a transfer line exchanger where the steam is recovery. Seven equations to describe the pyrolysis of ethane:

$$C_2H_6 \Leftrightarrow C_2H_4 + H_2 \quad (1)$$

$$C_2H_4 + 2H_2 \Leftrightarrow 2CH_4 \quad (2)$$

$$C_2H_4 \Leftrightarrow 0.25C_4H_6 + 0.125C_4H_8 + 0.125C_4H_{10} + 0.125H_2 \quad (3)$$

$$C_2H_4 \Leftrightarrow 2C + 2H_2 \quad (4)$$

$$C_2H_4 \Leftrightarrow C_2H_2 + H_2 \quad (5)$$

$$C_2H_4 + C_2H_6 \Leftrightarrow 0.952C_3H_6 + 0.381C_3H_8 + 0.62H_2 \quad (6)$$

$$C_2H_4 \Leftrightarrow 0.333C_6H_6 + H_2 \quad (7)$$

3. Analysis of data and model

The methodology for fuzzy programming (FP) has references at [5–8,14,16]. The approach proposed here is based on an interaction with the decision maker, the implementer and the analyst in order to find a compromised satisfactory solution for a fuzzy programming (FP) problem. In a decision process using FP model, source resource variables may be fuzzy, instead of precisely given numbers as in crisp linear programming (CLP) model [17,18]. For example, machine hours, labor force, material needed and so on in a manufacturing center, are always imprecise, because of incomplete information and uncertainty in various potential suppliers and environments. Therefore, they should be considered as fuzzy resources, and the FP problem should be solved by using fuzzy set theory [17–19]. A general model of fuzzy linear programming is formulated as:

$$\begin{aligned} &\text{Min}(z = Cx) \\ &\text{subject to} \quad \bar{A}x \tilde{\leq} \bar{b}, \quad x \geq 0 \end{aligned} \quad (8)$$

where x is the vector of decision variables and C are the coefficients of the objective function (real number); $\bar{A}$ and $\bar{b}$ are fuzzy quantities; the operations of addition and multiplication by a real number of fuzzy quantities are defined by Zadeh's extension principle [5]; the inequality relation $\tilde{\leq}$ is given by a certain fuzzy relation and the objective function, z, is to be maximized in the sense of a given FP problem. Carlsson and Korhonen [15] approach is considered to solve FP problem, which is fully trade-off, meaning that the solution will be with certain degree of satisfaction. First of all, formulate the membership functions for the fuzzy parameters of $\bar{A}$ and $\bar{b}$.

Very simply, fuzzy decision making selects from a set of crisp elements while possibility selects from a set of distributions. The underlying sets associated with fuzzy decision-making are fuzzy where one forms the decision space of crisp elements from operations ("and" in the case of optimization, that is, constraints) on these fuzzy sets. The underlying sets associated with possibilistic decision-making are crisp where one forms the decision space of distributions from operations on crisp sets. Possibilistic distributions encapsulate the best estimate about the value of an entity given the available information.

Fuzzy membership function values describe the degree to which an entity is that value [21]. A possibility of one means that the value of the entity has the highest possibility of being what distribution defines. If the fuzzy membership value is one, then it is definitely the value. Thus the nature of decision making in the presence of fuzzy/possibilistic uncertainties are quite different in semantics and optimization procedures since fuzzy optimization optimizes over sets of numbers and possibility optimizes over sets of distributions.

The problem (8) included linear functions of x whose coefficients are possibilistic variables. Such a function is called 'a possibilistic linear function'. Since the possibilistic variable coefficients are ambiguous parameters, the possibilistic linear function value is also ambiguous. The range of the possibilistic function value are restricted by a fuzzy number since the possibilistic variable coefficients are restricted by fuzzy numbers. Under a possibility distribution μ_A of a possibilistic variable α, possibility and necessity measures of the event that α is in fuzzy set B are defined as follows [22,23]:

$$\begin{aligned} &\Pi_A(B) = \sup \min(\mu_A(r), \mu_B(r)), \\ &N_A(B) = \inf \max(1 - \mu_A(r), \mu_B(r)) \end{aligned} \quad (9)$$

where μ_B is the membership function of the fuzzy set B. $\prod_A(B)$ evaluates to what extent it is possible that the possibilistic variable α restricted by the possibility distribution μ_A is in the fuzzy set B. On the other hand, $N_A(B)$ evaluates to what extent it is certain that the possibilistic variable α restricted by the possibility distribution μ_A is in the fuzzy set B.

