



Fig. 1. The chart for implementation of this approach at the mathematical modeling of the catalytic cracking

and cyclization of olefins with hydrogen transfer ( $A_{ij} = 4.62$  kJ/mol) are reversible at the process temperature 794 K during the processing of vacuum distillate with saturated to aromatic ratio 1.88 unit and reaction temperature range is 848–794 K. In addition, the reversibility of cracking olefins take into

account as the direct reaction of olefins aromatization in formalized scheme of hydrocarbon conversion due to the high reactivity of olefins according to the classical concepts of the catalytic cracking [2] and results of the quantum chemical calculation ( $\Delta G = -92.2$  kJ/mol).

## References

1. Parmon V.N. *Thermodynamics of nonequilibrium processes for chemists. Dolgoprudny: Intellect, 2015.*– 472p.
2. Kapustin V.M., Gureev A.A. *Technology of oil refining. Destructive processes. Part two.*– M.: Kolos, 2008.– 334p.

## COMPARATIVE EVALUATION OF DIFFERENT RADICAL INITIATORS, USED FOR PRODUCTION OF GRAFT COPOLYMERS, BASED ON ATACTIC POLYPROPYLENE

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**Introduction.** Nowadays the demand for production of polypropylene is extremely high in the world. Polypropylene takes the 3rd place by volume of consumption now, and this number has increased from 200 to 1200 thousand tons per year in Russia in 2000–2015. It's obvious that the need of this polymer will keep growing, therefore the technologies of production should be developed and the volume of it ought to be increased.

**Relevance.** Polypropylene is most commonly produced by propylene polymerization in presence

of the Ziegler–Natta catalyst [1, 2], yet at the end of the chemical process 2–3% of the final product is an atactic polypropylene (abbreviated APP). This material has much lower quality in comparison with the isotactic polypropylene; therefore it isn't used in industry and is commonly utilized. A hypothesis was made [3] that a modification of APP with different graft copolymers could improve its characteristics and makes it suitable for using in industry. This approach might also contribute to a solution of economic and ecological questions in the subject of

propylene production's waste.

**Purpose.** The selection of comonomer (styrene, dicyclopentadiene, abbreviated DCPD) for a graft copolymerization with APP, which will produce the product with better characteristics in comparison with APP. The selection of initiator (azoisobutyronitrile, abbreviated AIBN; benzoyl peroxide or BPO; potassium peroxydisulfate or KPS), which will give the highest practical product yield of the copolymer of the best quality.

**Method.** The radical copolymerization was processed in the heptane solution at the 80 °C temperature. The solution of APP in heptane and the solution of comonomer and initiator were prepared previously; then they were mixed together in a flask and this mixture was held for three hours. After the end of the reaction received copolymer was swaged in isopropyl alcohol, filtered out and dried firstly in air and then in vacuum. The speciation of graft copolymer was defined by the infrared spectroscopy.

**Results.** Maximum values of practical product yield depending on types of comonomer and initiator are represented in the table below. According to these results it can be concluded that the highest extent of reaction is reached by using AIBN and BPO with styrene.

In the low concentration area AIBN is not very effective, but the sharp increase of product yield takes place after reaching 5% concentration of AIBN. Then the product yield becomes constant so there's no use of increasing AIBN concentration further. The same tendency is shown in the experi-

**Table 1.** Maximum values of practical product yield depending on types of comonomer and initiator

Initiator	Comonomer	The highest practical product yield, %
AIBN	Styrene	85
	DCPD	24
KPS	Styrene	30
	DCPD	26
BPO	Styrene	85
	DCPD	26

ment with BPO. At the same time the copolymerization with DCPD has a low product yield with all three initiators.

The styrene copolymerization increases also the softening temperature from 70–90 °C to 105–120 °C, which could be interpreted as the elimination of low resistance to thermo-oxidative and light destruction. The mechanical strength of copolymer's films is also higher than of the film of APP itself.

**Conclusion.** According to the current day the volume of APP production is about 40 thousand tons per year. The introduction of APP copolymerization into industry seems rational because of the improvement of its physical properties and available data [4] about the positive effect of the addition of APP into bitumen and various coatings. The approach of this kind, as it was already mentioned upwards, could be the solution of an ecological problem and also might become a source of income.

## References

1. *Stereoselectivity in Ziegler-Natta polymerization of conjugated dienes. 2. Mechanism for 1, 2 syndiotactic polymerization of diene monomers with high energy s-cis 4 coordination* / Costabile C., Milano G., Cavallo L., Longo P., Guerra G., Zambelli A. // *Polymer*, 2004.– №45.– P.467–485.
2. Dolgoplosk B.A., Tinyakova E.I. *Organometallic catalysis in the processes of polymerization.*– Moscow: «Nauka», 1985.– 534p.
3. Battaerd H.A., Tregear G.W. *Graft copolymers.*– Leningrad: «Khimia», 1970.– 216p.
4. *The application of atactic polypropylene for the improvement of bitumen and asphaltic concrete* / Hochman L.M., Shemonaeva D.S., Steponyan I.V., Titov E.N. // *Car roads*, 1990.– №8.– P.11–13.