Chemistry and Technology of Fuels and Oils

2(630)'2022

Publisher— ICST «TUMA Group» LLC

Редактор
В. С. Дмитриева

Ответственный секретарь
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Формат 60 × 84 1/8.
Печать офсетная.
Усл. печ. л. 7.
Тираж 1000 экз.

Отпечатано в ООО ИПФ «СТРИНГ»
424006, Республика Марий Эл, г. Йошкар-Ола, ул. Строителей, 95

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Исследование возможности применения жидкого биокомпонента

в производстве товарного дизельного топлива

В статье представлено описание методики компаундирования нефтяного дизельного топлива и фракции 180-240°С, полученной из жидкого биопродукта пиролиза растительного сырья. Исследованы физико-химические свойства и групповой химический состав фракции растительного происхождения. Приводятся результаты физико-химических свойств полученных смесей дизельного топлива. Установлены допустимые концентрации биокомпонента при приготовлении смесевых биодизельных топлив.

Ключевые слова: биодизельное топливо, пиролиз растительного сырья, смесевые биотоплива, жидкий биокомпонент, низкотемпературные свойства.

DOI: 10.32935/0023-1169-2022-630-2-3-7

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Possibility of Liquid Biocomponent Usage in the Production

of Commercial Diesel Fuel

The article presents a description of the technique for compounding petroleum diesel fuel and a fraction of 180-240°C obtained from a liquid bioproduct of pyrolysis of plant materials. The physicochemical properties and group chemical composition of the fraction of plant origin have been studied. The results of the physicochemical properties of the resulting mixtures of diesel fuel are presented. Permissible concentrations of the biocomponent in the preparation of mixed biodiesel fuels have been established.

Key words: *biodiesel fuel, pyrolysis of plant raw materials, mixed biofuels, liquid biocomponent, low-temperature properties.*

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Принципы стабилизации состава тяжелого вакуумного газойля

при производстве технологических масел

Разработана и внедрена на промышленном предприятии установка выделения тяжелого вакуумного газойля стабилизированного состава из широкой фракции вакуумного газойля производительностью 65 000 т в год. Приведено описание принятых технических решений, выбранного оборудования и результаты эксплуатации установки. Выполнены экспериментальные исследования по отработке технологического режима

на лабораторной модели ректификационной колонны. В расчетах промышленной колонны с новой регулярной насадкой применялась ранее разработанная математическая модель многокомпонентной ректификации, где смесь представляется в виде псевдобинарной по фракциям. Кроме этого использовались программные пакеты при потарелочном расчете колонны. Осуществлен выбор основного и вспомогательного оборудования промышленной установки вакуумной перегонки.
Ключевые слова: вакуумный газойль, вакуумная ректификация,
производство масел мягчителей, проектирование технологической установки.
DOI: 10.32935/0023-1169-2022-630-2-8-13

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An Approach to Stabilize the Composition of Heavy Vacuum Gas Oil in the Production of Lubricating Oils
A heavy vacuum gas oil separation unit was developed and implemented at an industrial enterprise with a stabilized composition. The technical solutions, the selected equipment and the results of the installation operation are described. On a laboratory model of a distillation column, experiments were made to develop technological conditions. In calculations of an industrial column with a new regular packing applied previously developed mathematical model of multicomponent distillation. The mixture is represented as pseudo-binary in terms of fractions. In addition, software packages for plate-by-plate calculation of the column. The selection of the main and auxiliary equipment of the industrial vacuum distillation plant was carried out.
Key words: *vacuum gas oil, vacuum distillation, production of emollient oils, design of a technological plant.*

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Влияние поверхностной концентрации никеля на активность и селективность сорбентов Ni/ZnO-Al_2O_3 в реакционно-адсорбционном обессеривании олефинсодержащего сырья
Показаны преимущества процесса реактивной адсорбции для ультраглубокого обессеривания бензина каталитического крекинга и других углеводородных фракций. Для исследования влияния поверхностной концентрации никеля на активность и селективность процесса реактивной адсорбции был синтезирован ряд адсорбционно-каталитических систем Ni/ZnO-Al_2O_3 с различным содержанием никеля. Установлено, что на этапе хемосорбции при температуре 400 °С, давлении 0,5 МПа и массовой скорости подачи сырья 5,2 $ч^{-1}$ конверсия тиофена увеличивается до 94,8% с ростом поверхностной концентрации никеля до 8 ат/$нм^2$. Однако максимальное значение селективного фактора гидродесульфуризации/гидрирования достигается для адсорбционно-каталитической системы Ni/ZnO-Al_2O_3 с поверхностной концентрацией никеля 6 ат/$нм^2$.

