Effects of Wet CO Oxidation on the Operation of Engines and Power Generators

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A simplified method is used to determine the optimum water content in the flue gases of charcoal gasifiers to be utilized as alternative fuels in the operation of engines and gas turbines for power generation. Computational models of plug flow reactors and well stirred reactors are employed to simulate the reaction and post-flame zones, adopting different chemical mechanisms. In the simulations reactants enter the reactors at 1000 K, 1 atm and equivalence ratio 0.25. It was observed that mixtures about 3% to 4% in volume of water vapor allow to obtain optimal operation characteristics, including high blowout limit, low ignition delay, maximum reaction zone temperature, high CO2 prodution and low thermal NO formation. It was observed that increasing water contents reduce significantly ignition times up to 3% in volume, while blowout mass flow rates increase continuously up to 6 % in volume, the maximum value considered. Formation of NO decreases continuously with humidity after the flame zone, while there are peaks of NO formation within the flame zone below 1% in volume. Higher water vapor content decreases the final temperatures below 1700 K, leading to a lower thermal efficiency. The method can be used to estimate optimum operational conditions with other input parameters.

***Keywords**: Gasifier, carbon monoxide, power generator, engine, gas turbine*

Introduction

Operation of engines and power-generators has been made by using the flue gases produced by charcoal gasifiers (Morais, 1981; Ismail and Morais, 1983). Carbon monoxide, *CO*, is a main component of the mixtures produced by charcoal gasifiers, which are employed as alternative fuel. It is well known that oxidation of *CO* in the presence of water occurs more rapidly than oxidation in dry conditions, since water acts as a catalyst and is not consumed during the reaction (Dryer and Glassmann, 1973; Lewis and Von Elbe, 1985; Glassmann, 1996). Therefore addition of small amounts of water can yield a better combustion efficiency in power-generators and engines, once *CO* appear in the combustion process. On the other hand, the presence of liquid water or water vapor can reduce the final temperatures, leading to lower thermodynamic efficiencies and can, also, affect ignition conditions, blowout characteristics and the mechanisms of pollutant formation.[*]

A number of works has been published about water addition, in liquid or vapor form, in combustion processes. Dryer (1976) presented a review of concepts and applications related to the use of water in combustion systems, mentioning the use of water vapor in turbine operation during the 18th century. Greeves et al. (1978) investigated the utilization of water emulsions in diesel engines to reduce fuel consumption, ignition delay and emissions of *CO*, *NO* and *HC*. Rightley and Williams (1997) analysed the effect of addition of H_2 or H_2O on the propagation velocity of premixed flames of *CO* and O_2. Recently, Bhargava et al. (2000) compared experimental results, obtained by injecting humid air in aeronautical turbines, with simplified computational models involving a series of perfectly stirred reactors. They conjectured that water vapor presence reduces the concentration of the *O* radical, decreasing the formation of thermal *NO* and N_2O, while the larger concentration of *OH* decreases the amount of *NO* formed through the Fenimore mechanism, the so-called prompt-*NO*, which depends on the presence of *CH*, *CN* and *HCN* in the reaction zone.

Thus, the objective of this work is to investigate the optimum water content in the flue gases of charcoal gasifiers (assumed as mainly composed of *CO*) to be used as alternative fuel in gas turbines and engines. A simplified method is used to determine the optimum water content, based on computational models of plug flow and well stirred reactors. Different chemical mechanisms are considered with the help of CHEMKIN 3.5 and MATLAB 5.0. Optimal operation characteristics include a high blowout limit, low ignition delay, maximum reaction zone temperature, high CO_2 prodution and low thermal *NO* formation. Perfectly stirred reactors are used to study the flame zone characteristics and plug flow reactors are used to estimate ignition delays and *NO* formation after the flame zone.

