Archives of Occupational Health | Volume 5 | Issue 1 | January 2021 | 954-60.

Original

Modeling and Investigating the Production of Carbon Dioxide Gas Using HSC Software in the Tile Industry

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Abstract

Background: The study of the production and emission of greenhouse gases, including CO2 in the atmosphere, is one of the most important environmental issues and concerns of the international community. This study was conducted to investigate the effect of temperature and furnace fuel concentration changes on CO2 and CO production. **Methods**: In this study, using HSC Chemistry 6 software, the existing reactions for fuels used in the furnace, including CaCO3, MgCO3, Fe2O3, and Fe3O4, were simulated. The concentrations of carbon dioxide and carbon monoxide produced at different temperatures were investigated. **Results**: In the CaCO3 reaction, the temperature has a direct effect on carbon dioxide production but no effect on carbon monoxide production. In the MgCO3 reaction, the temperature has little effect on the production of both, and for the rest of the reactions, the effect of temperature depends on the molar composition and reaction conditions. **Conclusion**: In general, the results show that temperature affects the production of carbon dioxide and monoxide, so the emission of these gases to the environment can be reduced by adjusting the temperature of the furnace reactors.

Keywords: Carbon dioxide; Carbon monoxide; HSC software; Tile industry

Introduction

Greenhouse gases are gases that trap heat in the Earth's atmosphere.[1] The presence of greenhouse gases and their effect on the Earth is necessary because, in the absence of greenhouse gases, the Earth's temperature will drop to -17 degrees Celsius.[2, 3] Before the Industrial Revolution, the amount of greenhouse gas in the atmosphere was low, but with its onset, people's lifestyles changed, and with the growth of population and increasing use of fossil fuels such as oil and coal, as well as the growth of industrial societies, Atmospheric CO2 has risen, causing the Earth's temperature to rise.[2, 4-6] Greenhouse gases cause the sun's low-wavelength radiation to be reflected after passing through the clouds and increasing its wavelength from ultraviolet to infrared. These infrared rays are not dangerous and return to the ground after being hit by greenhouse gases, causing them to heat.[7]

Citation: Nakhjavani Sh, Bidel H, Nakhjavani M, Zavvar H, Momtaz SM, Halvani Gh, et al. **Modeling and Investigating the Production of Carbon Dioxide Gas Using HSC Software in the Tile Industry.** Archives of Occupational Health. 2021; 5(1): 954-60.

Article History: Received: 07 January 2019; Revised:15 May 2019; Accepted: 05 January 2020

[DOI: 10.18502/aoh.v5i1.5268]

According to the Paris Climate Agreement, greenhouse gas emissions should be reduced by 2030 so that global warming does not rise by more than 2 degrees Celsius compared to the start of the Industrial Revolution, but according to the United Nations, reducing emissions is one-third the amount needed to achieve the objectives of this agreement are needed. The United Nations Environment Program, which has been publishing its annual greenhouse gas emissions report since 2010, warned in a recent report that even if the Paris Agreement achieves its goals, global temperatures will rise by more than three degrees by 2100.[8] In its recent annual report, the World Meteorological Organization states that although greenhouse gas emissions have been reduced, CO2 accumulation in the Earth's atmosphere has reached unprecedented levels.[9] The International Committee on Climate Change also predicts that by 2100, atmospheric carbon dioxide levels will reach 590 PPM, which will raise the Earth's temperature to 1.9 degrees Celsius.[10]

The Environmental Protection Agency has also identified the most dangerous greenhouse gases: carbon dioxide, carbon monoxide, methane, nitrous oxide, nitrogen oxides, particulate matter, sulfur dioxide, and sulfur trioxide. Iran is one of the ten greenhouse gas-producing countries with a share of 1.65% of the world's total greenhouse gas emissions, which indicates the existence of environmental crises in the field of controlling the production and emission of greenhouse gases.[2, 11] Although carbon monoxide is a chemical asphyxiant gas that combines with hemoglobin in the blood, carbon dioxide is a simple asphyxiant gas that does not combine with hemoglobin in the blood and causes asphyxia by substituting oxygen.[12, 13] Carbon dioxide is considered an alternative gas and can be dependent on other pollutants in the room. High concentrations can endanger people's occupational health. Breathing carbon dioxide at low concentrations is not a problem, but the high concentration of this gas affects the function of the respiratory system and can damage the nervous system. High concentrations of carbon dioxide in the air also reduce the percentage of oxygen, and with a decrease in oxygen, people will experience nausea, vomiting, loss of consciousness, coma, and even in severe cases, death.[2, 12]

