

## Contents and short summary

- **Chemical Kinetic Modeling in Coal Gasification Processes: an Overview**

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### Abstract

Coal is the fuel most able to cover world deficiencies in oil and natural gas. This motivates the development of new and more effective technologies for coal conversion into other fuels. Such technologies are focused on coal gasification with production of syngas or gaseous hydrocarbon fuels, as well as on direct coal liquefaction with production of liquid fuels. The benefits of plasma application in these technologies is based on the high selectivity of the plasma chemical processes, the high efficiency of conversion of different types of coal including those of low quality, relative simplicity of the process control, and significant reduction in the production of ashes, sulphur, and nitrogen oxides. In the coal gasifier, two-phase turbulent flow is coupled with heating and evaporation of coal particles, devolatilization of volatile material, the char combustion (heterogeneous/porous oxidation) or gasification, the gas phase reaction/oxidation (homogeneous oxidation) of gaseous products from coal particles. The present work reviews literature data concerning reaction kinetic modelling in coal gasification. Current state of related kinetic models for heterogeneous/homogeneous oxidation of coal particles, included plasma assisted, is reviewed.

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- **Elongated Wire-Like Zinc Oxide Nanostructures Synthesized from Metallic Zinc**

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### Abstract

Elongated wire-like Zinc oxide, nanocombs and nanocrystals have been successfully synthesized on the silicon substrate from the metallic zinc as a starting material. The annealing temperature was as low as 450 °C in argon atmosphere mixed with about 3% oxygen. Structural analysis using the X-ray Diffraction (XRD) and Transmission Electron Microscopy (TEM) showed that the existence of two phases; nanowires and crystalline form. Moreover some nanoparticles aggregates were noticed to be attached in the bulk to the sides of the ZnO nanocrystals and sometimes these aggregate attached to the Zinc oxide hexagonal crystal and grow to form nanowire at different angles. Scanning electron microscopy (SEM) investigations for the zinc oxide nanostructure on the silicon substrate showed the formation of the nanocrystals in the gas flow direction and at the low energy sites over the silicon substrate. Photoluminescence (PL) measurements, performed at the room temperature, showed the existence of two basic emissions: narrow ultraviolet (UV) emission at 398 nm which attributed to the near band edge emission of the wide band gap and a very wide, more intensive, green emission at 471 nm corresponds to the crystal defects such as vacancies, interstitial sites in ZnO.

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- **Growth of 3C-SiC Films on Si (111) and Sapphire (0001) Substrates by MOCVD**

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**Abstract**

Thick silicon carbide films were grown on sapphire (0001) and silicon (111) substrates using metal organic chemical vapor deposition (MOCVD). Diethylmethylsilane (DEMS) has been used as a single precursor, which contain Si and C atoms in the same molecule, without any carrier or bubbler gas. Atomic structure, surface composition and morphology have been investigated by XRD, AES, SEM and AFM analysis. SiC films of 5-7 micron thickness were grown at a rate of ~ 40 nm/min on sapphire (0001) and Si (111) substrates. The films grown at low temperature (850 °C and 900 °C) on both substrates show crystalline 3C-SiC in the (111) orientation. XRD results show that the orientation of the crystal structure does not depend of the substrate orientation. AFM pictures of SiC films grown on sapphire (0001) exhibit more crystalline order as compared to films grown on the Si (111) substrates. AES of the grown films shows that in both cases the Si peak intensity is greater than that of carbon. This work shows promise for the development of alternative processes for developing low cost, large area substrates for application to III-nitrides LED and UV photodetector fabrication and also for gas detector application.

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- **SHS - Processes in the Carbonaceous Oxide System at High Nitrogen Pressure Values**

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**Abstract**

This paper contains study results of the nitride containing composites features formed in the compacted Al-TiO<sub>2</sub>-C-Si samples inside a high pressure reactor with various nitrogen pressure values. The nitriding and carbide-formation processes take place simultaneously with aluminothermic reduction of titanium oxide in the self-propagating high-temperature synthesis (SHS) mode. It has been found that the nitrogen pressure effect is manifested as insignificant reduction of the combustion temperature and increased durability of the synthesized composite. The SHS process in the nitric environment leads to practically complete reduction of titanium oxide, the free titanium being absent. The X-ray analysis has revealed that the basic SHS products are refractory compounds such as metal nitrides, carbides, and oxides. Increase in nitrogen pressure results in decrease of the specific electric resistance of the synthesized composites caused by growth of the electroconductive phases i.e. titanium carbides, nitrides, and silicides. Performed electron microscopic study including the energy dispersion analysis of the morphology and structure of the SHS products has revealed formation of the nano-sized titanium silicide crystals distributed between the complex carbonitride particles. The complex carbonitride composites synthesized in the high pressure reactor are of interest as high refractory and abrasive materials considering their physical and chemical properties.