Nomenclature

A = pre-exponential factor, 1/s
B = temperature exponent, dimensionless
CV = control volume, m^3
$c_{P,i}$ = specific heat of species i, J/(kg K)
h_i = specific enthalpy of species i, J/kg
$h^0_{f,i}$ = formation enthalpy of species i, J/kg
k = reaction constant, units depend on reaction order
M_i = molecular weight of species i, kg/kg-mol
$\dot{m}$ = total mass flow rate, kg/s
N = total number of species in the mixture, dimensionless
P = pressure, Pa
PFR = plug flow reactor
PSR = perfectly stirred reactor
R_o = universal gas constant, J/kg-mol/K
T = temperature, K
t = time, s
V = volume of reactor, m^3
v_x = axial velocity, m/s
$\dot{\omega}_i$ = reaction rate of species i, kg-mol/m^3/s
X_i = molar fraction of species i, dimensionless
x = axial coordinate, m
Y_i = mass fractions of species i, dimensionless
z = stoichiometric coefficient of water, dimensionless

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Greek Symbols

ϕ = equivalence ratio, dimensionless
ρ = mixture density, kg/m^3

Subscripts

e = relative to entrance
i = relative to a given species
mist = relative to mixture
s = relative to exit condition
0 = relative to initial condition

Chemical Mechanisms

The mechanism of *CO* oxidation with hydrogen-containing compounds is usually called wet oxidation. The *CO* oxidation proceeds through this route in practical systems, since even small quantities of hydrogen, of the order of 20 ppm, increase substantially the *CO* oxidation rate (Glassman, 1996).

Several chemical mechanisms of wet *CO* oxidation using hydrogen from water were considered in the analysis.

Simplified Mechanism

The simplest mechanism adopted was a single step or global reaction given by

$$CO+\frac{1}{2\phi}\left(O_2+3.76N_2\right)+zH_2O \underset{k_r}{\overset{k_f}{\rightleftarrows}} CO_2+\frac{1-\phi}{2\phi}O_2+ \\ +zH_2O+\frac{3.76}{2\phi}N_2 \tag{1}$$

where ϕ is the equivalence ratio. The molar fraction of water vapor X_{H2O} is related to the stoichiometric coefficient z of water by

$$X_{H2O}=z\left(1+z+2{,}38/\phi\right)^{-1} \tag{2}$$

and the molar concentration (kmol/m^3) of water vapor is obtained from $\left[H_2O\right]=X_{H2O}P/R_0T$, where P is the total pressure, R_0 is the universal gas constant and T is the gas temperature.

The reaction rates for the above mechanism were obtained by Dryer and Glassman (1973) by adjusting experimental results in plug flow reactors, with temperatures between 1000 and 1700 K:

$$d\left[CO\right]/dt=-k_f\left[CO\right]\left[H_2O\right]^{0.5}\left[O_2\right]^{0.25} \tag{3}$$

$$d\left[CO_2\right]/dt=-k_r\left[CO_2\right] \tag{4}$$

where

$$k_f=2.24\times10^{12}\exp\left[-20135/T\right]\quad\left(kgmol/m^3\right)^{-0.75}s^{-1}\ , \tag{5}$$

$$k_r=5.0\times10^{8}\exp\left[-20135/T\right]\quad s^{-1}\ . \tag{6}$$

Detailed Chemical Mechanisms

Descriptions of the detailed mechanism of *CO* oxidation are made, e.g., by Lewis and Von Elbe (1985), and by Glassmann (1996). The effects of small quantities of H_2O or H_2 in the *CO* oxidation rate are significant because the reaction rates between *CO* and *OH* are much greater than the reaction rates between *CO* and *O* or *CO* and O_2. The water-catalyzed reaction proceeds in the following manner:

$$CO+O_2=CO_2+O \tag{7}$$

$$O+H_2O=OH+OH \tag{8}$$

$$CO+OH=CO_2+H \tag{9}$$

$$H+O_2=OH+O \tag{10}$$

Reaction (7) is a chain initiating step, but it is slow and does not contribute significantly for production of CO_2. Step (9) is a chain propagating step, yielding *H* radicals which react with O_2, originating *OH* and *O* by the chain branching step (10). The *OH* radicals that are formed participate in step (9) and the *O* radicals formed participate in step (8). If H_2 is the catalyst, the following steps should be included:

$$O+H_2\rightarrow OH+H \tag{11}$$

$$OH+H_2\rightarrow H_2O+H \tag{12}$$

Consequently, all steps of the complete system H_2-O_2 must be included in the mechanism of wet *CO* oxidation. The presence of HO_2 creates another step for conversion of *CO* to CO_2:

$$CO+HO_2\rightarrow CO_2+OH \tag{13}$$

Reaction (13) is important at high pressures and in the initial stages of hydrocarbon oxidation. Reaction (9) is the most important in combustion processes. Any mechanism of hydrocarbon combustion in air involves H_2 and *CO* oxidation kinetics and most of the CO_2 that is formed results from reaction (9).