So far, various studies have been conducted to study the production and emission of greenhouse gases in the atmosphere around the world, but these kinds of studies are very limited in Iran. For example, a study by Usubharatana et al. (2006) showed that CO2 is the highest volume of greenhouse gas emissions.[14] HSC software can be used to study the amount of greenhouse gas, including carbon dioxide because HSC is a thermodynamic software whose main job is to simulate and predict the chemical reactions that can occur in any situation.[15, 16] The tile industry is one of the most important industries in Iran, and Iran ranks sixth in the production of ceramic tiles in the world, and Yazd provides one-third of the country's ceramic tiles. Due to the nature of the industry and the process of tile production, exposure to dust and particulate contaminants in these industries has been reported more than allowed.[17, 18] Also, the soil of the mines around Yazd is rich in carbon; thus, all the products of the factory lead to the production of carbon dioxide gas. Therefore, it is important to pay attention to the production of this pollutant, considering its adverse effects on human health. This study aimed to investigate the production of carbon dioxide at different temperatures using different furnace fuels from the perspective of occupational health.

Methods

In this study the HSC Chemistry 6 software was used to simulate and accurately study the changes in the reactions leading to the production of carbon dioxide and carbon monoxide. This software is used for thermodynamic calculations such as Gibbs free energy and fuzzy equilibrium diagrams of reactions. The Gibbs minimum free energy method was used to determine

[DOI: 10.18502/aoh.v5i1.5268]

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the equilibrium composition.[19] To ensure the accuracy of the model and its validation, some chemical equations from previously published articles were modeled with software and compared with the obtained results.[20] Gibbs free energy is a thermodynamic quantity that determines whether or not a chemical reaction occurs, which is denoted by ΔG (kJ) and can be defined as follows:

$\Delta G = H - TS$ (1)

Where H is the enthalpy, S is the entropy, and T is the temperature in Kelvin.[19, 21] According to the theory and research background, the amount of greenhouse gas produced in ceramic tile factories is a function of four independent variables: fuel type, temperature, oxygen concentration, and the amount of carbon in the fuel used. After field investigations, it was found that the oxygen concentration data in the factory could not be calculated, and this variable is unusable; therefore, the study was performed with the remaining three independent variables. Then, the type of fuel was investigated, and the concentrations were determined. If it is impossible to access the required values, predefined data can be used according to the type of reaction to perform chemical reactions. In the plant understudy, a total of six reactions inside the furnace resulted in the production of CO2, whose raw materials (fuel) were Fe2O3, Fe3O4, CaCO3, and MgCO3. The reactions are shown below:

CaCO3 = CaO + CO2 (2)

MgCO3 = MgO + CO2 (3)

3Fe2O3 + C = 2Fe3O4 + CO (4)

Fe2O3 + CO = 2FeO + CO2 (5)

Fe3O4 + C = 3FeO + CO (6)

Fe3O4 + CO = 3FeO + CO2 (7)

Specific concentrations of furnace fuels, including Fe3O4, Fe2O3, CaCO3, and MgCO3, were entered into HSC Chemistry 6 software. The amounts of carbon dioxide and carbon monoxide produced during each reaction was investigated at a molar ratio of 0.1 kM of fuel at different temperatures and concentrations. In this research, using the equations of the mentioned software, the conversion of fuel into energy and product, and the amount of carbon dioxide and carbon monoxide produced during each reaction was calculated.

Results

In each reaction, the raw material (fuel) with an initial concentration of 0.1 kM was injected into the furnace, and with the passage of time and increase in temperature during the reaction, the number of products produced and carbon monoxide and carbon dioxide was also investigated. However, some reactions may not produce carbon dioxide or carbon monoxide. In all shapes, the X-axis is the temperature in degrees Celsius, and the Y-axis is the concentration change in kM. Figure 1 shows the molar variations of calcium carbonate over temperature. According to the figure, at a temperature of 820-850 ° C, the amount of calcium carbonate reaches half of its initial amount, and the amount of carbon dioxide production increases sharply.

