Siberian Federal University

Petroleum chemistry

Course (module) Title

Petroleum Chemistry Guide

Course (module)

Krasnoyarsk, 2020

Table of Contents

Course (module) Guide Petroleum Chemistry

1. Course (module) Description

1.1. Course (module) overview

The course of Petroleum Chemistry provided a curriculum of postgraduate educational program 04.06.01 Chemical Sciences; specialization is 02.00.13 Petroleum Chemistry.

Natural gas and crude distillates such as naphtha from petroleum refining are used as feedstocks to manufacture a wide variety of petrochemicals that are in turn used in the manufacture of consumer goods. Petroleum Chemistry provides knowledge and generates skills in the field of technologies for producing the most bulk groups of petrochemical products; explains the principles of intensification and modernization of existing industries based on using of in-depth patterns of chemical transformations investigations. The course acquaints students with petrochemicals laboratory synthesis, petrochemical process operations and basic technological equipment. Technical and economic indicators calculation of chemical-technological processes is also discussed.

The discipline forms the ability to set and solves problems in the scientific and industrial direction; motivates postgraduate students for self-development and advanced training. Petroleum Chemistry subject promotes the ability to conduct independent research, teaching and expert consulting activities.

1.2. Special features of the course (module)

1. The course is split into 3 major sections. These are fundamentals of petrochemical production processes such as halogenation, etherification, dehydrogenation and other similar technologies; petrochemical industry overview and assessable resources for the organic synthesis industry; olefins chemistry and technology of polymer chemistry, In addition to conventional lectures, the course offers a range of other learning opportunities in which students actively participate. Moreover, students will be involved in online discussion and tests.
2. Provides broad technical information on petrochemical production processes, enabling a rapid immersion in the petrochemical field. Detailed course material with a glossary of the main technical terms used in petrochemical industry. There are new trends in production technology, petrochemical application characteristics to European and worldwide scale. Up to date petrochemicals production schemes are included.

1.3. Course (module) aim

• To acquaint with the main theoretical schools, approaches and concepts for solving problems in the field of organic substances chemical technology.
• To form abilities to search, analyze, critically reflect and generalize scientific and technical information, formalize the results of research work.
• To determine possible research areas towards the petrochemical synthesis.

1.4. Course (module) objectives

• Arranging of general refinery and petrochemical operations, their products and economic importance.
• Formation of skills for the invention of creating chemical-technological processes and materials innovative methods.
• Getting acquaint with the synthesis methods of some petrochemical products in the laboratory.
• Formation of professional skills of comparative analysis and selection of the optimal technology for the synthesis of organic synthesis products, taking into account the economic and environmental components.

1.5. Learning outcomes of the course (module)

By the end of the course, postgraduate students will be able to:

• create basic schematic diagrams for producing the most bulk products of petrochemical synthesis;
• select a laboratory methods for the synthesis of some petrochemical products in the laboratory;
• to carry out research activities independently in the relevant professional field using modern research methods and information and communication technologies;
• organize the work of a research team in the field of chemistry and related sciences;
• realize knowledge of the current state of science in the field of

petrochemistry;

- enter innovative production methods of different petrochemicals.

1.6. Teaching and Learning Methods

The course includes methodological information which will be educated by the students themselves, practice sessions and seminars session which is realized by distant form through electronic resources that are associated with the SibFU or in lecture halls of «Basic chair of chemistry and technology of natural energy resources and carbon materials»

2. Course Instructor(s) and Tutor(s), Contact Information

Vladimir A.Safin

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3. Course (module) Outline

4.1 Course (module) requirements

4.1.1. Required text(s)

Main literature

1. Petroleum Chemistry and Refining [Text]: monograph / ed. J. G. Speight. - London: Taylor & Francis, 1998. - xiv p. : ill. - (Applied Energy Technology Series / Editor: J.G. Speight¤). - Glossary: p. 247-262.
2. The chemisty and technology of petroleum [Text] / J. G. Speight. - 4th ed. - Boca Raton ; London ; New York : CRC Press : Taylor & Francis Group, 2006. - 919 p.
3. Applied process design for chemical and petrochemical plants [Electronic resource]. Vol. 1 / E. E. Ludwig. - 3th ed. - Electronic text data (28,8 МБ). -

