thermogravimetric analysis, grid heater and Curie-point pyrolyser. The oxidation of the char particles for the first two experimental techniques was obtained by applying the non-isothermal 'model of decomposition of functional groups in independent parallel reactions' and for the Curie-point pyrolyser an isothermal equation of the model was used. Data obtained with each technique has been extrapolated to other combustion conditions and other techniques. Effects of differences in heating rate, experimental environment, analysis and amount of sample are discussed, as well as the influence of heat evolution on the reaction order of reactions. The results provide criteria for the range of validity and possible extrapolation of experimental kinetic data.


There is potential in the heterogeneous reaction of NO with coal char as the basis for re-burning and post-combustion clean-up processes to control NOx combustion emissions. The reaction is also important in understanding NO formation and reduction during coal combustion. The kinetics of NO reduction by chars made from coals ranging in rank from lignite to low-volatile bituminous coal was examined in a packed-bed reactor at temperatures of 723-1173 K. Graphite and coconut charcoal were also studied. Low-rank chars were significantly more reactive than high-rank coals with the Ea (temperature required for 50% NO conversion) varying from 870 K for NDL to 1100 K for graphite for a given set of conditions. For all chars studied, the reaction was first order with respect to NO partial pressure and exhibited an activation energy (Ea) shift from 100-160 kJ/mol at low temperature to over 400 kJ/mol at high temperature. The Ea values were different and higher Eas at higher temperatures are opposite to what would be expected if a reaction is shifting from chemical rate control to mass transfer control and suggests different mechanisms or rate-determining steps at high temperatures. Although all chars exhibited an Ea at the shift temperature and the Ea within each temperature regime tended to increase with increasing rank. Also, the relative reactivity of char depended on organic char surface area and on inorganic contents.


Valuable tool for the study of the molecular dynamics of gas-phase and heterogeneous reactions and complex technical combustion processes, include laser-based in situ diagnostic techniques with high temporal, spatial and spectral resolutions. Results of recent experiments are presented in which the laser diagnostic techniques were used to examine elementary chemical gas-phase and catalytic reactions, combustion engines processes, as well as complex industrial and coal combustion.


It is possible that particulate matter emitted from solid-fuel combustors contains toxic metals in concentrations sufficient to endanger health. Metal contents are enriched in the sub-micron fraction, the one most likely to avoid capture by conventional collection devices and the one capable of deeper pulmonary ingestion. Mathematical models for predicting toxic metal emissions from solid-fuel combustors and of metals partitioning with respect to particle size is described. This model accounts for particle formation and growth by the combined effects of coagulation and metal vapour deposition. Based on experimental evidence, particle size distribution is subdivided into two ranges: the sub-micron fraction and much larger residual ash particles. Conservation equations are solved for the total number and mass concentrations of particles. The modelling is included in an existing procedure for solid-fuel combustors combustion and applied to predict lead and cadmium emissions from a laboratory coal-fired and from coal and waste treatment sludge. Predicted emissions of these two metals and the metals enrichment in the sub-micron class compared rather well with measured values. Discrepancies were attributed to the effect of gas-phase and surface chemical reactions that were not modelled, due to the absence of kinetic data.

00/02798 Modeling the fragmentation of non-uniform porous char particles during pulverized coal combustion Lin, G. Fuel, 2000, 79, (6), 627-633.

Char fragmentation during pulverized coal combustion was studied using an Australian bituminous coal. The coal was combusted with air in a drop tube furnace at a gas temperature of 1300°C. The char samples were collected at different levels of char burnout and their structure was examined using scanning electron microscopy. Approximately 40% of the char particles formed after pyrolysis were cenospheres with a highly non-uniform porous structure and a characteristic diameter over 90% being less than 10 μm. Analyses were also observed in the char samples with burnout levels between 30 and 30 vol%, which suggests that significant fragmentation occurs during the early combustion stage. A mathematical model was developed relating the fragmentation rate to the char particle number and particle size distribution. The formation of these macropores partially results because of the carbon removal from the surface of the thin shell due to surface oxidation. A percolation model was used to simulate the char structural changes during combustion in regime III and the predicted particle size distributions qualitatively agreed with the experimental measurements.


It is possible to modify the method for the preparation of coal for boilers by continuously pulverizing coal having a particle size of 0.1-0.5 mm from coal lumps by feeding the coal with an incombustible gas to a pulverizer to further oxidized coal having a particle size of 0.1-10 mm. Then the pulverized coal is fed to a cyclone with an incombustible carrier gas, the mineral contents in the pulverized coal are removed and the demineralized coal and the incombustible gas are withdrawn from the cyclone and fed to the boiler for combustion.


An experimental optimization has been carried out of operating regimes and ecological characteristics of a thermal contact pyrolysis reactor of a pilot plant with circulating spouted bed. It is shown how it is possible to obtain the medium-calorific pyrolysis gas with more than 80% of volatile combustion and more than 90% of coal sulfur capturing. In addition an optimal scheme of the thermal contact pyrolysis reactor operating in circulating fluidized bed is given.