Ключевые слова: реактивная адсорбция, селективное обессеривание,
адсорбционно-каталитические системы, поверхностная концентрация.
DOI: 10.32935/0023-1169-2022-630-2-14-20

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Study of The Nickel Surface Concentration Influence on the Activity and Selectivity of Ni/ZnO-Al_2O_3 Sorbents in Reactive-Adsorption Desulfurization of Olefin-Containing Feedstock

The advantages of the reactive adsorption process for ultra-deep desulfurization of FCC gasoline and other hydrocarbon fractions are shown. To study the influence of the surface concentration of nickel on the reactive adsorption activity and selectivity, several Ni/ZnO-Al_2O_3 adsorption-catalytic systems with different nickel contents were synthesized. It has been established that at the chemisorption stage at a temperature of 400°C, a pressure of 0.5 MPa, and an weight hourly space velocity of 5.2 h^{-1} the thiophene conversion increases to 94.8% with a nickel surface concentration increase to 8 at/nm^2. However, the maximum value of the hydrodesulfurization/hydrogenation selectivity factor is achieved for the Ni/ZnO-Al_2O_3 adsorption-catalytic system with a nickel surface concentration of 6 at/nm^2.

Key words: *reactive adsorption, selective desulfurization, adsorptive-catalytic systems, surface concentration.*

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Синтез и исследование никель-алюминиевых оксидных катализаторов на углеродном носителе

В работе исследованы образцы катализаторов, полученные импрегнированием активного угля оксидами NiO и Al_2O_3. Показано, что увеличение соотношения катионов никеля и алюминия в пропиточном растворе с 2:1 до 3:1 ведет к уменьшению среднего диаметра пор и увеличению площади удельной поверхности активного угля в 1,5 раза. Наибольшей площадью пор диаметром 10–200 нм обладают активные угли, импрегнированные оксидами никеля и алюминия с соотношением катионов металлов в пропиточном растворе 3:1, прокаленные в токе водорода. Термообработка никель-алюминиевых оксидных катализаторов на углеродном носителе при температуре 450°C в токе водорода приводит к увеличению размера пор и снижению площади удельной поверхности. Механическая активация оксидных катализаторов на углеродном носителе ультразвуковым воздействием увеличивает площадь внешней поверхности частиц в более чем два раза.

Ключевые слова: активные угли, оксид никеля, оксид алюминия, удельная поверхность,
размеры пор, микроскопия, рентгеноструктурный анализ, термический анализ.
DOI: 10.32935/0023-1169-2022-630-2-21-26

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Synthesis and Study of Carbon-Supported Nickel-Aluminum Oxide Catalysts

Activated carbons, which have a highly developed specific surface area and large pore sizes, have recently been increasingly considered as economically available carriers of catalytic systems for deep processing of heavy hydrocarbon feedstock. In this work, samples of catalysts obtained by impregnation of active carbon with oxides of NiO and Al_2O_3 were studied. It is shown that an increase in the ratio of metal cations Ni/Al in the impregnating solution from 2:1 to 3:1 leads to a decrease in the average pore diameter and an increase in the specific surface area of activated carbon by 1.5 times. Activated carbons impregnated with Ni/Al metal oxides with a ratio of metal cations in an impregnating solution of 3:1, calcined in a stream of hydrogen, have the largest pore area with a diameter of 10–200 nm. Heat treatment of Ni-Al oxide catalysts on a carbon carrier at a temperature of 450°C in a hydrogen flow leads to an increase in the pore size and a decrease in the specific surface area. Mechanical activation of oxide catalysts on a carbon carrier by ultrasonic action increases the area of the outer surface of the particles by more than two times.

Key words: *active carbons, nickel oxides, aluminum oxides, specific surface area, pore sizes, microscopy, X-ray diffraction analysis, thermal analysis.*

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Влияние гидротермальных флюидов на состав тяжелых нефтей

В работе исследованы закономерности преобразования состава тяжелых нефтей с разным генотипом при взаимодействии с гидротермальном флюидом при температуре 310 °С и давлении 50 МПа. При гидротермальном воздействии в составе тяжелой нефти типа А[1] снижается содержание насыщенных углеводородов и алканов линейного строения, увеличивается содержание ароматических углеводородов и смол. При гидротермальном воздействии на тяжелую нефть типа Б[2] в ее составе снижается количество ароматических углеводородов, увеличивается содержание асфальтенов и насыщенных углеводородов. Пик молекулярно-массового распределения н-алканов смещается в низкокипящую область, снижается содержание изоалканов. Это свидетельствует о том, что состав тяжелых нефтей влияет на доминирование тех или иных реакций, протекающих в гидротермальном флюиде.