Let α be a possibilistic variable. In context to the above example, let $B = (-\infty, g]$, i.e., B be a crisp (non-fuzzy) set of real numbers, which is not greater than g [24,25]. Then we obtain the following indices by possibility and necessity measures defined by:

$$\text{Pos}(\alpha \leq g) = \Pi_A((-\infty, g]) = \sup\{\mu_A(r) | r \leq g\} \quad (10)$$

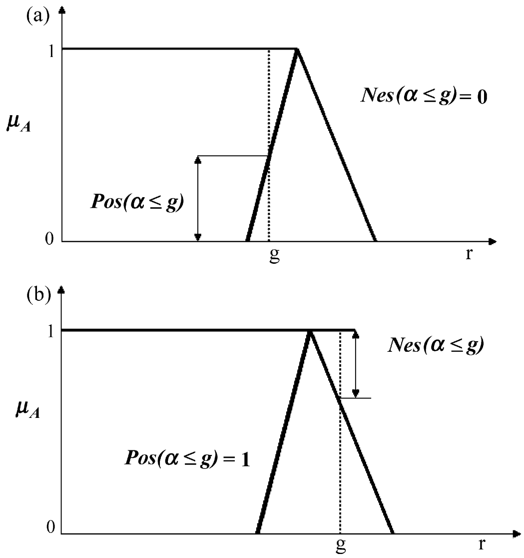

Fig. 1. Possibility and necessity measures of $\alpha \leq g$.

$$\mathrm{Nes}(\alpha \leq g) = N_{\mathrm{A}}((-\infty, g]) = 1 - \sup\{\mu_A(r)|r > g\} \quad (11)$$

$\mathrm{Pos}(\alpha \leq g)$ and $\mathrm{Nes}(\alpha \leq g)$ show the possibility and certainty degrees to what extent α is not greater than g. Those indices are depicted in Fig. 1.

Similarly, letting $B = [g, +\infty)$ we obtain the following two indices:

$$\mathrm{Pos}(\alpha \geq g) = \Pi_A([g, +\infty)) = \sup\{\mu_A(r)|r \geq g\} \quad (12)$$

$$\mathrm{Nes}(\alpha \geq g) = N_A([g, +\infty)) = 1 - \sup\{\mu_A(r)|r < g\} \quad (13)$$

$\mathrm{Pos}(\alpha \geq g)$ and $\mathrm{Nes}(\alpha \geq g)$ show the possibility and certainty degrees to what extent α is not smaller than g. Those indices are depicted in Fig. 2.

Following the study case, Schutt [19] has given data for effluent gas composition as a function of the optimal concentration of ethane, C_e:

$$N_{H_2} = 1.0044C_e - 4.036 \quad (14)$$

$$N_{C_2H_4} = 0.8022C_e + 3.950 \quad (15)$$

$$N_{C_3H_8} = 0.0083C_e - 0.205 \quad (16)$$

$$N_{CH_4} = 0.1786C_e - 2.500 \quad (17)$$

$$N_{C_4} = 0.0180C_e - 0.235 \quad (18)$$

$$N_{C_3H_6} = 0.0202C_e - 0.508 \quad (19)$$

$$N_{C_5} = 0.0203C_e - 0.662 \quad (20)$$

The conditions of the furnace must be checked to assure that coke deposition in the reactor coils will not be excessive. The criterion used is based on an equilibrium approach (EA) dimensionless parameter. Through experience in reactor design, it has been concluded that coke formation is not excessive if the approach to equilibrium of the primary decomposition of ethane is kept below 0.65. The EA constraint is defined as:

$$\mathrm{EA} = \frac{N_{C_2H_4} N_{H_2} P}{N_{C_2H_6} N K_1} \quad (21)$$

$$K_1 = 4.87 \times 10^{-6}\,\mathrm{e}^{0.0078T} \quad (22)$$

where P is the total pressure and N is the total moles. Since the coke formation mechanism is quite complex and not fully understood, a simple, but effective relationship has been developed to represent conditions, which give excessive coke formation. The heat flux, q, is the sum of energy fluxes. The energy balance associated to the furnace within the reaction zone varied by as much as 12 K. The equation is as follows:

$$\nabla q = \nabla \left(-k\nabla T + \sum h_i\,(-\rho D \nabla x_i)\right) \quad (23)$$

where k is the conductivity, T the furnace temperature, x the molar fraction by component and ρ is the mixture density. A simplified expression suggested by Maji et al. [20] for the calculation of mixture diffusivity (D) in the combustion of hydrocarbons was used. The expression is as follows:

$$D\,(\mathrm{m^2/s}) = \frac{AT^{1.75}}{P} \quad (24)$$

For developing the model, the necessity and possibilistic measures indicated Eq. (9) where considered, however, the costs are non-linear function of the decision variables considered in this article [26]. The model consists in a non-linear objective function and linear constraints. The final model is as follows:

$$\mathrm{Min}\left[\sum_n C_i x_i\right] \quad (25)$$

where C are the costs. The major costs used in this model are [26]:

$$\text{cost of reactor:} \quad C_R = C_{RB}\left[\frac{x_2 \ln(1 - x_1)}{(x_4/450\,\mathrm{kPa})K_1}\right]$$

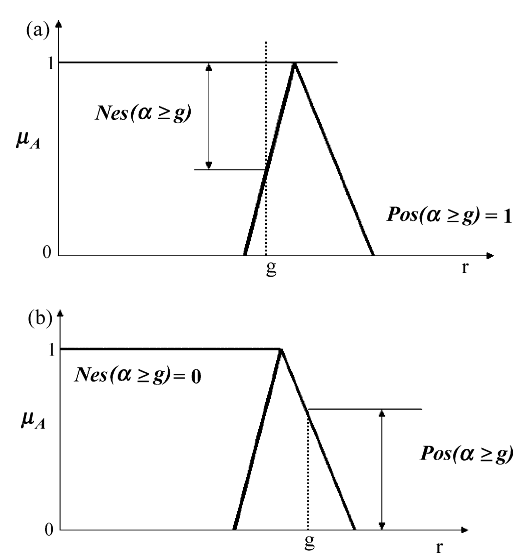

Fig. 2. Possibility and necessity measures of $\alpha \geq g$.

Table 1
a_i fuzzy intervals

	Ethane conversion (x_1)	Steam/hydrocarbon ratio (x_2)	Inlet temperature (x_3)	Inlet pressure (x_4)
Minimum	0.55	0.45	833	414
Average	0.59	0.52	910	490
Maximum	0.62	0.67	972	522

Table 2
b_i values

Variable	Value
Ethane conversion, x_1	1.00
Steam/hydrocarbon ratio, x_2	0.8
Inlet temperature, x_3 (K)	980
Inlet pressure, x_4 (kPa)	455

$$\text{cost of furnace}: \quad C_F = C_{FB}\left(\frac{q}{FC_p(x_3 - 900\,\text{K})}\right)^{0.78}$$

$$\text{cost of steam}: \quad C_S = C_{SB}{x_2}^{0.22}$$

where x_1 is the ethane conversion ($C_e = C_{e_0}(1 - x_1)$), x_2 the steam hydrocarbon ratio, x_3 the inlet temperature and x_4 is the inlet pressure. C_{RB}, C_{FB} and C_{SB} are basis costs that can be calculated using Guthrie correlations [26].