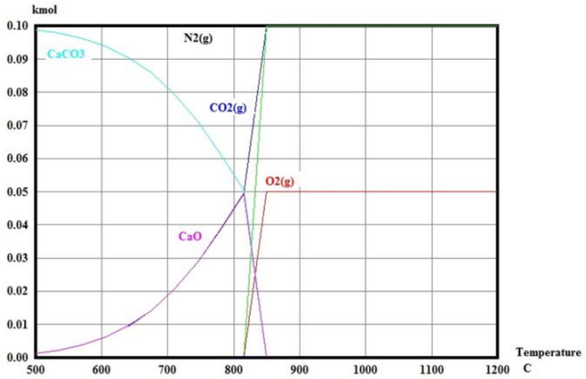

Figure 1. Molar changes of calcium carbonate by temperature. Injecting 0.1 kM of calcium carbonate into the furnace (Reaction 2)

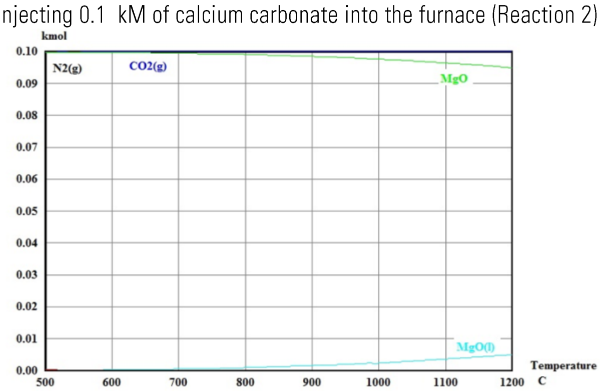

Figure 2. Molar changes of MgCO3 by temperature. Injecting 0.1 kM of MgCO3 into the furnace (R3)

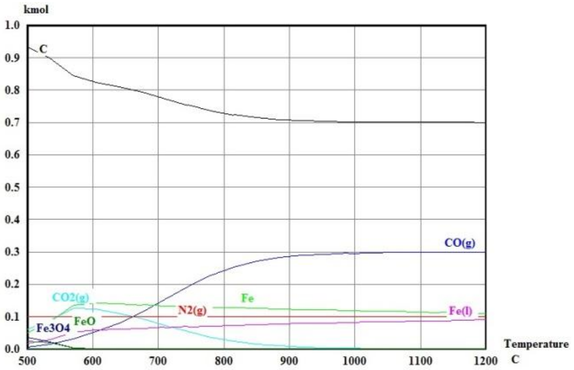

Figure 2. Molar changes of Fe2O3 in terms of temperature by injecting 0.1 kM Fe2O3 and 1 kM Carbon into the furnace (R4)

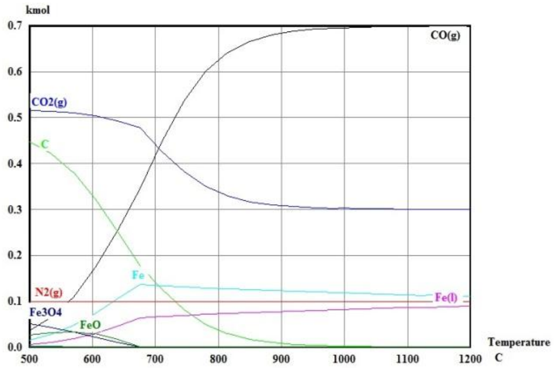

Figure 4. Molar changes of Fe2O3 by temperature. Injecting 0.1 kM Fe2O3 and 1 kM Carbon monoxide into the furnace (R5)

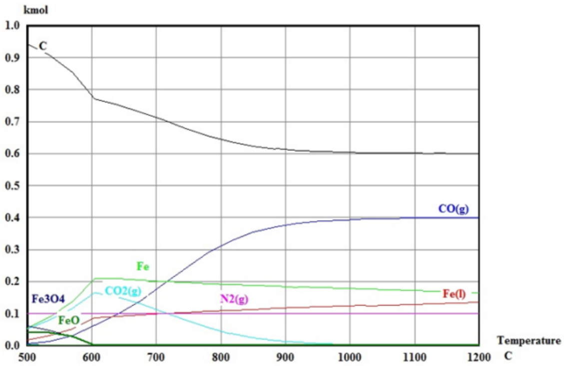

Figure 5. Molar changes of Fe3O4 by temperature. Injecting 0.1 kM Fe3O4 and 1 kM Carbon into the furnace (R6)

