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The exergy release mechanism and exergy analysis for coal oxidation in supercritical water atmosphere and a power generation system based on the new technology

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A B S T R A C T

The oxidation environment has important influence on the transformation of the energy contained in fuel and generation of pollutants. To the problem of nearly 50% exergy losses in coal oxidation at air atmosphere, this research intends to change oxidation atmosphere from air to supercritical water/oxidant and achieve efficient release of exergy in coal at about 650 °C with the aid of a high solubility and unique performance of heat and mass transfer of supercritical water. Therefore, firstly, based on the exergy analysis theory and the energy-utilization diagrams, the release mechanism of exergy of coal in supercritical water oxidation process is revealed. It is pointed out that supercritical water oxidation has changed the release pathways of chemical exergy, and decreased the level difference between chemical exergy and thermal energy, and more exergy is released. Meanwhile, there is also no exergy loss of physical heat transfer. As a result, supercritical water oxidation has higher exergy efficiency than conventional oxidation. Secondly, the exergy losses, level difference between chemical exergy and thermal energy as well as exergy efficiency, are quantitatively investigated. Results show that the exergy efficiency of supercritical water oxidation reactor may be as high as 80.1% and has increased by 27% relative to conventional boilers. Thirdly, based on supercritical water oxidation of coal, a concept power generation system is constructed. Exergy efficiency is calculated and exergy analysis is provided for the supercritical water oxidation power plant. Compared with conventional power plant, exergy efficiency in supercritical water oxidation plant reaches as high as 61.3% and 21% higher than that in conventional power plant. Finally, from the results obtained, it is believed that the commercial breakthrough of the supercritical water oxidation process will be possible when the corrosion and salt deposition in the reactor are solved.

1. Introduction

Coal is likely to be one of the main sources of primary energy for the next several decades based on its relatively low price compared with other fossil fuels and the largest proven resources in the world [1]. In the last decade China's coal consumption expanded by 135% and will remain the largest coal consumer [2]. However, in the conventional oxidation of coal, a large air surplus above the stoichiometric quantity is required, thus the efficiency decreases, and nearly 50% exergy of coal is lost [3]. Furthermore, forming NO_x and SO_2 polluted environment heavily [4]. Therefore, it is imperative to develop the new technology of clean and efficient utilization of coal. So far new technologies are being developed and conventional technologies are improved to obtain greater efficiencies and to control the emissions of toxic gases. Some examples include: oxidation in fluidized bed, pulverised coal combustion and use of SCW [5]. Among them, the study of coal oxidation in SCW is a hot topic for scholars in recent years.

SCW, which is water above critical temperature (374.0 °C) and critical pressure (22.1 MPa), it has unique properties and environmentally benignity [6]. Compared with normal water, SCW has the following behaviors:

(i) High heat capacity: owing to special temperature and pressure (such as 650 °C and 25 MPa), SCW has high heat capacity, and it is very suitable for energy recovery [7].
(ii) High solubility: due to the reduction of the number of hydrogen bond and the low dielectric constant of SCW, it becomes a nonpolar solvent [8]. So when organic com-

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Nomenclature

SCW	Supercritical Water	PIC	Physical Incomplete Combustion
SCWO	Supercritical Water Oxidation	GIC	Chemical Incomplete Combustion
EUDs	Energy Utilization Diagrams	HD	Heat Dissipation
TOT	Total Exergy	LGH	Leakage Gas Heat
PH	Physical Exergy	HT	Heat Transfer
CH	Chemical Exergy		
IC	Irreversible Combustion		
FG	Flue Gas		

pounds and gas are dissolved in SCW, they are immediately brought into intimate molecular contact in a single homogenous phase without interfacial transport limitations [9].

(iii) High diffusivities: because of the low viscosity, the SCW molecules and the solute molecules have high molecular mobility, therefore, it is easy to diffuse in SCW [10].

In addition, SCW has other features which can be found elsewhere, therefore, there is no longer much discussed. So, the following is the introduction of supercritical water oxidation (SCWO) technology.