Ключевые слова: гидротермальные процессы, тяжелые нефти, SARA-анализ, газовая хроматография, геохимические коэффициенты.

DOI: 10.32935/0023-1169-2022-630-2-27-30

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Effect of Hydrothermal Fluids on the Composition of Heavy Oils

The paper presents the results of comparative studies to identify the regularities in the transformation of the composition of heavy oils of different genotypes during their interaction with hydrothermal fluid at a temperature of 310 °C and a pressure of 50 MPa. Under hydrothermal impact, the content of saturated hydrocarbons and linear alkanes in the composition of heavy oil of type A[1] decreases, and the content of aromatic hydrocarbons and resins increases. During hydrothermal impact on heavy oil type B[2], the amount of aromatic hydrocarbons in its composition decreases, the content of asphaltenes and saturated hydrocarbons increases. The peak of the molecular weight distribution of n-alkanes shifts to the low-boiling region, and the content of iso-alkanes decreases. This indicates that the composition of heavy oils affects the dominance of certain reactions occurring in the hydrothermal fluid.

Key words: *hydrothermal processes, heavy oils, SARA analysis, gas chromatography, geochemical coefficients.*

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Теплоемкость нефтяных систем при высоких давлениях

Приведены результаты измерения удельной объемной теплоемкости четырех образцов нефтяных систем при изменении давления до 1 ГПа при комнатной температуре с помощью метода нагретой нити. Показано, что с увеличением давления удельная объемная теплоемкость исследованных образцов линейно возрастает со средним значением 0,051 МДж/(м^3·К) на 0,1 ГПа. Одинаковый темп роста удельной объемной теплоемкости наблюдался для всех исследованных образцов.

Ключевые слова: нефти, удельная объемная теплоемкость, высокое давление, метод нагретой нити.

DOI: 10.32935/0023-1169-2022-630-2-31-33

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Heat Capasity of Petroleum Systems at High Pressure

The heat capacity per unit volume c_p of four petroleum samples were measured at pressure up to 1 GPa at room temperature using the transient hot-wire method. It is shown that with increasing pressure c_p of the samples investigated increased linearly with an average value of 0.051 MJ/(m^3·K) for every 0.1 GPa. The same growth rate of c_p was observed for all samples investigated.

Key words: *heat capacity per unit volume, petroleum, high pressure, transient hot-wire method.*

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Состав серосвязанных структурных фрагментов в асфальтенах мазута тяжелой нефти и продуктах его термолиза

С использованием методов селективной химической деструкции, ИК-спектроскопии и хромато-масс-спектрометрии проведено сравнительное исследование состава структурных фрагментов, связанных через сульфидные мостики в молекулах асфальтеновых компонентов мазута тяжелой нефти и продуктах его термического и термокаталитического крекинга. Показано, что воздействие температуры в присутствии инициирующих добавок на основе ферросфер энергетических зол приводит к более глубоким изменениям структуры асфальтеновых компонентов.

Ключевые слова: мазут тяжелой нефти, асфальтены, термические процессы, серосодержащие структуры.
DOI: 10.32935/0023-1169-2022-630-2-34-37

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The Composition of "Sulfur-Bound" Structural Fragments in Asphaltene Molecules of Heavy Oil Fuel Oil and Products of Its Thermolysis

Using the methods of selective chemical destruction, IR spectroscopy and chromatography - mass spectrometry, a comparative study of the composition of structural fragments connected through sulfide bridges in the molecules of asphaltene components of heavy oil fuel oil and products of its thermal and thermocatalytic cracking was carried out. It is shown that the effect of temperature in the presence of initiating additives based on ferrospheres of energy ash leads to deeper changes in the structure of asphaltene components.