Boston : Butterworth-Heinemann, 1999. - 630 p.
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5. Applied process design for chemical and petrochemical plants [Electronic resource]. Vol. 3 / E. E. Ludwig. - 3th ed. - Electronic text data (24,4 МБ). - Boston : Butterworth-Heinemann, 1999. - 690 p.
6. Handbook of Vinyl Polimers. Radical Polymerization, Process and Technology [Text]: monograph / Y. Vagci; Ed. M.K. Mishra. - 2nd ed. - London: CRC Press, 2009. - 763 p.
7. Handbook of MTBE and Other Gasoline Oxygenates [Text] / ed.: H. Hamid, M. Ashraf Ali. - New York : Marcel Dekker, 2004. - 381 p.
8. Polymer Chemistry [Text]: monograph / W. R. Moore. - London: University of London Press LTD, 1967. - 270 p.
9. Petroleum Processing Handbook [Text]: monograph / ed. J. J. McKetta. - Basel; Hong Kong: Marcel Dekker, 2010. -774 p.
10. Practical Advances in Petroleum Processing [Text] / ed .: C. S. Hsu, P. R. Robinson. - Berlin: Springer, 2006 -. Volume 2. - 2006. - xv, 411 p.
11. Purification of laboratory chemicals [Electronic resource] / Wilfred L. F. Armarego, Christina L. L. Chai. - Electronic text data (20,1 MB). - Amsterdam: Butterworth-Heinemann, 2003. - 634 p. - Ver. with the title. screen. - Electron. version of the printer. publication.
12. Organic chemistry [Electronic resource] / J. Clayden. - Electronic text data (33,9 МБ). - [S. l. : s. n.], 2001. - 1490 p
13. Polymers a Property Database [Text]: monograph / ed .: B. Ellis, R. Smith. - 2nd ed. - London: CRC Press, 2009. - xxii p. : tabul. - Name and Synonym index: p.1089-1106.
14. Petroleum Refining. Tehnology and Economics [Text] / J. H. Gary, G. E. Handwerk, M. J. Kaiser. - 5th ed. - Boca Raton; London: CRC Press; London; New York: Taylor & Francis Group, 2007. - 463 p.
15. Essentials of Petroleum. A Key to Oil Economics [Text]: monograph / P. H. Frankel; foreword by M. A. Adelman. - London: Frank Cass, 2005. - xiii, 188 p.
16. Petroleum Refinery Process Economics [Text]: a monograph / R. E. Maples. - 2nd ed. - Tulsa: Penn Well, 2000. - xxix, 474 p.

The list of information and telecommunication resources required for mastering the discipline (module) is available via Internet network

1. www.eLIBRARY.RU - Scientific electronic library. Access mode is free.
2. www.sciencedirect.com - Elsevier Database. Access mode is free.

3. www.nature.com - Scientific journal Nature. The access mode is free.
4. www.scopus.com - Scopus peer-reviewed literature database. Access mode is free.
5. www.springerlink.co - Springer Database.
6. www.isiknowledge.com - Web of Science Database. Access mode is free.

4.1.2 Web page of the course (module)

You can receive the information about the postgraduate program 02.00.13 Petroleum Chemistry and about the course in SibU website: www.e.sfu-kras.ru. You must be logged in to access the materials. Course materials and required reading materials are available at the internet resources that are associated with the SFU.