Compared with traditional oxidation methods, SCWO is a clean and effective new technology. The kinetics is fast and the complete oxidation time was less than 1 min [11]. The products of hydrocarbon in SCWO process are carbon dioxide and water. Heteroatoms are converted into inorganic compounds, usually acids, salts or oxides in high oxidation state. Phosphorous is converted into phosphate and sulphur to sulphate. Meanwhile, a high density of the reaction medium intensifies the combined interaction of water with carbon and suppresses ash and tar formation, which is observed during decomposition of heavy organic substances in gaseous medium. The relatively low temperature of SCWO conversion impedes formation of NO_x and SO_x, and closeness of this system excludes emissions of fine ashes [12].

At present, the research on the application of SCWO is mainly focused on the following two types: waste treatment and energy recovery.

Waste treatment: the main application of the SCWO is the disposal of wastewaters and sludges [13]. Gong et al. investigated the influence of temperature, time, water density and oxidation coefficient on the supercritical water oxidation reaction of quinazoline and related reaction products in batch reactors [14]. Xu et al. studied the SCWO of a pesticide wastewater under a wide range of operation conditions in two reaction plants [15]. There are many studies about waste treatment in SCWO, the paper is no longer to repeat.

Energy recovery: many theoretical study points out that the SCWO process would be much more efficient if its energy could be recovered as work based on recovering the heat released by waste oxidation and generating steam [16]. Bermejo et al. performed a SCWO of coal for theoretical study of power generation plant using a transpiring wall reactor and the efficiency is 37% and it will increase to 40% when there is an extra intermediate reheating process [5]. Franco Donatini et al. presented a SCWO of coal for power generation system with pure oxygen, and the gross and net thermodynamic efficiencies have been estimated to be about 44% and 28%, respectively [17].

To the best of our knowledge, there have been almost little reports on the exergy release mechanism and exergy analysis for SCWO of coal so far. In this manuscript, an efficient release mechanism of exergy of coal in SCWO atmosphere and a new concept power generation system based on SCWO of coal are presented. Five sections are included. In Section 2, main parameters and factors affecting SCWO of coal are analyzed and determined; In Section 3, the calculation principle of exergy efficiency is present; In Section 4, an efficient release mechanism of exergy of coal in SCWO process is disclosed and exergy efficiency is analyzed quantitatively. In Section 5, a SCWO power plant is constructed and described, and its theoretical exergy efficiency is calculated, and the comparison of exergy efficiency between SCWO power plant and conventional power plant is discussed in detail. At the end, some conclusions and remarks highlighting some further research tasks are reported in Section 6.

2. The determination and selection of main parameters and factors affecting SCWO of coal

The effect of coal oxidation in SCW is influenced by various factors, such as reaction temperature, pressure, residence time, feed concentration, combustion environment, heating rate, coal types, and the structure of reactors. The major factors will be analyzed as follows:

Reaction temperature: coal oxidation reaction in SCW includes two parallel processes: gasification by water and oxidation by oxygen [18]. According to authors preliminary study in Fig. 1 [19], reaction temperature has an important role on gasification performance of organic compounds in SCW. As suggested by the authors' research results on biomass gasification, high temperature favors gasification of biomass. There is, however, a limit to higher temperature which improves performance. The gasification results improve slowly when the temperature reaches 1000 K (about 727 °C). The appropriate range of temperature is 770–1000 K (about 497–727 °C) in order to obtain hydrogen fuel. In addition, referring to experimental results [20], as temperature increases from 600 °C to 700 °C, gasification efficiency (mass of gaseous product/mass of dry matter in the water-coal-slurry) and hydrogen gasification efficiency (mass of hydrogen gas/the mass of hydrogen in dry matter in the water-coal-slurry) are already greater than 100%, so the reaction temperature is designed for 650 °C in this research.

Reaction pressure: Fig. 2 gives the influence of pressure on glucose gasification in SCW. It can be seen that pressure, from 20 MPa to 35 MPa, has no great effect on the biomass (glucose) gasification [19]. This tendency is also achieved in Hawaii Natural Energy Institute and State Key Laboratory of Multiphase Flow in Power Engineering experiments [22]. So the pressure is designed for 25 MPa, little above water critical pressure 22.1 MPa in this study.

Coal types: the impact of coal compositions on power plant availability and its operating efficiency is uncontested [24]. Among the coal compositions, moisture is one of the important factors corresponding net efficiency of the overall power plant [25]. For example, brown coal is characterized by heterogeneity in chemical composition and physical properties, low caloricity caused by the presence of water, oxygen and mineral components. Hence, they cannot be used for power generation without preliminary prepara-