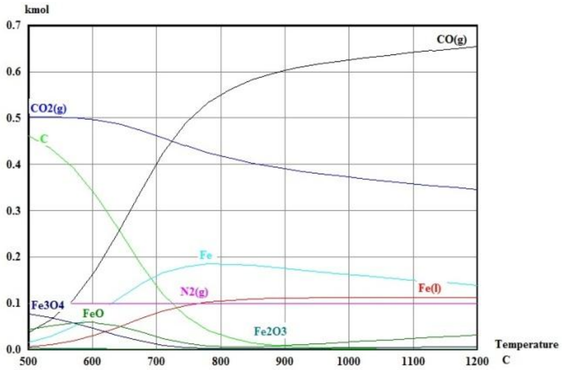

Figure 3. Molar changes of Fe3O4 by temperature. Injecting 0.1 kM Fe3O4 and 1 kM Carbon monoxide into the furnace (R7)

Figure 2 shows the decomposition of MgCO3 by temperature. As can be seen, at the initial temperatures of the furnace, the raw material used, and the concentration of carbon dioxide change slightly linearly until the end of the reaction.

Figure 3 shows the molar variations of Fe2O3 in the presence of carbon over temperature. As can be seen, at 1000 ° C, the increase in carbon monoxide production stops, and after that, the increase in temperature will not affect its concentration, while carbon dioxide reaches its maximum at 580 degrees.

Figure 4 shows the molar changes of Fe2O3 in the presence of one kM of carbon monoxide over temperature. As can be seen at 1000 ° C, the upward trend in carbon monoxide production and the downward trend in carbon dioxide production stop and then stabilize.

Figure 5 shows the molar variations of Fe3O4 in the presence of carbon over temperature. Based on the figure, it can be seen that increasing the temperature to 1000 ° C increases the production of carbon monoxide. Carbon dioxide peaks at 600 degrees.

Figure 6 shows the molar variations of Fe3O4 in the presence of one kM of carbon monoxide over temperature. As can be seen, carbon monoxide is increasingly produced up to 1200 ° C, while the production of crane dioxide from the temperature of 600 degrees onwards has a decreasing trend.

Discussion

This study was conducted to investigate carbon dioxide production in one of the tile industries of Yazd province using HSC Chemistry software. After determining the fuels used in the furnace, the production of carbon dioxide and carbon monoxide was investigated using simulation software at different temperatures and based on a specific concentration of fuel. According to Figure 1, during the reaction and at all concentrations of calcium carbonate, the amount of calcium oxide gradually increases from 500 to 820°C, and at 850°C, carbon dioxide production increases sharply, and calcium carbonate decomposes

[DOI: 10.18502/aoh.v5i1.5268]

completely. Carbon monoxide is not produced at all. Figure 2 shows the results of the concentration of material leaving the furnace during the magnesium carbonate decomposition reaction at different temperatures. At all concentrations of magnesium carbonate at 500 to 510°C, the molecular bonds are completely broken. The concentration of carbon dioxide is linearly maintained until the end of the reaction, and the change in concentration is very slight under the influence of temperature. This reaction does not produce carbon monoxide.

The effect of temperature on materials concentration of leaving the furnace during the reaction of Fe2O3 and carbon in Figshows3 show that at a 0.1 molar ratio of Fe2O3 and 1M of carbon, the temperature has a direct effect on the production of carbon dioxide and carbon monoxide. As the temperature rises to 1000 degrees, the carbon monoxide production increases sharply, and after that, the temperature increase will not affect its concentration. Carbon dioxide reaches its maximum at 580 degrees Celsius, and with further increase in temperature due to the decomposition of this gas, the amount of carbon dioxide decreases, and with the reaction of carbon and oxygen, the amount of carbon monoxide increases again. However, for the molar ratio of 4 kM or more of fuel, the simulation showed that with increasing temperature, the concentration of carbon dioxide was not a function of temperature at all, and the concentration of carbon monoxide gradually increased to a small amount and was not a function of temperature. So at a temperature of 580 degrees and the above molar ratio, the concentration of carbon dioxide is about 0.8 kM and remains constant until the end of the system, and at the same temperature, the amount of carbon monoxide is 0.1 kM. The same behavior was observed for higher concentrations.

The results of calculations during the reaction of Fe2O3 and carbon monoxide, according to Figure 4, show that for the molar ratio of 0.1 Fe2O3 and carbon monoxide, temperature directly affects the concentration of carbon dioxide and carbon monoxide. A rise in temperature to 1000 degrees causes a sharp increase in carbon monoxide production, and then an increase in temperature will not affect its concentration, while carbon dioxide concentration has dropped dramatically to that temperature. However, for molar ratios of 4 and more, the simulation showed that carbon monoxide was completely removed from the reaction and that as the temperature increased, the concentration of carbon dioxide was not a function of temperature at all; as at 500 degrees, the concentration of carbon dioxide is one kM and remains constant until the end of the system.