00/02801 Pilot scale study of trace element vaporization and condensation during combustion of a pulverized sub-bituminous coal Sun, C. L. Fuel Processing Technology, 2000, 63, (2-3), 149-165.

Trace metal emissions from coal-fired power plants are largely associated with the fly ash. The work reported here is part of a larger effort to develop a fundamental model for transformation of trace metals in coal to air toxic emissions from coal-fired power plants. Because the time-temperature history of the combustion gases determines the condensation behavior and gaseous species, experimental study of these phenomena require a realistic post-combustion environment. Pilot-scale combustion of a Powder River Basin coal was conducted using realistic post-combustion conditions. Trace element distributions were measured in the submicron fly ash at the inlet to the electrostatic precipitator. Flame temperature had a dramatic effect on the amount of certain trace elements such as arsenic and selenium in the submicron ash, indicating that these elements vaporize during the combustion process. The amount of vaporization was not sensitive to coal grind. There is evidence for the reaction of arsenic and selenium vapors with the flue gas (supermicron) ash in the post-combustion flue gas via a surface reaction. The correlation between arsenic and calcium in the ash suggests the formation of calcium arsenate. No such correlation was observed between selenium and calcium.


The main focus of the modellisation was focused on the evolution under heat treatment of the so-called α, β and γ-resins fractions usually used for the characterization of pitch. Pechs and reactions modelling to predict toxic metal emissions from solid-fuel combustors and of metals partitioning with respect to particle size is described. This model accounts for particle formation and growth by the combined effects of coagulation and metal vapour deposition. Based on experimental evidence, particle size distribution is subdivided into two ranges: the sub-micron fraction and much larger residual ash particles. Conservation equations are solved for the total number and mass concentrations of particles. The modelling is included in an existing procedure for solid-fuel combustors combustion and applied to predict lead and cadmium emissions from a laboratory coal-fired and from coal and waste treatment sludge. Predicted emissions of these two metals and the metals enrichment in the sub-micron class compared rather well with measured values. Discrepancies were attributed to the effect of gas-phase and surface chemical reactions that were not modelled, due to the absence of kinetic data.


In this study, a simple model to predict the evolution of the combustion characteristics of solid-gas mixtures in a closed vessel was extended to a wide range of dust suspensions in the general case of vented explosions. The model was tested to obtain a risk evaluation and to improve safety conditions in industrial plants. A simple representation of the combustion phenomena based on energy transfers between particles and the action of specific molecules is presented. The pressure venting due to the vent breaking is calculated from thermodynamic characteristics given by the model and taking into account the mass rate of discharge of the different products deduced from the standard orifice equations. The application conditions determine the fuel ratio of the used mixtures, the nature of the chemical kinetics and the calculation of a universal set of parameters. The proposed model is compared to Barknecht's experimental results and shows the model representativeness for various dust suspensions (corn.

310 Fuel and Energy Abstracts September 2000
The gas purification involves employing an alkali or alkaline earth metal under standard free energy is less than that for formation of its sulfates so as to make a lean exhaust NOx chemical adsorbed or absorbed to the oxides. The use of the catalysts gives improved SOx-poisoning protection and the exhaust gases improved NOx purification.

Pyrolysis kinetics of lignocellulosic materials—three independent reactions model

The pyrolysis reactions with lignocellulosic materials in the presence of nitrogen and air was used to study the behaviour of biomass components, such as cellulose, lignin and hemicellulose. The results were compared and the pyrolysis kinetics of cellulose detected. Using simple independent reactions model it was not possible to model the thermal decomposition of xylan and lignin with acceptable criteria. Thermograms were detected for pine and eucalyptus woods and pine bark, under inert (nitrogen) or oxidizing (air) conditions. The pyrolysis of these lignocellulosic materials was modelled with good approximation by three first-order independent reactions. One of these reactions is associated with the primary pyrolysis of cellulose, its parameters being obtained by fitting the model to the TG data. The other two parameters are the activation energies and pre-exponential factors for the pyrolysis of the remaining two pseudo-components and two additional parameters related to the biomass composition. This report also presents a method to determine the biomass composition. Comparative studies were made from calculated results and data from the literature, and they were in agreement with one another.

Release of biomarkers from sulfur-rich kerogens during hydrous pyrolysis

The pyrolysis of these kerogens was modelled using a two-step mechanism with linear temperature programming in the presence of nitrogen and air. The instantaneous evolution of the volatile components, such as water, especially when clay minerals are involved in the process. Laboratory tests have been undertaken on a suite of 12 mineral samples to evaluate these sources. SDM calculates mean values of the Eulerian source models in the non-premixed regime. Various numerical methods may be found in the literature to calculate such turbulent flames, using either Reynolds averaged Navier–Stokes techniques (RANS) or large eddy simulation (LES). These methods are not suitable for coupling with other simulations. The computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction. However, the sources of fluctuations of mixture fraction and their fluctuations in computational fluid dynamics codes, Euler–Lagrange spray modelling may provide the mean source of mixture fraction.