The primary nitrogen oxide formed in combustion systems is *NO*. In some systems, appreciable NO_2 is produced, usually as a result of $NO \rightarrow NO_2$ conversion in low temperature mixing regions of nonpremixed systems (Turns, 1996). *NO* is formed through several mechanisms, for example, the Fenimore mechanism and the thermal process of Zeldovich, or it can come from nitrogen present in the fuel.

It can be inferred that *NO* originates mainly from the thermal process in the cases presented here, since the *CO* molecule does not contain *N* atoms, the mixture is lean (equivalence ratio = 0.25), and formation of radicals *CH* and *HCN* is not significant. According to Heywood (1988), the extended mechanism of Zeldovich, responsible for production of thermal *NO*, is given by:

$$N+NO=N_2+O \tag{14}$$

$$N+O_2=NO+O \tag{15}$$

$$N+OH=NO+H\ . \tag{16}$$

Table (1) shows a mechanism with 24 reactions, including steps (7) and (9), the H_2-O_2 mechanism and the Zeldovich mechanism. Kinetic data were taken from CHEMKIN 3.5 (1999) input files. Some steps, shown in Tab.(1), include colision factors dependent on size and form of a third body. In Tab.(1), E_a is the activation energy, b is the temperature exponent and A is the pre-exponential factor in the reaction constant $k=AT^b\ \mathrm{exp}\tilde{(}E_a/RT)$.

The GRI-Mech mechanism (1999), including 55 species and 335 steps, allows to simulate the burning of methane (CH_4) in air, and the Konnov mechanism (1998), including 127 species and about 1100 steps, allows to simulate the burning of propane (C_3H_8) and lower hydrocarbons in air. In the present work, only the steps involving the *CO* oxidation and *NO* formation in the GRI-Mech and Konnov mechanisms are considered. This is performed automaticaly by the CHEMKIN 3.5 software.

Table 1. Kinetic constants for a mechanism with 24 steps.

Reaction	*A* mol-cm-s-K	*b* -	E_a cal/mol
CO+O2 = CO2+O	1.60E13	0.0	41000
CO+OH = CO2+H	1.51E07	1.3	758
H+O2 = O+OH	5.10E16	0.82	16510
H2+O = H+OH	1.80E10	1.0	8830
H2+OH = H2O+H	1.2E09	1.3	3630
OH+OH = H2O+O	6.0E08	1.3	0
H+OH+M = H2O+M	7.5E23	2.6	0
H2O/20.0/			
O2+M = O+O+M	1.9E11	0.5	95560
H2+M = H+H+M	2.2E12	0.5	92600
H2O/6.0/ H/2.0/ H2/3.0/			
H2+O2 = OH+OH	1.7E13	0.0	47780
H+O2+M = HO2+M	2.1E18	1.0	0
H2O/21.0/ H2/3.3/ O2/0.0/ N2/0.0/			
H+O2+O2 = HO2+O2	6.7E19	1.42	0
H+O2+N2 = HO2+N2	6.7E19	1.42	0
HO2+H = H2+O2	2.5E13	0.0	700
HO2+H = OH+OH	2.5E14	0.0	1900
HO2+O = OH+O2	4.8E13	0.0	1000
HO2+OH = H2O+O2	5.0E13	0.0	1000
HO2+HO2 = H2O2+O2	2.0E12	0.0	0
H2O2+M = OH+OH+M	1.2E17	0.0	45500
H2O2+H = HO2 + H2	1.7E12	0.0	3750
H2O2+OH = H2O+HO2	1.0E13	0.0	1800
N+NO = N2+O	2.7E13	0.0	355
N+O2 = NO+O	9.0E09	1.0	6500
N+OH = NO+H	3.36E13	0.0	385

* data from CHEMKIN 3.5 input files.
** constants for the direct reactions.

