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Correction to: Beneficiation of coal using supercritical water and carbon dioxide extraction: sulfur removal

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In the original publication, there were few amendments to be made in Section 3.2 Extractive reactions involved. The updated version of the section is provided in this correction.

The original article has been corrected.

3.2 Extractive reactions involved

Water molecule dissociates to form hydrogen ion and hydroxyl ion that both participate in further extraction reactions. At room temperature, the ions are in small concentration, and the dissociation increased with temperature up to about 300 °C, and then, it rapidly drops, as shown in Fig. 1 (Kritzer and Dinjus 2001). Thermal energy promotes the diffusion and reaction of the ions with the elements in the coal matrix.

$$H_2O \rightarrow H^+ + OH^-$$

Carbon dioxide dissolves in water to form carbonic acid following the reaction below:

$$CO_2 + H_2O \rightarrow H_2CO_3$$

$$H_2CO_3 \rightarrow HCO_3^- + H^+$$

$$HCO_3^- + OH^- \rightarrow CO_3^{2-} + H_2O$$

Carbonic acid can then react to dissolve metals into solution or to form carbonate salts. (M = Ca, Mg, etc.)

$$CO_3^{2-} + M^{2+}_{(mineral)} \rightarrow MCO_{3\,(s)}$$

$$MCO_{3\,(s)} + H_2CO_3 \rightleftharpoons M^{2+}_{(aq)} + 2HCO_3^-$$

$$MCO_{3\,(s)} + \text{heat} \rightarrow MO + CO_2$$

The CO_2–H_2O mixture is acidic which will help to break down complex mineral structure and provide access to metal ions. Many complex reactions have been hypothesized regarding the specific forms of sulfur. Although this paper does not attempt to study these reactions, a comprehensive analysis of the reaction network can further help understand the molecular mechanism involved so that a rational design for industrial level extraction plants can be made.

For pyrite, iron and sulfur can react with various forms of hydrogen, carbonate, and oxygen ions to ultimately form iron, iron sulfates, sulfur dioxide, and hydrogen sulfide. Pyrite can also be converted into sulfate. Reactive sulfur species COS may also be formed, via a network of reactions as

$$FeS + H_2CO_3 \rightarrow FeCO_3 + H_2S$$

$$SO_2 + H_2O \rightleftharpoons H_2SO_3$$

$$SO_2 + 2H_2O \rightleftharpoons H_2 + H_2SO_4$$

$$4SO_2 + 4H_2O \rightleftharpoons 3H_2SO_4 + H_2S$$

The original article can be found online at https://doi.org/10.1007/s40789-020-00324-1.

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$$H_2S + CO \rightarrow COS + H_2$$

$$H_2S + CO_2 \rightarrow COS + H_2O$$

Organic sulfur is found in coal as mercaptans (RSH), disulfides (RS-S-R'), sulfides (R-S-R'), and thiophenes (heterocyclic). Organic sulfur is thus integrated into the carbon structure and difficult to remove. Oxidative ions convert organic sulfur to sulfates which can be dissolved in water or form sulfur dioxide.

$$RSH + H_2O \rightarrow ROH + H_2S$$

$$RSH + CO_2 \rightarrow ROH + COS$$

Interaction of fluid with the coal may also cause lower organics to liquefy or gasify to produce carbon dioxide, hydrogen gas, or methane. More complex studies of the reactions involved can be found in other recent studies (Morimoto et al. 2008; Tian et al. 2016; Zhang et al. 2018).