Computational modeling of the combustion of coal water slurries containing petrochemicals

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The combustion predictive model was developed based on the results of experiments with coal water slurry and coal water slurry containing petrochemicals. Unlike other known models, it takes into account the effect of liquid flammable component (in particular, engine oil waste) on the main mass and heat transfer as well as other physical and chemical processes in the combustion chamber. The main differences, conditions and characteristics of the combustion of coal water slurries containing petrochemicals and without additives have been studied theoretically with different defining parameters: fuel composition, component properties, and furnace chamber temperature. Temperature fields and volumetric concentration distribution of combustion products in the furnace chamber are established for fuel compositions based on water, coal, and industrial oil waste. Temperatures and concentrations for both the initial fuel components and their combustion products are established at different points of the furnace chamber for various component concentrations, properties, and furnace air temperatures. The main research findings are the quantitative differences between the characteristics of ignition and combustion of slurries with and without a liquid fuel component. These differences are critical to illustrate the benefits of using coal water slurries containing petrochemicals in heat and power plants. Adding as little as 10% (relative mass fraction) of waste industrial oils was shown to significantly reduce the ignition delay times and improve the combustion efficiency of fuel compositions. Possible ranges, in which the ignition delay of slurry fuels can be reduced, and the displacement of their ignition zones in the combustion chamber were...
### Nomenclature

- **\( a \)**: absorption coefficient
- **\( A \)**: prefactor in Arrhenius equations
- **\( A' \)**: ash content (dry basis) [%]
- **\( A'' \)**: ash content (as received) [%]
- **\( A_{char} \)**: particle effective surface area [m²]
- **\( A_{char}^{B20,C02} \)**: stoichiometric coefficient indicating the ratio of mass of unreacted char to the mass of consumed oxygen
- **\( B_m \)**: Spalnd mass number
- **\( B_T \)**: Spalnd heat transfer number
- **\( C_D \)**: particle drag coefficient
- **\( C_{O2} \)**: the concentration of oxygen [kg/m³]
- **\( c_P \)**: specific heat [J/(kg·K)]
- **\( C' \)**: fraction of carbon (as received) [%]
- **\( D \)**: mass diffusion coefficient [m²/s]
- **\( D_b \)**: binary gas diffusion coefficient [m²/s]
- **\( D_{O2} \)**: the oxygen diffusion coefficient [m²/s]
- **\( D_{o} \)**: binary steam diffusion coefficient under reference conditions [m²/s]
- **\( d_p \)**: particle diameter [m]
- **\( E \)**: activation energy [J/mol]
- **\( E_{char} \)**: activation energy of char [J/mol]
- **\( E_{kin} \)**: gas combustion activation energy [J/mol]
- **\( E_p \)**: radiation flux density [J/mol]
- **\( f_{r} \)**: mass fraction of ith component
- **\( f_{v} \)**: vapor mass fraction
- **\( \phi_{V} \)**: vapor mass fraction at the surface
- **\( h \)**: enthalpy [J/kg]
- **\( h_j \)**: enthalpy of the jth component (H₂O, O₂, CᵢHᵧ, C) [J/kg]
- **\( H' \)**: fraction of hydrogen (as received) [%]
- **\( k \)**: turbulent kinetic energy [m²/s²]
- **\( k_{char} \)**: reaction rate constant [m/s]
- **\( k_{comb} \)**: empirical coefficient
- **\( k_{EBU} \)**: eddy breakup model constant
- **\( k_{kin} \)**: pre-exponential factor of gas combustion reaction
- **\( k_p \)**: combustion rate of char [kg/(m² s)]
- **\( k_{char} \)**: rate constant of the chemical reaction [m/s]
- **\( k_{diff} \)**: rate of devolatilization in the diffusion regime [s⁻¹]
- **\( k_{diff, char} \)**: rate constant of the chemical mass transfer [m/s]
- **\( k_{diff, kin} \)**: rate of devolatilization in the kinetic regime [s⁻¹]
- **\( k_{vol} \)**: the rate of devolatilization [s⁻¹]
- **\( L_{s,V} \)**: latent heat [J/kg]
- **\( M \)**: molecular mass [kg/kmol]
- **\( m_{char} \)**: char oxidation rate [kg/s]
- **\( m_{p} \)**: mass flow rate of particles [kg/s]
- **\( m_{vol} \)**: the mass of volatiles released from particle [kg]
- **\( m_{vol, vol} \)**: the total mass of volatiles in the initial coal particle [kg]
- **\( m_{dry} \)**: molar mass of environment matter (vapor excluded) [kmol]
- **\( \Delta m_{J} \)**: mass rate of change of the jth component (H₂O, O₂, CᵢHᵧ, C) [kg]
- **\( m_{p} \)**: mass of a single particle [kg]
- **\( m_{p} \)**: mass flow rate of particles [kg/s]
- **\( M_{i} \)**: molecular mass of ith component [kg/kmol]
- **\( M'_{vapor} \)**: vapor molar mass [kmol]
- **\( N' \)**: fraction of nitrogen (per fuel operating condition) [%]
- **\( N_r \)**: the number of reagents
- **\( N_{Vol} \)**: diffusion Nusselt number
- **\( p \)**: pressure [N/m²]
- **\( p_{s,V} \)**: saturated vapor pressure at the droplet temperature [N/m²]
- **\( p_e \)**: operating pressure [Pa]
- **\( Pe \)**: Peclet number
- **\( Q \)**: caloric value [J/kg]
- **\( Q' \)**: lower fuel heating value [MJ/kg]
- **\( Q'_{hi} \)**: higher fuel heating value [MJ/kg]
- **\( R \)**: gas constant [kJ/(kg·K)]
- **\( r_{char} \)**: radius of char [m]
- **\( R_{EBU} \)**: eddy breakup model reaction rate
- **\( R_{kin} \)**: kinetic model reaction rate
- **\( R_{vol} \)**: reagent combustion rate (including volatiles)
- **\( Re \)**: Reynolds number
- **\( S \)**: source terms
- **\( Sc \)**: Schmidt number
- **\( Sh \)**: Sherwood number
- **\( S \)**: the rate of mass change due to the interface interaction
- **\( S_{r} \)**: the rate of momentum change due to the interface interaction
- **\( S' \)**: fraction of sulfur (as received) [%]
- **\( T \)**: temperature [°C]
- **\( T_b \)**: liquid boiling temperature [°C]
- **\( T_g \)**: gas temperature [°C]
- **\( T_p \)**: particle temperature [°C]
- **\( ν \)**: velocity [m/s]
- **\( ν_{rad} \)**: volatiles (dry ash-free state) [%]
- **\( w \)**: release rate of reaction products [m³/s]
- **\( W^w \)**: moisture content of analytical sample of coal in an air-dry state [%]
- **\( W^* \)**: moisture content (as received) [%]
- **\( Z_{r0} \)**: number of particles release points
- **\( Z_{r} \)**: mass fraction of particles size-class b
- **\( x_{r,i} \)**: mass concentration of ith reactant
- **\( x_{r,y,z} \)**: longitudinal, wall-normal and tangential coordinates

