

00/00566 Steady-state and dynamic behaviour of fixed-bed catalytic reactor for Fischer-Tropsch synthesis: I. mathematical model and numerical methodLiu, Q.-S. *et al.* *J. Nat. Gas Chem.*, 1999, 8, (2), 137-150.

The paper discusses the simulation procedure of fixed-bed catalytic reactors. A two-dimensional heterogeneous model simulates the Fischer-Tropsch synthesis fixed-bed reactor. In addition, a method for solving the fixed-bed reactor model equations during Fischer-Tropsch synthesis is detected.

00/00567 Study of coals by high resolution solid state nuclear magnetic resonanceYang, B. *et al.* *Sci. China, Ser. A: Math., Phys., Astron.*, 1999, 42, (3), 305-309.

Six different coal samples from four countries were analysed using a high-resolution solid state nuclear magnetic resonance method. Twelve structural parameters of the samples were measured and compared against Chinese coals. The most significant result obtained was from the spectral editing experiment, in which an ^{15}N NMR spectrum was obtained.

00/00568 A study of the chemical and physical processes governing CO_2 laser-induced pyrolysis and combustion of RDXLee, Y. *et al.* *Combustion & Flame*, 1999, 117, (3), 600-628.

The flame structure of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) propellants under laser-assisted combustion was studied to better understand related chemical and physical processes in the gas phase. Experiments were conducted from 0.1-3 ATM in pressure with heat fluxes of 50-600 W/cm^2 . Gaseous products were extracted through the use of quartz microprobes and analysed by a triple quadrupole mass spectrometer (TOMS). Temperature profiles were measured using micro-thermocouple techniques to investigate reaction zones in RDX flames. Flame behaviour was observed using a high-magnification video system. Major species in RDX flames were identified as H_2 , H_2O , HCN , H_2CO , NO , HNCO , N_2O , and NO_2 at low masses ($m/z \leq 47$). In addition to these species, H_2CNH with $m/z = 29$ was found to exist in the near-surface reaction zone as an important minor species. Higher molecular weight species were found at m/z values of 47, 54, 56, 70, 81, and 97; with the daughter mode operation of TOMS, they were identified as HONO , $\text{C}_2\text{H}_2\text{N}_2$, $\text{C}_3\text{H}_4\text{N}_2$, $\text{C}_2\text{H}_2\text{N}_2\text{O}$, $\text{C}_3\text{H}_3\text{N}_3$, and $\text{C}_3\text{H}_3\text{N}_3\text{O}$, respectively. Increasing heat flux and decreasing pressure stretched out the reaction zones and were useful for investigating reactions near the deflagrating surface. However, the conditions appeared to have no effect on major reaction pathways. Two-stage chemical reaction pathways in the gas phase were explicitly identified from the major species profiles at all experimental conditions. Also, the reactions of minor high-mass species occurred in the primary reaction zone. The decomposition of RDX at the surface showed evidence of the two competing branch reactions into $\text{H}_2\text{CO} + \text{N}_2\text{O}$ and $\text{HCN} + \text{HONO}$, as well as two subsequent reactions: $\text{H}_2\text{CO} + \text{N}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{CO} + \text{N}_2$ and $2\text{HONO} \rightarrow \text{H}_2\text{O} + \text{NO} + \text{NO}_2$. With the consideration of the previous four reactions, the branching ratio for the two decomposition pathways of RDX was estimated to be about 2:1. For all experimental conditions, temperature profiles had a near-surface region where temperature increased very slowly; the extent of this zone increased as the near-surface reaction zones expanded. After this region, the temperature profiles increased to final flame temperatures without any dark zone temperature plateau. Based on comparisons of species and temperature profiles, this near-surface region is believed to be related to the consumption of NO_2 , production of NO and H_2O , and production and consumption of high-mass species.

00/00569 A study of thin-flame quasisteady sphericosymmetric combustion of multicomponent fuel droplets. Part II: parametric studiesMukhopadhyay, A. and Sanyal, D. *Int. J. Energy Res.*, 1999, 23, (11), 979-987.

A parametric study of thin flame sphericosymmetric multicomponent droplet combustion has been carried out in this second part of the work, based on the model developed in the companion paper. In this section, the effects of ambient pressure and temperature and initial droplet composition have been analysed. It has been shown that droplet surface temperature and droplet life increase with increasing pressure. Droplet life increases with a reduction in ambient temperature, a decrease in initial concentration of the volatile component and an increase in boiling point of the less volatile component.