4.1.3. Course (module) materials (seminar notes, assignments for classroom activities and sessions)

Prior to attending the lections some preparation can be very valuable. Consultation on the Petroleum Chemistry module is carried out by electronic resources that are associated with the SFU or face-to-face. There are various materials for self-preparation, for lections or practical classes, which are available a week before the class on the web page of the discipline provided by My SFU Resource. The materials can be in form of simple text documents while others may be audio or video files, or online exercises. Most of them are supplementary intended for independent study and are not supposed to replace the practical sessions. The great benefit is that you can return and revisit them when you want. Home assignments involve printed reports, oral or visual presentations.

4.1.4 Required feedbacks

The supervisor might use the web page of the discipline located on My SFU Resource as a communication channel. It is important that you become familiar with checking and accessing it regularly. Make sure that you have access to the correct module pages, and get in touch with your lector or programmer administrators in any other cases.

The postgraduate students must be ready to discuss the aim and methodology of them own research activities in the field of petroleum chemistry. They have to justify a selection of appropriate laboratory or technological methods that have been chosen for a research implementation. The discussion is realized via

face-to-face discussion or via the electronic resources.

4.2. Course (module) Structure

4.2.1 Internal education

Learning activities	Total credits (academic hours)	Semester
		3
Total	2 cr. (72 a. h.)	2 cr. (72 a. h.)
Lectures	0,72 cr. (26 a. h.)	0,72 cr. (26 a. h.)
Practice sessions / Seminars,	-	-
Self-study of the students:		
Study of the theoretical course (including preparation for final attestation)	1,28 cr. (46 a. h.)	1,28 cr. (46 a. h.)
Final Attestation	credit	credit

4.3 Time schedule course (module) and course (module) outline

4.3.1 Internal education

№	Topic	week, №	Learning Activities (lecture, lab, class assignments, assessment and other)	Hours	Self-study Assignments	Reading
1	Goals and objectives of the course. The basic feedstock for the organic synthesis industry. The role of Russia in the	1	**Lecture 1.** The basic feedstock for the organic synthesis industry. The role of Russia in the international market for organic synthesis products formation. Material balances of petrochemical processes	2	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	The literature listed in 4.1 paragraph. The articles and materials are indexed by Scientific

	formation of the international market for organic synthesis products.	2	**Lection 2.** Methods for technological indicators calculating.	2	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	Databases listed in 4.1 paragraph.
		3	**Lection 3.** Material balances of petrochemical processes	2	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	
2	Processes of halogenation, hydrolysis, hydration, dehydration, esterification.	4, 5	**Lection 4 - 5.** Chemistry of halogenation, hydrolysis, hydration, dehydration, esterification processes.	4	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	The literature listed in 4.1 paragraph. The articles and materials are indexed by Scientific Databases listed in 4.1 paragraph.
		6, 7	**Lection 6 - 7.** Selection of equipment for halogenation, hydrolysis, hydration, dehydration, esterification processes realizing.	4	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	
		8, 9	**Lection 8 - 9.** Technological indicators of halogenation, hydrolysis, hydration, dehydration, esterification processes.	4	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	

3	Alkylation, oxidation, hydrogenation, dehydrogenation processes.	11, 12	**Lection 10 –11.** Chemistry of alkylation, oxidation, hydrogenation, dehydro-genation processes.	4	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	The literature listed in 4.1 paragraph. The articles and materials are indexed by Scientific Databases listed in 4.1 paragraph.
		14	**Lection 12.** Technological indicators of alkylation, oxidation, hydrogenation, dehydro-genation processes.	2	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	
		16	**Lection 13.** Selection of equipment for alkylation, oxidation, hydrogenation, dehydro-genation processes.	2	Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	
4	Final attestation	18	**Credit**			

5. Assessment

5.1 Form of assessment

Home assignment will involve some form of printed and oral reports, or downloadable file on the web page of the discipline within the specified period. The students must realize successfully not less than 6 oral reports during the course.