Simplified Computational Models

Analysis of the reactive processes in complex flows in combustors, turbines, engines and other systems can be made, e.g., by combination in series or in parallel of perfectly stirred reactors (PSR) and plug flow reactors (PFR). Simplified models of reactive systems are useful to understand the coupling between the conservation laws of mass and energy with chemical kinetics. For example, a PSR allows to estimate blowout conditions and theoretical maximum temperatures, while a PFR allows to estimate *NO* formation and to investigate ignition delays, simulating combustion processes in chambers of power-generators and engines. The blowout condition determines the maximum load condition for continuous flow combustors. The reaction zone in burners can be modelled by one or two PSR with recirculation. Turns (1996) presents a detailed description of several simplified reactive models, however a brief review of the PSR and PFR models is presented here.

Perfectly Stirred Reactors (PSR)

A perfectly stirred reactor is an ideal reactor where perfect mixing occurs inside the control volume (*CV*).

Conservation of mass equation for a species *i* in a PSR, assuming steady state, is given by

$$\dot{\omega}_i M_i V + \dot{m}\left(Y_{i,e} - Y_{i,s}\right) = 0\,, \quad \text{for } i = 1, 2, 3, ..., N \text{ species} \tag{17}$$

where $\dot{\omega}_i$ is the reaction rate, M_i is molecular weight, $Y_{i,e}$ and $Y_{i,s}$ are mass fractions of species *i* entering and exiting the reactor, respectively. The total mass flux $\dot{m}$ and volume *V* of the reactor are given parameters.

Exit mass fractions $Y_{i,s}$ are equal to mass fractions inside the reactor, since perfect mixing is assumed after the reactants enter the *CV*. Composition within the reactor is the same everywhere, therefore the composition at the exit must be the same at any point inside the *CV*. With this information, the reaction rates are of the form

$$\dot{\omega}_i = f\left(\left[X_i\right], T\right) = f\left(\left[X_i\right]_s, T\right) \tag{18}$$

where the mass fractions Y_i and molar concentrations $[X_i]$ are related by

$$Y_i = \frac{\left[X_i\right] M_i}{\sum_{j=1}^{N} \left[X_j\right] M_j} \tag{19}$$

Equations (17), written for each species, yield *N* equations involving *N* + 1 unknowns: *N* mass fractions and temperature. An energy balance provides the additional equation required for closure. Neglecting variations in kinetic and potential energies, the steady-state energy equation for steady and adiabatic flow in a control volume is given by $h_s = h_e$, where h_e and h_s are specific enthalpies of the entering and exiting mixture, respectively. In terms of composition, the energy equation becomes

$$\sum_{i=1}^{N} Y_{i,s} h_i(T_s) = \sum_{i=1}^{N} Y_{i,e} h_i(T_e) \tag{20}$$

where

$$h_i = h_{f,i}^0 + \int_{T_{ref}}^{T} c_{p,i}\, dT \tag{21}$$

and h_i is specific enthalpy, $h_{f,i}^0$ is formation enthalpy, and $c_{P,i}$ is the specific heat of species *i*.

The mass flux $\dot{m}$ or, alternatively, the residence time, is a parameter for the problem. Initially small values of mass flux are chosen to allow combustion for a given equivalence ratio. Making a progressive increase in $\dot{m}$, or decrease in residence time, the system of equations has no solution or it yields the same input values. This gives the blowout limit, which indicates that there is not enough time for the reaction to occur within the reactor. Curves relating blowout mass flux with equivalence ratio in a PSR are similar to curves obtained in experimental reactors and turbines. To solve the *N* + 1 non-linear equations obtained, equations (17) through (21), an iterative method, such as the generalized Newton-Raphson method, must be employed.

Plug Flow Reactor

The following assumptions are made in the case of a PFR: 1) steady state, steady flow with constant area; 2) no mixing or diffusion in axial direction; 3) one-dimensional flow; 4) frictionless and adiabatic flow; and 5) ideal gas behavior.

