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Exergy, can it be used to reflect the environmental issues of a fuel?

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Abstract: Can exergy be used to reflect the environmental issues of a fuel? This article elaborates if and how exergy can be used to reflect the environmental issues of a fuel, and details the processes for some typical fuels. The results show that the exergy method can be well used to reflect the environmental issues of a fuel. The case studies further show that coal samples (1,324.99–1,437.47 kJ/kg) have higher total environmental impacts than the biomass samples (381.02–1,078.81 kJ/kg), and the environmental impacts are mainly contributed by CO₂ (52.72%–99.37%), followed by ash (0.18%–35.93%), SO₂ (0%–11.77%) and NO₂ (0.16%–8.75%).

Keywords: exergy; fuel; environmental issue; coal; biomass.

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1 Introduction

Exergy is defined as the maximum theoretical work when the material or system gets complete thermodynamic equilibrium with the 'dead' environment (Szargut et al., 1988; Dincer and Rosen, 2020). It can well evaluate not only the quantity of an energy but also the quality of the energy (Sciubba and Wall, 2007).

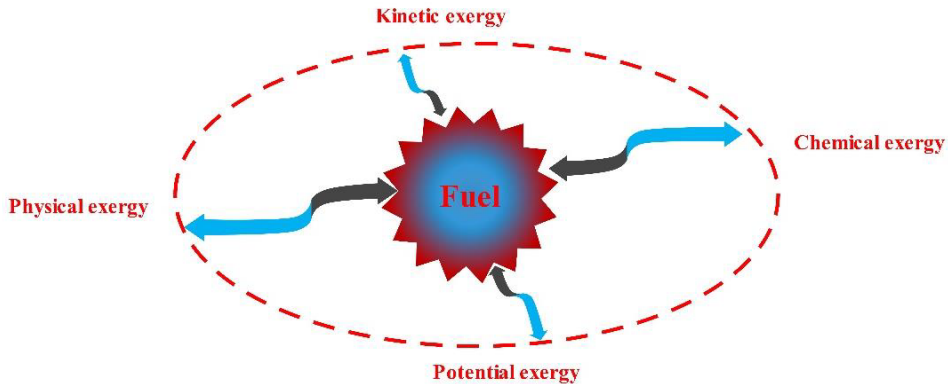
Exergy has been widely used to evaluate/measure the energy qualities of fuels, i.e., the energy resources of fossil fuels (Chen and Chen, 2007), biomass fuels (Zhang et al., 2020), etc. Although there are generally four forms (kinetic, potential, physical, and chemical) of exergy for a fuel (Figure 1), the chemical exergy accounts most of the total energy, it is therefore more meaning than the (total) exergy for a fuel. Therefore, the exergy of a fuel mainly refers to the chemical exergy of the fuel.

For an energy process or system, a fuel is usually used during the process (i.e., decomposition, combustion, etc.) or to drive the system (i.e., boiler, engine, etc.). Because there are generally losses in the energy qualities (even the process or system has no losses in the energy quantities and/or the energy efficiency is 100%) during the process or in the system, exergy can be effectively used to evaluate or diagnose the process/system. On the other hand, if the process or system has no losses in the energy quantities, the energy efficiency is then 100%, and the energy analysis method fails (it can not tell the energy losses or diagnose the process/system). Consequently, exergy analysis method is widely used to evaluate or diagnose the process/system, i.e., biomass drying process, biomass valorisation process, ammonia production process, air separation unit, engine system, power plant system, solar-biomass hybrid system, biogas driven multi-generation system, biomass driven ammonia-water solution cycle, biomass integrated gasification combined cycle (IGCC), etc.

To evaluate or diagnose the energy process/system from an exergy aspect, calculation or estimation of the exergy of the fuel used is very fundamental and important (the first step). Consequently, many scholars proposed or developed various formulae/relationships to calculate or estimate the exergy of fuels, i.e., Shieh and Fan (1982) proposed a formula to estimate the exergy of waste materials based on the element contents and ash contents, Song et al. (2012) developed equations to estimate the exergy of dry biomass involving

the element contents and ash contents, Qian et al. (2017) developed an equation to estimate the exergy of dry biomass involving the element contents, He et al. (2018) proposed neural network method to estimate the standard chemical exergy of fuels, Zhang et al. (2020) proposed relationships to calculate the exergy of woody biomass, wheat straws, oat straws, rice residues (rice husk and rice straw), etc.

Figure 1 Exergy of a fuel (see online version for colours)



Exergy has been widely used to assess or evaluate the properties, processes and systems of a fuel. However, can it be used to reflect the environmental issues of a fuel? Many researchers tried to do work on this. Huijbregts et al. (2006) proposed the fossil cumulative energy demand (CED) as an indicator for the environmental performance of products and processes. Bösch et al. (2007) proposed cumulative exergy demand (CExD) to depict total exergy removal from nature to provide a product by summing up the exergy of all resources required. Dewulf et al. (2008) proposed the extraction of cumulative exergy from the natural environment (CEENE). Zhu et al. (2005) proposed the concept of cumulative exergy consumption (CExC) for the treatment of emissions (CExCT) and equivalent cumulative exergy consumption (ECExC) to analyse the total environmental impact (EI) of industrial processes. Yang and Chen (2014) proposed a series of extended indicators based on exergy to evaluate the sustainability of biogas projects in China. Huang et al. (2022) converted the internal and total exergy loss flows as well as the life-cycle consumed material (including utility) to the values of EI points. Balcom et al. (2021) used an extended exergy analysis (EEA) to quantify the resources used in the disposal process.

