MULTIPLE LINEAR REGRESSION OF C9 FRACTION INVERCED EMULSION OLIGOMERIZATION

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The production of hydrocarbon resins by low-temperature oligomerization in an emulsion of the 2nd kind is considered. Correlation dependences between yield, resin characteristics and process conditions are established. Statistical analysis of the yield and physicochemical characteristics of hydrocarbon resins was performed.

Keywords – petroleum resin, emulsion oligomerization, fraction C9, correlation, multiple linear regression.

Introduction

In the process of synthesis of ethylene/propylene by pyrolysis, a significant number of liquid by-products (about 30%) are obtained. C9 fraction, containing unsaturated aromatics (styrenes and indenes), to produce aromatic oligomers. Aromatic oligomers (so-called petroleum or hydrocarbon resins) have a wide range of applications as film-forming agents in lacquer-paint and anticorrosive coatings [1, 2].

We propose to use the emulsion method of oligomerization of unsaturated hydrocarbon of C9 fraction of diesel pyrolysis liquid by-products. This method can significantly reduce the process temperature and reaction time compared to the industrial methods of oligomers (hydrocarbon resins) synthesis [3].

Emulsifiers of the second kind form an emulsion of the "water-in-oil" type. Characterized by the value of hydrophilic-lipophilic balance (HLB) from 3 to 6. The use of emulsifiers of the second kind (water-in-oil emulsion) allows for reducing the amount of water in the reaction mixture. This increases the productivity of the reaction equipment and reduces energy costs.

Experimental results and discussion

Composition of the reaction mixture of 2nd kind emulsion oligomerization:

– the dispersion medium - liquid pirolisis by-products fraction C9 (density – 936 kg/m^3; bromine number – 68 g Br_2/100 g, molecular weight – 102, the content of unsaturated compounds to 45 %wt. especially: styrene - 17,85 % viniltoluene - 6,99 %, dicyclopentadiene - 18,00 %, indene 1,25 %.);
– the disperse phase – water;
– emulsifier – used 2nd kind emulsifiers (Polyglycerol polyricinoleate – HLB = 6; Ester A (a mixture of mono- and di-glycerides of oleic acid) HLB = 3)
– the initiator is soluble in the disperse phase (2nd kind emulsion) - Benzoyl Peroxide 1.0 %wt. (in terms of fraction C9).

The pH of the reaction mixture is 2.8. The study was performed at a reaction time of 180 min. The main studied process parameters:

– the reaction temperature was 303-353 K,
– the emulsifier concentration – 0.6-1.0 % (in terms of water),
– mixing intensity (Re = 6870-10120),
– the volume ratio fraction C9: water - [1:1] - [1:5].

Microsoft Excel was used for the correlation index calculations. As confirmed by the average correlation indices (per module), the emulsion oligomerization temperature has the least effect on the process. The most significant effect (0.81) on the yield of oligomers has the reaction duration. The results are shown in Table. 1.

Table 1

Correlation of petroleum resins characteristics and reaction conditions

Characteristic	Correlation index				
	reaction duration	temperature	emulsifier concentration	phase ratio	mixing intensity
Yield	0,81	0,30	0,03	0,51	0,51
Bromine number	-0,83	-0,27	0,08	-0,57	-0,06
Molecular weight	-0,28	0,02	0,59	0,24	0,05
Softening point	0,11	0,15	0,31	0,23	-0,05
Color index	0,54	0,45	-0,52	0,05	-0,26

Multiple linear regression is suggested (Eq. 1). For it`s construction, the parameters that have the most significant impact on the course of the oligomerization reaction are selected.

Table 2

Factors identified multiple linear regression

mixing intensity (**M**) b3	the volume ratio of the phases (**R**) b2	reaction duration (**D**) b1	b0
0,0046	0,0924	0,0603	-8,9825

The dependence of the oligomer yield (Y) on the considered parameters (multiple linear regression) is described by the equation:

$$Y = -8{,}9825 + \mathrm{D} * 0{,}0603 + \mathrm{R} * 0{,}0924 + \mathrm{M} * 0{,}0046 \quad (1)$$

The calculated Fisher criterion is 95,593. It`s indicates the high adequacy of the proposed multiple linear regression [4].

Conclusion

The main correlations of the yield and petroleum resins characteristics to the reaction conditions are established. It is confirmed that the product yield depends on all process conditions. Multiple linear regression is suggested.

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