The following system of ordinary differential equations is obtained:

$$\frac{d\rho}{dx} = \frac{\dfrac{\rho \overline{R}_0}{\mathrm{v}_x c_P M_{mist}} \sum_{i=1}^{N} M_i \dot{\omega}_i \left(h_i - \dfrac{M_{mist}}{M_i} c_P T \right)}{P\left(1 + \dfrac{\mathrm{v}_x^2}{c_P T}\right) - \rho \mathrm{v}_x^2}\,, \tag{22}$$

$$\frac{dT}{dx} = \frac{\mathrm{v}_x^2}{\rho c_P}\frac{d\rho}{dx} - \frac{1}{\mathrm{v}_x \rho c_P}\sum_{i=1}^{N} h_i \dot{\omega}_i M_i \;, \tag{23}$$

$$\frac{dY_i}{dx} = \frac{\dot{\omega}_i M_\mathrm{i}}{\rho \mathrm{v_x}} \;, \tag{24}$$

where x is the axial coordinate, v_x is axial velocity, and ρ is mixture density. In equations (22) and (23) the variables M_mist and P can be written in terms of T, ρ e Y_i. Initial conditions to solve equations (22) through (25) are

$$T(0) = T_0; \quad \rho(0) = \rho_0; \quad Y_\mathrm{i}(0) = Y_{i0},\; i = 1, \dots , N$$

To solve the problem, it is necessary to adopt a method to integrate stiff systems of ordinary differential equations, since chemical reactions have, in general, many different time scales.

Results

Figures (1) and (2) show temperatures, blowout mass rates, CO_2 and NO_2 formation at the flame zone within a combustion chamber, assuming it can be represented by a PSR; and Figs. (3) and (4) show final temperatures, ignition delays, CO_2 and NO_2 formation after the flame zone, assuming it can be represented by a PFR.

Five different mechanisms were tested in the simulations: I) KON: mechanism with Konnov steps; II) GRI: mechanism with GRIMech steps; III) TB1: mechanism with steps from Tab. 1; IV) VPS: mechanism with global reaction Eq. (1) and variable properties using data from CHEMKIN 3.5; and V) CPS: mechanism with global reaction Eq. (1) and constant properties.

The PSR volume used was 67.4 cm^3 and the mass flux was 7 g/s, corresponding to a the reaction zone volume, and the PFR diameter was 5.8431 cm and the velocity 2.6815 cm/s, yielding a mass flux of 7 g/s, to simulate the volume and the mass rates in a given internal combustion engine. In all cases the inlet temperature was 1000 K, pressure 1 atm and equivalence ratio ϕ = 0.25, which are typical conditions of flue gases in charcoal gasifiers. Since the global mechanism is fitted for low pressures, all detailed mechanims were compared at 1 atm, despite engines can operate at higher pressures. The total mass flow rate was kept constant, with water vapor added at the same temperature and pressure as the *CO*.

The simulation programs in the CHEMKIN 3.5 collection were utilized for mechanisms I, II, III and IV, while MATLAB 5.0 programs were written for mechanism V. A listing with an example run written in MATLAB 5.0 is presented in Tab. 2, showing the values used in the simulations for case V. As can be seen in Tab. 2, the code is quite simple, since it is assumed a single step reaction and constant properties. The CHEMKIN 3.5 collection contains an extensive data bank with temperature dependent properties and a built-in chemical kinetics solver, being suitable for detailed calculations.

Temperatures and CO_2 production did not present significant variations between 1 and 6 % water content in volume for all PSR models. However a small content of water (< 0.1 %) did not allow ignition of the mixture. In the case of the PFR models I and II, the temperatures and CO_2 production had a consistent decrease with water content increase, from 0 to 6% water content.

All five models presented maximum temperatures at about 3 % of water volume in the PSR. Except by model V, the PSR models have shown a maximum CO_2 production at about 4 % water volume. The detailed models I, II and III in the PFR presented decreasing temperatures and CO_2 production with increasing water content. Model IV presented highest temperature in the PFR with about 3 % volume of water and model V presented temperatures constant above 3 % water content. CO_2 production was identical in both models IV and V in a PFR, with maximum values around 3 % water content.