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- **Towards a Better Understanding of the Chemical Reactions Between Iron Carbide and Silicon Carbide**

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**Abstract**

This article contains the research results of the equilibrium interaction of iron carbide (Fe<sub>3</sub>C) with silicon carbide (SiC) in a temperature interval of 700-2000 K with the formation of iron silicides (Fe<sub>3</sub>Si, Fe<sub>2</sub>Si<sub>3</sub>, FeSi, FeSi<sub>2</sub>), by using the program of the Finnish metallurgical company Outokumpu HSC Chemistry-5.1 for Windows with regard to the electrothermal production of ferrosilicium from siliceous and carbon-containing raw materials.

On the basis of the received regression equations connecting the Gibbs energy change with the temperature and the silicon content in a ferroalloy, the response surfaces (change of the Gibbs free energy -  $\Delta G_T^0$ ) and their horizontal sections for three groups of ferroalloys were constructed with the program Mathcad. The silicon

content in the first group of alloys is 14.3-23 %, in the second group of alloys – 23-33.3 % and in the third group of alloys – 33.3-42.8 %. It was established, that the reactions between  $\text{Fe}_3\text{C}$  and  $\text{SiC}$  with the formation of iron silicides in the range of temperatures 700-2000 K are possible, and the probability of these reactions increases with increasing the mole ratio  $\text{Fe}_3\text{C}/\text{SiC}$  from 0.166 to 1.0. As a result of the reactions the low-silicon ferrosilicium can be obtained, answering to a grade FS20 with Si content from 19 to 27 % and consisting of a mixture of  $\text{Fe}_3\text{Si}$  and  $\text{FeSi}_3$ , and also the ferrosilicium corresponding to a grade FS25 with a Si content from 23 to 29 % and consisting of a mixture of  $\text{Fe}_3\text{Si}_3$  and  $\text{FeSi}$ . It was found, that at the technological temperature of 1900-2000 K the maximum Si content in the received ferrosilicium can't be more than 37.7-38.8 %. Production of the medium-silicon and the high-silicon ferrosilicium answering to grades FS45- FS90 from the  $\text{Fe}_3\text{C}$ - $\text{SiC}$  mixture is impossible from a thermodynamic point of view.

The received information extends our knowledge about the iron silicides formation during the electrothermal production of ferrosilicium with a silicon content in the alloy from 19 to 90 %.

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- **Seasonal Variations of Lipid Content and Composition in Starfish *Asterias amurens* Lütken**

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**Abstract**

The total lipid content, lipid classes and fatty acid composition in the internal organs of starfish (*Asterias amurens*) were analyzed to determine the effects of seasons (winter and spring). The non-polar and polar lipid fractions obtained from starfish internal organs were analyzed through two seasons using thin layer chromatography (TLC) and gas liquid chromatography. Total lipid content of internal organs was 10.18% in spring and 8.21% in winter as wet weight basis. The predominant lipid class in spring was triglyceride whereas free fatty acids were the main lipid class in winter. The most abundant fatty acid of non-polar lipid fraction was eicosamonoenoic acid (C20:1) in spring having the highest proportion (29.2% of total fatty acid) as compared to the winter. Eicosapentaenoic acid (EPA) was also found significantly ( $P < 0.05$ ) higher in spring compared to winter in the non-polar lipid fraction. On the other hand, comparatively lower amount of EPA was observed in spring than winter in the polar lipid fraction. Proportions of other fatty acids in non-polar and polar lipid fractions were also varied seasonally. This result might be useful for commercial production of lipid from internal organ of starfish with a view to potential use in food, pharmaceutical, cosmetics and other non-food industries.

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- **Sorptive and Separation Properties of Ultrafiltration Membranes on the Basis of Sulfonate-Containing Polyamide with Respect to Bovine Serum Albumin**

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**Abstract**

Investigation of sorption of bovine serum albumin in the static mode and in ultrafiltration conditions by membranes produced from statistic copolymers of aromatic polyamides synthesized by polycondensation of the sodium salt of 4, 4'-diaminodiphenylamine-2-sulfo-acid and *m*-phenylenediamine in various ratios with chloroanhydride of isophthalic acid has been carried out. Interconnection has been established between the charge of protein macromolecules, concentration of fragments containing ionic groups in the aromatic polyamide and sorptive, separation and transport characteristics of membranes on its basis. It has been shown that dominant forces that determine membrane/protein interaction in the systems under consideration are coulomb forces, but the contribution of hydrophobic interactions is also significant. The results of mathematical processing of experimental data indicate that there is a good compliance of sorption isotherms with Langmuir's model. Depending on the concentration of fragments containing ionic groups in the polyamide and *pH* of the solution, the calculated values of maximum sorption in sorbent/sorbate systems under consideration vary in the range of 0.028 to 0.338 mg/cm<sup>2</sup>. Dynamic investigations have shown that selectivity of the membranes is 85 to 98%. To assess the sorptive activity of the membranes in the course of ultrafiltration, indicators of sorption and sorptive losses calculated on the basis of the ratio of the change of mass content of protein in the process of filtration to the initial value have been used. Depending on the material used to

