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CONSIDERATION OF SAFETY INDICATORS IN SELECTING AUXILIARY SUBSTANCES FOR CHEMICAL-TECHNOLOGICAL PROCESSES OF OIL REFINING

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The paper gives study results on the indicators in accordance with which the selection of auxiliary substances (reagents) for chemical-technological processes of oil refining is carried out. Methods of expert assessment for decision-making based on multi-criteria parameters are proposed.

Emergency depressurization of process equipment at hydrocarbon processing plants can cause a major accident with attendant emissions of toxic substances, destruction and damage to expensive equipment, process stops, fires and explosions [1].

Currently, when selecting auxiliary substances (reagents) for chemical-technological processes of oil refining, technological parameters (flow, concentration, corrosivity, rheological properties, thermal and chemical stability, impact on the quality of the target product and its output, etc.) and economic indicators (cost, availability, etc.), almost without taking into account the indicators characterizing the impact of reagents on workers and the environment (the threshold limit value (TLV), hazardous materials (HAZMAT), toxicity, etc.). This circumstance determined the purpose of this study, which is to study the procedures and indicators in accordance with which the selection of auxiliary substances (reagents) for chemical-technological processes of oil refining and the development of expert assessment methods for decision-making taking into account the multi-criteria parameters is carried out.

Problems of choice of reagents and the need to take into account indicators characterizing safety arise at the design stage of the chemical process, for example, the choice of isobutane alkylation catalyst with olefins or concentrated sulfuric acid (2nd class HAZMAT) or hydrofluoric acid (1st class HAZMAT); solvent selective purification of petroleum oils (phenol (2nd class HAZMAT), furfural (3rd hazard class) and N-methylpyrrolidone (4th hazard class), comparative technological indicators are given in Table 1); alkanolamines for the desulfurization of hydrocarbon gases (monoethanolamine (2nd class HAZMAT), diethanolamine (3rd class HAZMAT), methyldiethanolamine (3rd class HAZMAT), the comparison of physicochemical properties is given in Table 2); hydrogen sulfide scavengers from fuel oil, etc.

An analysis of the practice of using reagents in existing plants shows that often more toxic and hazardous excipients are preferred. It should be noted that exports in the conditions of multi-criteria technological and economic parameters are difficult to make a choice in favor of one or another reagent.

Currently, various expert assessment methods are used for decision-making: operations research method, utility theory method, hierarchy analysis method, use of fuzzy set theory elements, their combination (fuzzy hierarchy analysis method) and others [2-8], method of accounting for safety indicators when choosing reagents for chemical-technological processes of oil refining using elements of the theory of fuzzy sets.

Table 1. – Comparative technological indicators of solvents for selective purification of oils

Indicators	N-methylpyrrolidone	Phenol	Furfurol
Molar mass, g·mol^{-1}	99	94	96
Density at 66 °C, g/cm^3	0.996	1.040	1.110
Kinematic viscosity at 50 ° C, mm^2/c	1,01	3,24	1,15
Digule moment, Db	4,10	1,70	3,57
Boiling point Melting point Flash point	204 -24,2 91	182 +41,1 79	162 -38,6 59
Surface tension at 20 °C, мН/м	39,9	38,2 (50 °C)	43,9
Solubility in water, %	100,0 (20°C)	100,0 (above 66°C)	100,0 (20°C)
Formation of an azeotropic mixture with boiling water	No	Yes	Yes
Heat of evaporation, kJ / kg	493,1	479,1	451,1
raw materials consumption, kg/t	0,1	0,4	0,8
TOE/t raw material	0,83-1,24	1,65	1,24

Table 2. – Physico-chemical properties of alkanolamines

Indicators	Monoethanolamine (MEA)	Diethanolamine (DEA)	Methyldiethanolamine MDEA
Molar mass, g·mol^{-1}	61,1	105,1	119,2
Density at 20 °C, g/cm^3	1,015	1,011	1,030
Boiling point congelation	170,3 10,3	268,4 27,5	231 –21
Vapor pressure at 60 ° C, Pa	860	4,7	27
Dynamic viscosity, kPa/s (at Temperature)	18,9 (25°C)	352 (30°C)	101 (20°C)
Specific heat capacity, kJ/(kg˚C) (at 30 °C)	2,72	2,47	1,71

The following successive steps are provided: to determine the input variables of technological, economic parameters and safety indicators; to fuzz the input data by finding the values on the corresponding graphs of the term membership function; determine the degree of truth of conditions for each of the rules of fuzzy inference systems; construct the resulting membership functions for the output parameters, taking into account the degree of truth of all production rules; calculate the resulting (clear) value of the output variable by defuzzification using the center of gravity method; decide on each reagent.

The technique allows us to unify the procedure for selecting a reagent for chemical-technological processes and it is reasonable to determine the auxiliary substance that is most preferable, taking into account technological and economic parameters and safety indicators.

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