Table 2. Matlab function to simulate wet CO oxidation in a plug flow reactor.

```
function yp=plug(t,y);
% Wet CO oxidation in PFR with single step reaction and constant
% properties. Input initial concentrations Ci0 (kmol/m3) of reac-
% tants and temperature To(K), then copy the comment lines
below
% in the command window and press [enter] to execute program:
% y0=[Cco0;Ch2o0;Co20;Cco20;Cn20;To];     % comment line 1
% t=[0 0.1]; ode23s('plug',t,y0);                   % comment line 2
hfo2 = 0 ; hfco = -110527*10^3; hfco2=-393522*10^3 ; % J/kmol
Cpco =   36.2776*10^3 ; Cpo2 = 37.8257*10^3;        % J/kmol-K
Cph2o = 51.0059*10^3 ; Cpn2 = 35.9060*10^3 ;       % J/kmol-K
Cpco2 = 60.4053*10^3 ;                                           % J/kmol-K
Ro = 8.314*10^3;  % J/kmol-K; Po = 101.325*10^3;  % N/m^2;
To = 1000; % K;    To1= 298;  % K;     fi = 0.25;
A  = 2.24*10^12;          % ((kmol/m^3)^-0.75)*(1/s);
B  = 5.0*10^8;               % (1/s)
C  = -1.674*10^8;         % J/kmol;          c  = C/Ro;
D = 0.5*Cpo2 + Cpco-Cpco2;     E  = hfco-hfco2-(D*To1);
F = 0.5*Ro+D;  G  = Cpo2-Ro;  H  = Cpco2-Ro;
J  = Cpn2-Ro;    K = Cpco-Ro;  L  = Cph2o-Ro;
yp=[exp(c/y(6))*(B*y(4)-A*y(1)*(y(2)^0.5)*(y(3)^0.25))
0
exp(c/y(6))*(B*y(4)-A*y(1)*(y(2)^0.5)*(y(3)^0.25))/2
-exp(c/y(6))*(B*y(4)-A*y(1)*(y(2)^0.5)*(y(3)^0.25))
0
-exp(c/y(6))*(B*y(4)-A*y(1)*(y(2)^0.5)*(y(3)^0.25))*(E+
F*y(6))/ (y(3)*G+y(5)*J+y(1)*K+y(2)*L+y(4)*H)
];
```

*ode23s is a solver for stiff differential equations

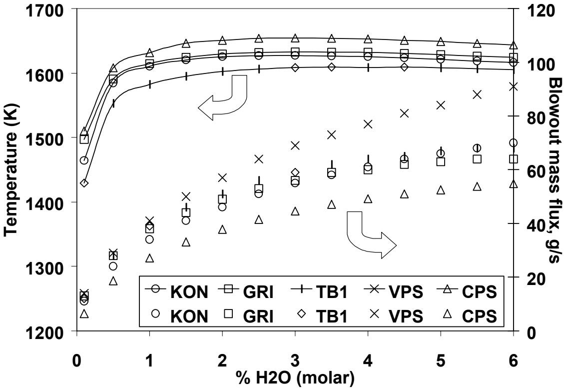

Figure 1. Influence of water vapor molar fraction on temperature, K, and blowout mass flux, g/s, of a perfectly stirred reactor, for several chemical mechanisms. Symbols with lines: temperatures, symbols without lines: blowout mass flux.

The detailed models I and II predicted a much larger *NO* production in a PSR (flame zone) than model III, with peaks at about 0.5 % volume of water, since many more pathways of *NO* formation were considered, besides the Zeldovich mechanism. After this peak there was a continuous decrease of *NO* production with increasing water content for models I and II in a PSR

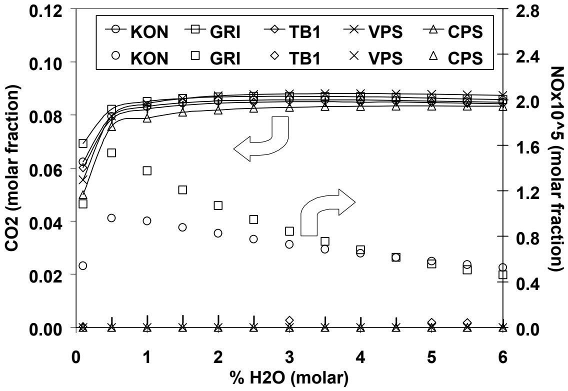

Figure 2. Influence of water vapor molar fraction on CO2 and NO molar fractions of a perfectly stirred reactor, for several chemical mechanisms. Symbols with lines: CO2 molar fraction, symbols without lines: NO molar fraction.