Key words: *heavy oil fuel oil, asphaltenes, thermal processes, sulfur-containing structures.*

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Система контроля закоксованности катализатора гидрирования ацетилена в этан-этиленовой фракции

Производство ацетилена окислительным пиролизом природного газа основано на сложном химико-технологическом процессе. Одним из основных этапов этого процесса является гидрирование в этан-этиленовой фракции в присутствии катализатора. Как и при протекании многих технологических процессов при гидрировании ацетилена образуются побочные продукты реакции, вызывающие закоксованность катализаторов и снижающие их активность. В работе представлена система контроля закоксованности катализатора, основанная на использовании системы усовершенствованного управления и генетического алгоритма. Использование предлагаемой системы контроля позволяет перейти от плановой регенерации катализатора к его регенерации по фактическому состоянию закоксованности.

Ключевые слова: системы усовершенствованного управления (APC), генетический алгоритм, гидрирование ацетилена, закоксованность, этан-этиленовая фракция, адиабатический реактор.
DOI: 10.32935/0023-1169-2022-630-2-38-41

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Control System of Coking of the Catalyst for Hydrogening of Acetylene in Ethane-Ethylene Fraction

The production of acetylene by the oxidative pyrolysis of natural gas is based on a complex chemical-technological process. One of the main stages of this process is the hydrogenation of acetylene in the ethane-ethylene fraction. To increase the efficiency of the hydrogenation process, catalysts are used in the reactors. As in the course of many technological processes, hydrogenation produces by-products of the reaction, which cause coking of the catalysts and reduce their activity. The article presents a catalyst coke control system based on the use of an advanced control system (APC) and a genetic algorithm. The use of the proposed control system makes it possible to switch from the planned catalyst regeneration to its regeneration based on the actual state of coking.

Key words: *advanced control system (APC), genetic algorithm, acetylene hydrogenation, coking, ethane-ethylene fraction, adiabatic reactor.*

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Разработка экологически безопасного кислотного состава для обработки высокотемпературных геотермальных карбонатных коллекторов

В работе рассматривается разработка экологически безопасной кислотной композиции для обработки высокотемпературных карбонатных коллекторов. Особенностью данной кислотной композиции является использование в составе нетоксичной и высокотемпературной гликолевой кислоты с экологически безопасными добавками, что делает ее пригодной для обработки геотермальных скважин — экологически чистого источника энергии.

Ключевые слова: геотермальные источники, карбонатный коллектор, гликолевая кислота, поверхностно-активное вещество, ингибитор коррозии, кислотная обработка.
DOI: 10.32935/0023-1169-2022-630-2-42-45

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Development of Eco-Friendly Acid Composition for the Treatment of High Temperature Geothermal Carbonate Reservoirs

This paper discusses the development of an environmentally friendly acid composition for the treatment of high-temperature carbonate reservoirs. A feature of this acidic composition is the use of non-toxic and high-temperature glycolic acid with environmentally friendly additives, which makes it suitable for treating geothermal wells – an environmentally friendly source of energy.

Key words: *geothermal springs, carbonate reservoir, glycolic acid, surfactant, corrosion inhibitor, acid treatment.*

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Животная биомасса как сырье для производства продуктов основного органического синтеза

В обзоре рассмотрена биомасса животного происхождения как потенциальное возобновляемое сырье для получения CO_2-нейтрального топлива, не оказывающего влияние на баланс углекислого газа в атмосфере. Оценка характеристик животных биомасс позволит определить потенциал их интегрирования в современные процессы нефтехимии и биохимии. В работе описаны основные характеристики биомасс животного происхождения, их структурные и элементные составы. Проведена оценка количества и энергетической ценности отдельных видов.

Ключевые слова: биомасса, животная биомасса, вторичная биомасса, CO_2-нейтральное топливо, основной органический синтез, экологически чистое топливо.

DOI: 10.32935/0023-1169-2022-630-2-46-50

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Animal Biomass as a Raw Material for Obtaining Products of Basic Organic Synthesis

The review considers biomass of animal origin as a potential renewable raw material for the production of CO_2-neutral fuel, which does not affect the balance of carbon dioxide in the atmosphere. Evaluation of the characteristics of animal biomasses will make it possible to determine the potential for their integration into modern processes of petrochemistry and biochemistry. The paper describes the main characteristics of biomasses of animal origin, their structural and elemental compositions. An assessment of the quantity and energy value of certain species has been carried out.