Figure 5 shows that for the molar ratio of 0.1 Fe3O4 with carbon, the direct effect of temperature on carbon dioxide and carbon monoxide is observed. As the temperature rises to 1100 degrees, it causes a sharp increase in carbon monoxide production and will not affect its concentration. While carbon dioxide reaches its maximum at 600°C and decreases further with increasing temperature due to decomposition, the amount of carbon dioxide decreases, and with the reaction of carbon and oxygen, the amount of carbon monoxide increases again. However, for molar ratios of 4 and more, the concentrations of carbon dioxide and carbon monoxide gradually increase slightly from 680°C and are no longer a function of temperature. At a molar ratio of 10, the concentration of carbon dioxide is about 0.9 kM and has remained constant from 540°C until the end of the system, and in the whole reaction, the amount of carbon monoxide is about zero. The same behavior is observed for higher concentrations, and carbon monoxide is removed from the system.

During the reaction of Fe3O4 and carbon monoxide, as shown in Figure 6, the temperature has a direct effect on the carbon dioxide and carbon monoxide concentration. As the increase in temperature to 1200 degrees causes a sharp increase in

[DOI: 10.18502/aoh.v5i1.5268]

carbon monoxide production and carbon dioxide at a temperature of 500 to 600 degrees is almost unchanged and decreases to a temperature of 1200 degrees. At equal molar ratios, carbon dioxide increases in concentration up to 600°C and then reaches a constant concentration of up to 750°C, which is no longer affected by temperature. Carbon monoxide also increases in concentration up to the same temperature, and then the temperature does no effect on its concentration. However, at a molar ratio of 4, carbon monoxide and carbon dioxide increase in concentration up to 600°C, after which increasing the temperature does not affect the concentration of these two gases. The simulation showed that in the molar ratio of 7 and more, with increasing temperature, the concentration of carbon dioxide increases to a certain temperature, and then it is not affected by temperature. Carbon monoxide is gradually removed from the system completely.

Due to the increase or decrease in the production of pollutants due to the reactions of the fuels used, it can be concluded that the production of carbon dioxide compared to carbon monoxide occurs at lower furnace temperatures. The reaction of Fe2O3 and carbon is more dangerous than other reactions due to the low temperature to reach the maximum concentration of carbon dioxide and carbon monoxide. However, it should be noted that in the magnesium carbonate reaction, the production of carbon dioxide continues linearly from the initial moments of the reaction and continues with the consumption of magnesium carbonate up to 1200 degrees. The reaction of calcium carbonate, which is the maximum concentration of carbon dioxide at 850°C, should also be considered. The production of carbon dioxide and carbon monoxide in reactions of iron with carbon or carbon monoxide occurs at almost the same temperature range that can be used to control pollutant emissions. In a general view, in all reactions between the temperatures of approximately 500 to 1200 degrees, the concentration of contaminants produced increases, and at higher temperatures, the concentration is not affected by the reaction temperature.

Conclusion

Carbon dioxide and carbon monoxide have adverse effects on human health. The tile industry is one of the industries that, due to the nature of work and the large volume of products, and the widespread use of furnaces and fuels, is a good platform for producing and releasing these pollutants. Considering the mentioned temperatures at which carbon dioxide or carbon monoxide production has started or increased, it can be concluded that to control the production and emission of carbon dioxide and carbon monoxide from the furnaces, setting the furnace temperature is the best action. Also, by prioritizing the use of fuels, the least hazardous fuels can be used, or alternative fuels with lower hazard levels and the production of less harmful products can be used. It will also be useful to replace other types of furnaces. The strength of this study is to investigate the production of carbon dioxide and carbon monoxide pollutants due to the consumption of furnace fuels from the perspective of occupational health and propose control measures. The limitation of the study is the limited access to information. Future studies are recommended considering the adverse effects on safety, toxicity effects, and in general, the occupational health effects of pollutants produced in the workplace.

Conflict of interest statement

There is no conflict of interest between the authors.

Acknowledgments

The authors would like to express their gratitude to the esteemed employees and officials of the industry under study. This study with the code of ethics IR.SSU.SPH.REC.1396.157 is approved by the Research Council of Shahid Sadoughi University of Medical Sciences, Yazd.

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[DOI: 10.18502/aoh.v5i1.5268]

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[DOI: 10.18502/aoh.v5i1.5268]