5.2 Grading scale

Grade policy for both home assignments and the final exam is:

- A (excellent work) 91–100 points
- B (above average work) 81–90 points
- C (average work) 71–80 points
- D (below average work) 50–70 points
- F (failed work) < 50 points

Students are assessed by results of practical work, tests, and a final attestation. Progress assessment:

- 50 % home assignments;
- 50 % credits.

6. Attendance Policy

Students are expected to attend and participate in classes and should notify lecturer of excused absences in advance, where possible. Students who have an excused absence are expected to make arrangements with lecturer for alternative assignment.

Every topic has a home assignment work that should be done. The final mark will be made by the same grade policy as for a final exam.

7. Required Course (module) Participation

Students should be able to:

- defend the writing reports (50 points maximum),
- write an answer on 2 questions, demonstrate covered material (50 points maximum).

8. Facilities, Equipment and Software

The implementation of the course provides for the availability of lecture rooms (personal computers, printers, copier, projector, demonstration materials) with access to webpages of the E-learning SibFU through web site: www.sfu-kras.ru. The training process for this course uses standard Microsoft Office programs.

List of required software.

1. Windows XP or later operating system from Microsoft® Windows family.
2. Microsoft® Office Professional Plus 2010 Russian Academic OPEN No Level.
3. ESET NOD32 Antivirus Business Edition for 2750 users.
4. Adobe Acrobat Pro Extended 9.0 WIN AOO License IE Acrobat Pro Extended, License Certificate from Softline (10.12.2008, indefinitely).
5. Ascon Compass-3D, License Certificate №E-08-000123 (11.09.2008); №E-7-00107 (12.12.2017, indefinitely).
6. AutoCAD, free software.

Annex 1. Example of Questions to the Credit

1. Initial substances for the processes of basic organic and petrochemical synthesis.

2. Olefins as a feedstock for organic synthesis processes.

3. Aromatic hydrocarbons as feedstock for organic synthesis processes.

4. Methods for obtaining halogen derivatives. Substitution reactions, addition reactions (halogenation, hydrohalogenation, halohydrination).

5. Cleavage reactions (dehalogenation, dehydrohalogenation, chlorolysis, pyrolysis).

6. Radical-chain paraffin chlorination. Chlorination reactions of paraffins, olefins, aromatic hydrocarbons. The mechanism of radical-chain chlorination. Liquid-phase chlorination processes (products, initiation methods, batch and continuous reactors).

7. Gas-phase chlorination (products, initiation method, reactors).

8. Ionic catalytic chlorination. Ionic catalytic processes of chlorine introduction: chlorination of olefins and acetylene, chlorohydrination, hydrochlorination, substitution into the benzene nucleus.

9. Hydrolysis processes. Hydrolysis mechanisms of aliphatic and aromatic chlorine derivatives. Products: alcohols, phenols.

10. Processes of dehydrochlorination. Reaction mechanisms of chloroalkanes and chlorohydrin dehydrochlorination. Products: olefins, chlorolefins and oxides.

11. Hydration of olefins - dehydration of alcohols. Hydration-dehydration reaction mechanisms, by-products, selectivity, technological parameters, products.

12. Oxidation. Radical chain oxidation. Processes with a radical chain oxidation mechanism. Obtaining hydroperoxides. Getting phenol and acetone.

13. Heterogeneous catalytic oxidation. Processes of heterogeneous catalytic oxidation of hydrocarbons. Acrylic acid production. Obtaining ethylene oxide.

14. Dehydrogenation. Classification of dehydrogenation reactions. Carbon-carbon, carbon-oxygen, carbon-nitrogen dehydrogenation, dehydrocyclization, dehydrocondensation, oxidative dehydrogenation reactions.

15. Technologies for dehydrogenation. Parameters, catalysts, selectivity.

16. Hydrogenation. Regularities of hydrogenation processes. Classification of reactions, technological parameters, catalysts, selectivity.

17. Technological processes of hydrogenation. Liquid-phase hydrogenation, catalysts, reaction units, technological scheme for hydrogenation of esters of higher acids into alcohols.