Key words: *biomass, animal biomass, secondary biomass, CO_2-neutral fuel, basic organic synthesis, ecofriendly fuel.*

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Будущее российской гелиевой промышленности в Восточной Сибири, проблемы и пути их решения

В статье рассмотрено мировое производство и потребление гелия. Проведен анализ и оценен способ выделения гелия из природного газа. Выявлены и обсуждены потенциальные проблемы российской гелиевой

промышленности в Восточной Сибири. Предложены варианты долгосрочного хранения гелия. Рассмотрена проблема транспортировки гелия в России и пути ее решения.
Ключевые слова: гелий, Амурский газоперерабатывающий завод, хранение гелия, мембранные технологии, транспортировка гелия.
DOI: 10.32935/0023-1169-2022-630-2-51-56

D. Yu. Tremaskin, I. A. Golubeva
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The Future of Helium Industry in Eastern Siberia,
Problems and Solutions
The world production and consumption of helium are analyzed. Potential problems of the helium industry in Eastern Siberia have been identified. Variants of long-term storage of helium are proposed. The problem of helium transportation in Russia and the ways of its solution are considered.
Key words: *helium, Amur gas processing plant, helium storage, membrane technologies, helium transportation.*

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STUDY ON VIBRATION ENERGY CONVERSION EFFICIENCY
OF THE DRILL STRING ABSORPTION & HYDRAULIC SUPERCHARGING DEVICE
The vibration of a drill string can cause multiple hazards in the process of drilling operations. The conversion of excessive vibration energy of the drill string into the rock breaking energy can provide the dual effect of reducing the risks and improving the rock breaking efficiency of drilling. To address the task, a drill string absorption & hydraulic supercharging device has been developed. However, the design and exploitation of the drill string absorption & hydraulic supercharging device needs a comprehensive understanding of the characteristics of conversion of the drill string's vibration energy. Based on the drill string dynamics experimental device, a simulation test platform has been developed to evaluate the efficiency of conversion of the vibration energy. The analysis of the test results is used to evaluate the conversion characteristics of the vibration energy of the bottom hole drill string. The results show that the energy conversion efficiency depends on the elastic stiffness and installation position of the drill string absorption & hydraulic supercharging device, the overall rotational speed, and the WOB (weight on bit) of the conversion device. With increase in the elastic stiffness, the conversion efficiency of the vibration energy first increases and then decreases. The closer the installation position of the drill string absorption & hydraulic supercharging device is to the bit, the better the conversion efficiency. With increase in the rotational speed, the conversion efficiency of the vibration energy increases. With increase in the WOB, the conversion efficiency of the vibration energy first increases

and then decreases. The research results provide the background for the development and application of speed raising tools based on conversion of the drill string vibration.

Keywords: *drill string vibration; energy conversion and utilization; rock breaking efficiency; drilling parameters; elastic stiffness.*

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DEVELOPMENT AND APPLICATION OF A KIND OF CHEMICALCEMENTING STRONG WALL AGENT

It is an important technical measure to solve the borehole wallinstability in mud shale formation to improve the bearing capacity of borehole wall while drilling through the interaction between drilling fluid and formation. By using the method of functionalization of polymer and introducing functional groups with strong adhesion and cementation properties, a new type of chemical cementing strong wall agent SLGB-1 was developed, forming strong wall drilling fluid technology. The solid wall performance was evaluated by lap shear strength test, core uniaxial compression test and scanning electron microscope analysis. The results show that SLGB-1 adsorbed on the rock surface can improve the shear strength of rock sample in water and enhance the compressive strength of rock sample after soaking, and the performance of SLGB-1 is significantly better than the existing borehole wall stabilizer. The strong solid wall drilling fluid can cement the loose minerals in the micro-pores and micro-cracks of rock samples, effectively consolidate and plug them, so as to enhance the mechanical stability of rock while drilling. Two Wells were field tested with the rigid-wall drilling fluid technology. The test sections were regular in well diameter, and well diameter enlargement rate was low (< 10%), which was significantly lower than that of the offset Wells.