produce the membrane and *pH* of the solution being filtered, sorptive losses range from 5 to 33%. Their minimum value is observed when *pH* is higher than the isoelectric point of the protein, i.e. in the field where protein macromolecules and the surface of the membrane have like charges.

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- **Petroleum Sorption by Thermally Treated Rice Husks Derived from Agricultural Byproducts**

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**Abstract**

Agricultural byproducts or residues are widely produced in Kazakhstan and their utilization as a sorbent material for petroleum spill can be developed as low cost, high tech environmental technology. Rice husk, an agricultural waste, was used as petroleum sorbent material. The present study examines the sorption capacity of thermally treated rice husk for different petroleum products. Results showed that the petroleum sorption capacity of this material prepared at 700 °C was 15 g/g for heavy crude petroleum. The material obtained by thermal treatment of rice husk has very good buoyancy characteristics, high petroleum sorption capacity and high hydrophobicity. The effects of heating temperature, contact time and petroleum density on the petroleum sorption capacity of thermally treated rice husks were further studied on the basis of phase composition, microstructure and morphology using X-ray diffraction analysis, FTIR spectrometry, optical digital microscopy and scanning electron microscopy (SEM). The results of the SEM and optical microscopy studies strongly indicate that thermal treatment is a suitable method to improve structure of husk particles regarding porosity compared to virgin samples. The research provides the basis for development of a new environmental material with optimal characteristics, providing efficient sorption of petroleum and petroleum products from aqueous medium.

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- **Food Chemistry: a Kazakhstan Perspective on the Maillard Reaction and Acrylamide Formation in Common Foods**

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**Abstract**

The Maillard reaction is largely responsible for the colour, flavour, aroma and texture of fried, baked and roasted foods, including bread, biscuits, breakfast cereals and other foods made from wheat grain, French fries and crisps made from potato and a wide range of other popular foods. However, it also results in the formation of undesirable products, including the neurotoxin and probable carcinogen, acrylamide, and furans. Kazakhstan is a major wheat producer and exports wheat grain to many countries, including countries within the European Union. The European Commission has already issued "indicator levels" for the presence of acrylamide in food products. Although these are not regulatory limits, food producers strive to keep the levels of acrylamide in their products beneath the indicator levels in order to avoid intervention from food safety authorities and the associated bad publicity. Sourcing raw material with low acrylamide forming potential would enable food producers to achieve this without expensive changes to processes and this is likely to be an increasingly important issue for suppliers. This review describes the Maillard reaction, the evolving regulatory scenarios in Europe and the USA and the implications for Kazakhstan as a grain exporter.

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- **Study of Asphaltene Structure Precipitated from Oil Sands**

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## **Abstract**

In the paper microscopic structure and physicochemical characteristics of asphaltenes were investigated. Asphaltene was precipitated from natural bitumen of oil sand of Munaily-Mola deposit using organic solvent of petroleum ether. According to results of our work, we found that the largest yield of asphaltens was reached by using the petroleum ether in 40-fold amount in relation to the initial hitch of bitumen. Chemical composition of precipitated asphaltenes aggregates were studied on FT-Infra red spectrometer Spectrum-65 at 450-4000 cm<sup>-1</sup>. At the Infrared spectrum, that the broad absorption band of asphaltenes at 3000-3600 cm<sup>-1</sup> are characterizing the presence of polycyclic aromatic hydrocarbons and aliphatic chains in the samples of asphaltens. Elemental composition of the samples of asphaltenes on the installation of x-ray fluorescent spectrometer "Focus-M2". Also found the presence of two crystalline phases. One - quartz content is less than one percent. Another phase is also present in very small quantities and is represented by a single line of diffraction  $d = 4.158 \text{ \AA}$ . The microstructures and microanalysis of asphaltenes were investigated with a scanning electron microscopy (Quanta 3D 200i) at an accelerated voltage of 20 kV and a pressure of 0.003 Pa at National Nanotechnological Laboratory of Open Type of Kazakh National University. Microscopic images showed that the asphaltenes have a medium-ordered structure, the main component of the surface is represented by amorphous carbon.

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## **IMPORTANT INFORMATION**

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