00/00570 A study of thin-flame quasisteady sphericosymmetric combustion of multicomponent fuel droplets. Part I: modelling for droplet surface regression and non-unity gas-phase lewis numberMukhopadhyay, A. and Sanyal, D. *Int. J. Energy Res.*, 1999, 23, (11), 963-977.

In the first part of this two-part work, a model for sphericosymmetric thin-flame combustion of multicomponent fuel droplets has been developed. The model incorporates effects of droplet surface regression and gas-phase Lewis number. It is observed that both these factors greatly affect the results. The investigation also reveals the transient nature of the combustion process.

00/00571 A vitrinite reflectance kinetic model incorporating overpressure retardationCarr, A. D. *Marine & Petroleum Geology*, 1999, 16, (4), 355-378.

The models currently used to predict maturation and hydrocarbon generation in petroleum basins use time and temperature as controlling parameters. A small number of studies have indicated that overpressure can retard maturation. Although some of the published information from experimental investigations appears to be conflicting, careful examination of the experimental conditions shows that both vitrinite reflectance and hydrocarbon generation are retarded by overpressures. Overpressure appears to result in the retention of volatiles within the molecular structure which prevents the molecular reorganization necessary to produce higher reflectance values. Using a database containing vitrinite reflectance from both overpressured and normally pressured wells, a kinetic model (PresRoTM) has been developed in which overpressure modifies the Arrhenius (A) factor. The model has been tested on two different basins (South China Sea and Sable), exhibiting a range of time-temperature-overpressure characteristics. The results suggest that the maturity and timing of the onset of hydrocarbon generation differ significantly from those predicted by current models.

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00/00572 Break-even price of distributed generation under uncertaintyAng, B. W. *et al.* *Energy*, 1999, 24, (7), 579-589.

This paper presents a stochastic model for evaluating distributed generation investment under uncertainty. The objective is to estimate the break-even price and its probability distribution. The model is developed based on the probabilistic influence diagram technique and the main uncertain variables are explicitly represented by probability distribution functions. The model is used to study a photovoltaic generation project.

00/00573 Climate Change Levy creates winners tooCook, A. *Energy World*, 1999, October, 273, 2.

For a tax that is designed to be revenue neutral, the Climate Change Levy has attracted an awful lot of noise from some very big guns. Business and industry have lined up against the tax, claiming that it will increase their costs and harm Britain's competitiveness. However, local authorities, for example, are among Britain's large employers, they stand to save more on their National Insurance than they pay out in the energy levy. By channelling these savings into energy efficiency programmes, local authorities can help millions of fuel poor claim their right to a warm home.

00/00574 Decomposition of aggregate CO_2 emissions in the OECD: 1960-1995Sun, J. W. *The Energy Journal*, 1999, 20, (3), 147-155.

This paper analyses the change of aggregate CO_2 emissions in the OECD from 1960 to 1995 based on a complete decomposition approach. The study indicates that developed countries have achieved a considerable decrease in their CO_2 emissions mainly due to improved energy efficiency and fuel switching. However, some member countries of the OECD have found it difficult to achieve the environmental targets set at Rio de Janeiro in 1992, and should reconsider their energy policies in light of information given at the UN Climate Change Conference in Kyoto.

00/00575 District heating and market economy in LatviaLund, H. *et al.* *Energy*, 1999, 24, (7), 549-559.

From the Soviet time, Latvia inherited a number of district-heating systems fuelled with Russian natural gas or imported heavy fuel oil. From a fuel efficiency point of view there is no reason to preserve the district heating systems unless the boilers are replaced by CHP. However, 50% of the electricity consumption is imported, and the import prices are low because the production prices in neither Estonia nor Lithuania fully include the long-term capacity costs. Thus, Latvia has two major long-term strategic choices to make: (1) should the country try to reduce the energy demand, and (2) should the country try to replace the import of electricity by domestic production. In implementing the latter solution, Latvia could benefit from cogeneration, if the local district heating systems are preserved. This article seeks to form a strategy to develop the use of Latvian wood resources in local cogeneration. Even though cogeneration from a business economic point of view is not feasible with today's import prices, the Latvian balance of payments would benefit immediately from the implementation of such technologies.