Keywords: *mud shale, strong wall agent, chemical wall fixation, while drilling, performance evaluation method.*

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Study on Fracture Development Characteristics of Low Permeability Oilfield and Its Influence on Horizontal Well Pattern Deployment

In order to study the influence of natural fracture and artificial fracture on reservoir well pattern deployment and development, Chang 6 fractured reservoir in Tang 9 oilfield is taken as the research object, through core, microscopic

slice and microseismic artificial fracture monitoring, the development characteristics of natural fractures and artificial fractures in the reservoir are studied, and the production conditions of horizontal wells and fractures in different directions are analyzed. It is found that the natural fractures in the core of Chang 6 reservoir in Tang 9 oilfield are well developed, the occurrence is mainly high-angle oblique fractures or vertical fractures, the fractures with dip angle more than 70 degrees account for the majority, the surface density of micro-fractures is generally 0.1–0.3 cm/cm^2, the average 0.2 cm/ strip cm^2 is about 108 m, which is much longer than the distribution length of natural fractures. The initial annual decline of the parallel fracture direction of the oil well is 28%, and the annual decline of the vertical fracture direction is 42%. It is considered that the development effect of the parallel fracture direction of the horizontal section is better, mainly because the horizontal section is in the process of fracturing production. The influence of fracture on production is much greater than that of the original fracture direction of the reservoir. This is different from the understanding of well pattern deployment in conventional fractured reservoirs, and the result has practical guiding significance for the development of similar reservoirs.
Keywords: *low permeability oil field, fracture characteristics, horizontal well, well pattern deployment.*

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Analysis on Fracture Mechanism and Overflow Gas Production Law of High Pressure Fractured Gas Reservoir

Taking the fractured gas constant volume body as the research unit, considering the boundary conditions such as the height of the constant volume body, the cross-sectional area of the constant volume body, the initial formation pressure, the initial bottom hole pressure and the initial overflow, a mathematical model of the average pressure of the fractured formation of the constant volume body varying with the overflow time is proposed; With the help of programming language, the model is solved. Taking well ST1 as an example, the results show that with the increase of fracture dip angle, the fracture width increases and the fracture permeability also increases; The permeability of fractured gas reservoir is most affected by matrix stress, followed by dip angle and fracture spacing. With the constant volume overflow, the overflow flow decreases rapidly in the initial stage, and then remains stable for a long time until it decreases again in the end; With the increase of throttle back pressure and gas influx, the annular gas holdup increases. The mathematical model of average pressure of fractured formation with constant volume can calculate the change value of average pressure with time, and can guide the design of kill fluid density and the loading of backpressure target value in the process of circulating exhaust.
Keywords: *high pressure gas reservoir, fracture, fracture width, overflow, formation pressure.*

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FORMATION DAMAGE AND PROTECTION TECHNOLOGY
FOR MEDIUM-LOW PERMEABILITY RESERVOIR IN LATE DEVELOPMENT STAGE

The first member of Dongying formation is the main production reservoir of Nanpu 1-5 block in Jidong Oilfield located in northern Bohai Bay Basin, China. The formation was put into development as early as 2005, and it has entered late development stage. Formation characteristics changed constantly during the development by waterflooding, formation damage mechanisms were not well understood, which resulted in the incompatibility of formation protection technology with the reservoir so that further formation damage happened. For wells newly putted into production, significantly lower production was obtained than the expected for years. Based on the measurement and comparison of formation characteristic, remaining oil distribution and damage mechanisms in early and late development stage, formation protection drilling fluid are conducted and optimized. The reservoir analysis results show that with constant development, pore-throat sizes decrease, heterogeneity intensify, and remaining oil is mostly trapped in the the low permeability strip, where water block damage rate is 10–29%, solid damage rate is about 10%, and the damage rate of liquid sensitivity is 5–10%. The synergy of broad-spectrum film-forming plugging and water blocking prevention was utilized to optimize formation protection drilling fluid system, the recovery value of the intercepted permeability recovered to more than 92%. Field application of the system on 17 wells showed an excellent formation protection effect, which meet the urgent formation protection needs of the late development of Nanpu 1-5 block. The technological ideas can be a valuable reference for other similar reservoir in China and around the world.

Keywords: *waterflooding development, late development stage, remaining oil distribution, formation damage mechanism, formation protection drilling fluid.*

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EFFECTS OF MAGNETIC FIELDS ON COMBUSTION AND EXPLOSION

Magnetic fields affects chemical reactions through acting on irons, electriferous groups and magnetic particles. Gas combustion and explosion are a chain reaction process of free radicals, which are paramagnetic species. Magnetic fields can affect gas combustion and explosion by acting on the key species, free radicals, of chain reaction. Magnetic fields has great potential in the field of energy and combustion. The effects of magnetic fields on combustion and explosion are reviewed from three aspects : flame characteristics, engine performance and emission, and explosion intensity. Theory, in a general sense, and theoretical methods development have a role. The theory of magnetic fields acting on free radicals is summarized. Free radicals are affected by gradient magnetic force, magnetic force, gravity and buoyancy. Free radicals are subjected to gradient magnetic force, magnetophoresis force, gravity and buoyancy in the magnetic fields. We discuss in this review all these topics in some detail with an emphasis on issues and methods. Even so, our review is selective, rather than comprehensive, out of necessity.