18. Gas-phase hydrogenation.

19. Hydration of olefins - dehydration of alcohols. Hydration-dehydration reaction mechanisms, by-products, selectivity, technological parameters, products.

20. Technologies for hydration of olefins. Sulfuric acid and direct hydration, features of these technologies.

21. Esterification. The reaction mechanism of esterification. Reversibility,

equilibrium of reactions, homogeneous and heterogeneous catalysis, products.

22. Alkylation of aromatic compounds. Alkylating agents, catalysts, reaction mechanism, side reactions. Alkylation technological parameters. Main products. Reaction units for alkylation with liquid and gaseous olefins.

23. Alkylation of paraffins. Composition of products of the catalytic process, by-products. Technological process, theoretical

Annex 2. Example of Self-Study Assignment

1. The solubility of sodium chloride in water at 290 K is 35.8 kg/100 kg of water. Express the solubility as the following:

(a) Mass fraction and mass percent of NaCI

(b) Mole fraction and mole percent of NaCI

(c) kmol NaCI per 1000 kg of water

2. Determine the volume of oxygen obtained under standard conditions, by the decomposition of 100 kg of potassium chlorate.

3. The capacity of the tubular ethylene polymerization reactor at 170 MPa is 6,000 kg of polyethylene per hour. The reactor has a diameter of 0.06 m and a length of 1000 m. Determine the volumetric feed rate of ethylene (at the stated pressure and gas temperature 190 ° C), if the ethylene conversion is 12.5%.

4. One way to obtain Acrylonitrile (monomer for the production of Nitron fiber) is the oxidative ammonium propylene. On oxidative ammonium received: 1254 kg of propylene; 2360 kg of oxygen; 516 kg of ammonia and water vapor. It was obtained 1000 kg of Acrylonitrile, as well as a number of by-products: acrolein, hydrocyanic acid, acetonitrile, methane and carbon dioxide. At the same time, part of propylene and oxygen were not reacted — respectively 161 kg and 903 kg.Calculate the yield of Acrylonitrile from the theoretically possible, the conversion of propylene and oxygen. Write the equation of the target reaction and reactions of formation of by-products.

Course Petroleum Chemistry

Basic Information

This is a course, which contributes to postgraduate educational program 04.06.01 Chemical Sciences, specialization is 02.00.13 Petroleum Chemistry.

Course period	From September 1st till December 31st, 3 semester (15 weeks)
Study credits	2 ECTS credits
Duration	72 hours
Language of instruction	English
Academic requirements	– M. Sc degree in Petroleum Engineering, Engineering, Chemistry , Environmental Sciences or equivalent (transcript of records), – good command of English (certificate or other official document)

Course Description

Natural gas and crude distillates such as naphtha from petroleum refining are used as feedstocks to manufacture a wide variety of petrochemicals that are in turn used in the manufacture of consumer goods. Petroleum Chemistry provides knowledge and generates skills in the field of technologies for producing the most bulk groups of petrochemical products; explains the principles of intensification and modernization of existing industries based on using of in-depth patterns of chemical transformations investigations. The course acquaints students with petrochemicals laboratory synthesis, petrochemical process operations and basic technological equipment. Technical and economic indicators calculation of chemical-technological processes is also discussed.

The discipline forms the ability to set and solves problems in the scientific and industrial direction; motivates postgraduate students for self-development and advanced training. Petroleum Chemistry subject promotes the ability to conduct independent research, teaching and expert consulting activities.

Special Features of the Course

1. The course is split into 3 major sections. These are fundamentals of petrochemical production processes such as halogenation, etherification, dehydrogenation and other similar technologies; petrochemical industry overview and assessable resources for the organic synthesis industry; olefins chemistry and technology of polymer chemistry, In addition to conventional lectures, the course offers a range of other learning opportunities in which students actively participate. Moreover, students will be involved in online discussion and tests.
2. Provides broad technical information on petrochemical production processes, enabling a rapid immersion in the petrochemical field. Detailed course material with a glossary of the main technical terms used in petrochemical industry. There are new trends in production technology, petrochemical application characteristics to European and worldwide scale. Up to date petrochemicals production schemes are included.