### Greek symbols

- **\( \alpha \)**: convective heat transfer coefficient [W/(m²·°C)]
- **\( \alpha_g \)**: absorption coefficients of gas
- **\( \alpha_p \)**: absorption coefficients of particles
- **\( \beta \)**: temperature exponent in Arrhenius equation
- **\( γ_p \)**: particle dispersion coefficient
- **\( Δ \)**: difference
- **\( δ \)**: particle size before volatile emission [mm]
- **\( δ_{char} \)**: char dimensions [mm]
- **\( ε \)**: rate of dissipation of turbulence kinetic energy [m²/s³]
- **\( ε_p \)**: particle radiation emissivity
- **\( μ \)**: dynamic viscosity [Pas]
- **\( ν_{i} \)**: stoichiometric coefficient of \( x_{r,i} \) species
- **\( ξ \)**: coefficient of scattering anisotropy
- **\( ρ \)**: density [kg/m³]
- **\( σ \)**: Stefan-Bolzmann constant [J/K]
- **\( τ \)**: stress tensor
- **\( τ_{t} \)**: tensor of turbulent stress
- **\( τ_{φ} \)**: tensor of viscous stress
- **\( φ \)**: fraction of char heat absorbed by gas (relative to particles)
- **\( Χ \)**: fraction of heat release from char burning goes into the gaseous phase

### Suffixes and superscripts

- **\( char \)**: char
- **\( conv \)**: convection
- **\( devol \)**: devolatilization
- **\( diff \)**: diffusion (regime)
- **\( eb \)**: eddy breakup
- **\( i \)**: ith component in the mixture
- **\( in \)**: conditions at the inlet
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