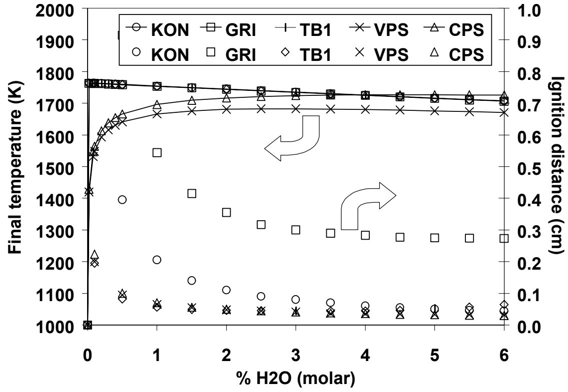

Figure 3. Influence of water vapor molar fraction on final temperature, K, and ignition distance, cm, of a plug flow reactor, for several chemical mechanisms. Symbols with lines: temperatures, symbols without lines: ignition distance.

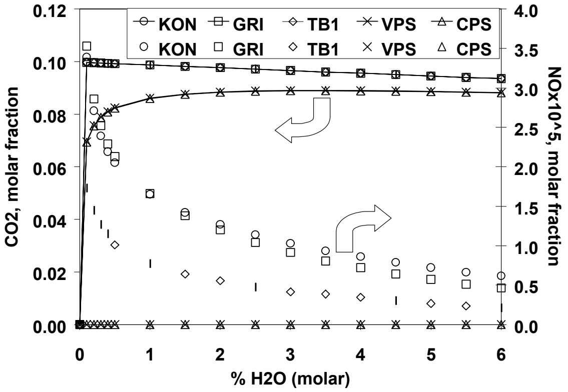

Figure 4. Influence of water vapor molar fraction on *CO_2* and *NO* molar fractions of a plug flow reactor, for several chemical mechanisms. Symbols with lines: *CO_2* molar fraction, symbols without lines: *NO* molar fraction.

The thermal *NO* profiles obtained with mechanism III in a PFR were similar but 50 % lower than the *NO* profiles obtained with mechanisms I and II, indicating that the Zeldovich mechanism does not describe accurately all the *NO* production in the post-flame zone in the case of wet *CO* oxidation. *NO* production presented a continuous decrease with increase of water content. There is no production of *NO* in the simplified models since there is no radical production.

Ignition delays decreased strongly up to 3% water content, with model II (Grimech) presenting values much larger than the other models. Above 3 % water content the ignition delay remained approximately constant for all PFR models.

Blowout mass flow rates presented similar trends for all PSR models, increasing more strongly up to 3 % water content. There were no significant differences among blowout curves of models I, II and III. Model IV presented the largest blowout mass fluxes, 15 % above the detailed models, while model V presented the lowest blowout mass fluxes, 10% below the detailed models, indicating that models IV and V are not appropriate for blowout estimates.

Conclusions

A simplified method was developed to determine the optimum water content in the flue gases of charcoal gasifiers to be used as alternative fuels in the operation gas turbines and engines for power generation.

Numerical simulations of perfectly stirred reactors and plug flow reactors with several chemical mechanisms for wet *CO* oxidation were performed to estimate the reaction zone temperature, *NO* and *CO_2* formation, ignition delay and blowout mass flow rate.

A combustion chamber with 67.4 cm^3 volume was considered with reactants entering at 1000 K, 1 atm, $\phi = 0.25$, and mass flow rate of 7 g/s. The water content was varied from 0 to 6 % in volume.

It was verified that the water content in the specified range has a strong influence on ignition delay, blowout mass rate and *NO* formation, but not a significant influence on temperatures and CO_2 production, above 1% water content in volume.

Considering maximum reaction zone temperature, high blowout mass flow rate, low ignition delay and low *NO* production it was found that water contents between 3 and 4 % volume would allow to attain optimum operational conditions in engines and power generators, for the assumed parameters.

The method presented can be applied to any input conditions using detailed mechanisms.

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