Course Aims

- To acquaint with the main theoretical schools, approaches and concepts for solving problems in the field of organic substances chemical technology.
- To form abilities to search, analyze, critically reflect and generalize scientific and technical information, formalize the results of research work.
- To determine possible research areas towards the petrochemical synthesis.

Course Objectives

- Arranging of general refinery and petrochemical operations, their products and economic importance.
- Formation of skills for the invention of creating chemical-technological processes and materials innovative methods.
- Getting acquaint with the synthesis methods of some petrochemical products in the laboratory.
- Formation of professional skills of comparative analysis and selection of the optimal technology for the synthesis of organic synthesis products, taking into account the economic and environmental components.

Learning Outcomes of the Course

By the end of the course, students will be able to:

- create basic schematic diagrams for producing the most bulk products of petrochemical synthesis;
- select a laboratory methods for the synthesis of some petrochemical products in the laboratory;
- to carry out research activities independently in the relevant professional field using modern research methods and information and communication technologies;
- organize the work of a research team in the field of chemistry and related sciences;
- realize knowledge of the current state of science in the field of petrochemistry;
- enter innovative production methods of different petrochemicals.

Course Outline

Week	Topic	Lections / Practice session / Assignments	Hours[1] (Internal education)
1-4	Goals and objectives of the course. The basic feedstock for the organic synthesis industry. The role of Russia in the formation of the international market for organic synthesis products.	**Lecture 1.** The basic feedstock for the organic synthesis industry. The role of Russia in the international market for organic synthesis products formation. Material balances of petrochemical processes. **Lection 2.** Methods for technological indicators calculating. **Lection 3.** Material balances of petrochemical processes **Self-study assignments.** Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	2 2 2 15.33

[1] Hours designed for Classroom sessions, Web-sessions, Home Assignments etc.

5-7	Processes of halogenation, hydrolysis, hydration, dehydration, esterification.	**Lection 4-5.** Chemistry of halogenation, hydrolysis, hydration, dehydration, esterification processes. **Lection 6-7.** Selection of equipment for halogenation, hydrolysis, hydration, dehydration, esterification processes realizing. **Lection 8-9.** Technological indicators of halogenation, hydrolysis, hydration, dehydration, esterification processes. **Self-study assignments.** Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	4 4 4 15.33
8-11	Alkylation, oxidation, hydrogenation, dehydrogenation processes.	**Lection 10 –11.** Chemistry of alkylation, oxidation, hydrogenation, dehydrogenation processes. **Lection 12.** Technological indicators of alkylation, oxidation, hydrogenation, dehydrogenation processes. **Lection 13.** Selection of equipment for alkylation, oxidation, hydrogenation, dehydro-genation processes. **Self-study assignments.** Exact topics for self-study assignments are depended on the line of academicals research that is conducted by the students.	4 2 2 15.33
15	Final attestation (Credit)		

Lecturer and Contact Information

Vladimir A.Safin

Associate Professor at School of Petroleum and Natural Gas Engineering, Siberian Federal University

(room 313) 82/6, Svobodny prospect, Krasnoyarsk, Russia.

Tel: +7(391) 2-062-879. E-mail: VSafin@sfu-kras.ru

Assessment

Grade policy for both home assignments and the final attestation is:

- A (excellent work) 91–100 points
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Web page of the course

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Core reading

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3. Applied process design for chemical and petrochemical plants [Electronic resource]. Vol. 1 / E. E. Ludwig. - 3th ed. - Electronic text data (28,8 МБ). - Boston : Butterworth-Heinemann, 1999. - 630 p.
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