Keywords: *magnetic fields, combustion and explosion, free radicals, gradient magnetic force.*

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AN ONLINE PIECEWISE LINEAR REPRESENTATION METHOD FOR HYDRAULIC FRACTURING TIME SERIES

Characteristic problems of data collection in the process of fracturing operations are due to high frequency of data collection and complex downhole operating environment. In order to compensate noise and fluctuations in the fracturing data, we propose to apply an online piecewise linear representation method for hydraulic fracturing time series to re-describe the original sequence. First, the unique engineering characteristics of start and stop sanding in fracturing scenarios are combined, integrating the fitting errors to segment the sliding window; second, a mechanism of online optimization of the fitting form is proposed for adjacent fitting line segments with similar trends. When optimization is performed, the degree of optimization is calculated using the trend factor and the vertical distance factor. Finally, the original series is replaced by the fitted line segment. Based on actual fracturing data, we experimentally compare a proposed method with a variety of benchmark methods. The results show that thy developed method can retain important information of the original sequence to the greatest extent while coarse-graining the original sequence. Applying the linear representation method of the fracturing data, the computing time of the upper-level task can be further reduced and the task performance improved.

Keywords: *time series; hydraulic fracturing; piecewise linear representation; data denoising.*

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MOLECULAR SIMULATION OF HYDRATION CHARACTERISTICS OF MONTMORILLONITE UNDER POTASSIUM SALT INHIBITOR

The hydration of the shale is an important factors to the stability of borehole wall, and montmorillonite as the main component of the shale, its hydration inhibition mechanism is of great significance to maintain the stability of borehole wall of the shale. In this paper, molecular simulation software Material Studio is used to study the inhibition mechanism of potassium salt hydration inhibitors from a microscopic perspective. The results show that under the same conditions, montmorillonite has the smallest layer spacing, the largest diffusion coefficient, the smallest coordination number and the best inhibitory effect. On the whole, the parameters of potassium nitrate are significantly higher than potassium silicate and potassium carbonate; Hydration degree is low, potassium chloride inhibitor on the mechanical parameters of montmorillonite increase degree is one of the biggest, followed by potassium nitrate, potassium carbonate and potassium silicate; The effect of potassium formate on the mechanical strength of montmorillonite was similar to that of potassium chloride at higher hydration degree. Therefore, different hydration inhibitors should be selected for different hydration degrees.

Key words: borehole wall stability, hydration expansion, molecular simulation, inhibitors.

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MOLECULAR DYNAMICS SIMULATION OF CO_2 HYDRATE GROWTH AND INTERMOLECULAR WEAK INTERACTION ANALYSIS

The growth of carbon dioxide (CO_2) hydrate in CO_2 aqueous solution (box A), and in CO_2 aqueous solution with structure I (sI) CO_2 hydrate cell as seed (box B) under the same conditions of 275 K and 10 MPa, were simulated respectively. The total simulation time is 5000 ns. The nucleation process is very slow, so it is difficult to observe CO_2 hydrate growth in box A without CO_2 hydrate seed, CO_2 just accumulates to form bubbles, while H_2O still remains liquid, the F4 order parameter remains about -0.1. By contrast, beautiful CO_2 hydrate in box B grows rapidly, CO_2 is trapped in the cages formed by H_2O molecules, F4 rises from 0.12 to 0.7 due to the formation of sI hydrate. The density of CO_2 hydrate in box B is as high as 1.25 g/cm^3, higher than that of seawater, which is beneficial to its permanent sealing on the seabed. In box B, in accordance with the independent gradient model based on Hirshfeld partition (IGMH) analysis, a H_2O molecule forms four hydrogen bonds with surrounding H_2O molecules, CO_2 only has van der Waals interaction with surrounding water cages. In the actual large-scale CO_2 storage process, especially for the rapid storage of CO_2 in the form of hydrate, it is strongly recommended to pre-add CO_2 hydrate crystals into the solution to achieve the purpose of rapid growth of CO_2 hydrate.

Keywords: *molecular dynamics, CO_2 hydrate, order parameter, IGMH.*