Subject to:

$$\text{Nec}\left[\left(\sum_n \bar{a}_i x_i \le b_i\right) \ge \alpha\right] \leftrightarrow \sum (a_i)x_j + \sum \alpha(\bar{a}_i - a_i)x_i \le b_i \tag{26}$$

$$\text{Pos}\left[\left(\sum_n \bar{a}_{ij} x_i \le b_i\right) \ge \alpha\right] \leftrightarrow \sum (a_i)x_i + \sum (1-\alpha)(\bar{a}_i - a_i)x_i \le b_i \tag{27}$$

where α is the level or degree of optimism for the satisfaction of the constraint. Here a_i and b_i are triangular fuzzy numbers: $0/a_i/\bar{a}_i$ and $0/b_i/\bar{b}_i$ crisps and $\alpha \in [0\,1]$ with $\alpha = 0.0, 0.25, 0.50, 0.75$ and 1.00 is used (these values were selected arbitrarily) [25]. Any values between [0 1] can be used. The values of a and b can be found in Tables 1 and 2.

4. Results and discussion

Briefly speaking, the possible optimal solution is a solution, which is optimal for at least one possible objective coefficient. On the other hand, the necessarily optimal solution is a solution, which is optimal for all objective coefficients. A necessarily optimal solution does not always exist. When no necessarily optimal solution exists, plenty possibly optimal solutions should exist. The idea is that Eqs. (25) and (27) incorporate a possibilistic right-hand side with a possibilistic outcome left side where the constraints are a set of distribution so that one must take into account all the possible distribution. Eqs. (25)–(27) can be solved using any non-linear programming algorithm or software package as GAMS.

Since the furnace has to be thermally efficient to be economical, the optimum combination of variables will tend to balance in the total cost. In Tables 3 and 4, are shown the values of the decision variables to different degree of optimism. The optimum values were obtained when the degree of optimism is equal to 1.0, where: the conversion is equal to 0.61, the steam/hydrocarbon ratio is equal to 0.61, the inlet temperature is 865 K and the inlet pressure is 445 kPa. The combination when $\alpha = 1.0$ is realistic because EA is below 0.65, the composition of the effluent gas is more according to our filed data and the heat flow was below 14,200 kJ/m^2 K. On the other hand, Table 5 depicts the total cost of the plant (objective function) is very sen-

Table 3
Composition of the effluent gas at different degrees of optimism and operating conditions

Component	α				
	0.00	0.25	0.50	0.75	1.00
H_2	35.0	34.8	35.1	34.6	35.0
CH_4	5.1	5.1	4.9	4.8	5.2
C_2H_2	0.2	0.15	0.15	0.16	0.15
C_2H_4	33.1	32.8	33.1	32.5	33
C_2H_6	23.8	23.8	24.0	23.7	23.6
C_3H_6	1.0	0.9	0.9	0.9	0.9
C_3H_8	0.19	0.19	0.18	0.19	0.19
C_4	0.45	0.45	0.49	0.45	0.45
C_5	1.16	1.18	1.18	2.7	0.21

Table 4
EA at different degrees of optimism

	α				
	0.00	0.25	0.50	0.75	1.00
EA	0.61	0.58	0.58	0.60	0.60
Heat flux (kJ/m^2 K)	13,810	13,821	13,800	13,801	13,804

Table 5
Operating costs (US$) at different degrees of optimism

α	Cost (US$)
0.00	2.61
0.25	2.61
0.50	2.62
0.75	2.61
1.00	2.55

sible to α. When the value of α is over 0.50 the cost is practically constant.

It is worth noting that the result can change if another fuzzy function is used (S-shape or Gaussian). We used triangular fuzzy function because this function adjusted satisfactory to our data. Moreover, the objective function is independent of the average used because the possibility and necessity measures are satisfied of the same manner.

5. Conclusion

Real world problems are not usually so easily formulated as mathematical models or fuzzy models. Sometimes qualitative constraints and/or objectives are almost impossible to represent in mathematical forms. The fuzzy solutions have not yet been investigated considerably. In this paper, we formulated a fuzzy problem for studying the pyrolysis of ethane. The most important results indicated that using fuzzy programming with a degree of optimistic equal to 1.0, a good result can be obtained and the furnace is economically attractive.

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