Generally, the methods or indicators mainly concentrate on the resources needed or consumed (Huijbregts et al., 2006; Huang et al., 2022), the EUs of pollutions or emissions may not be considered (Bösch et al., 2007; Dewulf et al., 2008), or only the EI of CO₂ was concentrated (Zhu et al., 2005; Yang and Chen, 2014). The above methods may also encounter a problem: how to compare the EIs of different pollutions or emissions which have different exergy values?

The novelty of this work is to clarify and demonstrate how exergy can be used to reflect the environmental issues of a fuel. The specific objectives are:

- a to formulate how exergy can be used to reflect the environmental issues of a fuel
- b to detail the process of using exergy to reflect the environmental issues of some typical fuels (i.e., coal and biomass).

2 Environmental issues of a fuel

The characteristic of a fuel is that it has chemical energy in itself, and the chemical energy is mainly released through combustion. Figure 2 shows the energy release process of a fuel. When a fuel is completely combusted, the products are generally incombustible gases and ash (if the fuel contains ash). The gases are mainly CO_2 , SO_x , NO_x , etc. The ash compositions mainly include oxides, i.e., K_2O , Na_2O , SiO_2 , P_2O_5 , etc. Usually, these emissions may impact the environment through greenhouse effect, ozone depletion, photochemical smog, acid rain, soil compaction, etc.

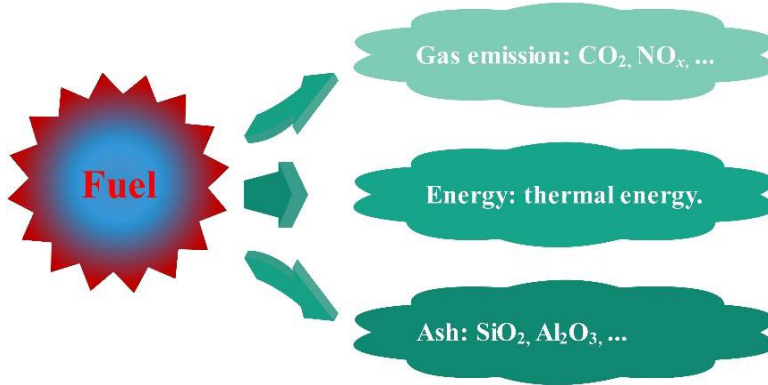
Many methodologies have been adopted to study the EI of emissions, e.g., greenhouse gas (GHG) methodology, life cycle assessment (LCA), etc. Among all the methods, the GHG method is much more intuitive and simpler, and it can be well used to index the EI of a fuel through presenting the amounts of some typical GHG emissions released from the utilisation of the fuel, i.e., CO_2 , CH_4 , etc. However, the method still suffers from some problems:

- a the other gas emissions which may also have environmental effects (i.e., NO_x , SO_2 , and ash) are not considered
- b the method does not have a uniform basis for indexing the EIs of different emissions (i.e., NO_x , SO_2 , and ash).

Then, the EIs of different emissions can not be compared, for example, one can not directly compare the EIs of 1.1 kg of CO_2 and 0.9 kg of SO_2 , because they are not the same emission and they actually have different units or bases for indexing the EIs (i.e., the unit or basis for the EI of CO_2 is mainly greenhouse effect whereas the unit or basis for the EI of SO_2 is mainly acid precipitation). Further, the EIs of different emissions can not be added directly, for example, one can not directly add the EI of 1 kg of CO_2 to the EI of 1 kg of SO_2 . Consequently, if the different fuels release different emissions, the EIs of the different emissions can not be compared, and the EIs of the different fuels can not be compared either. For example, if a coal releases 1 kg of CO_2 , 1 kg of SO_2 and 1 kg of ash whereas a biomass releases 1.1 kg of CO_2 , 0.9 kg of SO_2 and 1 kg of ash, what are the EIs of the two fuels? How can we compare the EIs of the two fuels? The difficulties mainly come from the facts that:

- a the released CO_2 and SO_2 have different units or bases for the EIs
- b the coal ash and biomass ash may have different units or bases for the EIs (the coal ash and biomass ash may have different types and concentrations of compositions).

These are fundamentally due to the fact that the GHG methodology does not have the same basis for indexing the EIs of different emissions [i.e., CO_2 , NO_x , SO_2 , and ash compositions (i.e., Al_2O_3 , K_2O , Na_2O , MnO , SiO_2 , etc.)].

Figure 2 Energy release process of a fuel (see online version for colours)

3 Environmental issues of a fuel through exergy

Exergy can be used as a measure of the difference between the fuel and the environment, and more difference indicates higher EI (Liu and Li, 2015). Because the EI of a fuel is mainly from the EIs of the emissions from the fuel, the EI of the fuel can therefore be represented by the EIs of the emissions from the fuel (Zhu et al., 2005). For a complete conversion or utilisation of a fuel, its EIs are mainly from its products, and the products are mainly gas emissions and ash components. The EI of a fuel is therefore calculated based on the EIs of the gas emissions and ash components from the fuel.

The EI of a fuel can be presented by:

$$EI = EI_{\text{Gas}} + EI_{\text{Ash}} \quad (1)$$

where

EI is (total) environmental impact of fuel.

EI_{gas} and EI_{Ash} are the EIs of emission gases and ash, respectively.

The EI of emission gases (EI_{Gas}) can be calculated through:

$$EI_{\text{Gas}} = \sum m_i ex_i \quad (2)$$

where

i is the emission gas i

m_i and ex_i are the mass and chemical exergy of i , respectively.

The chemical exergy values of some gases are shown in Table 1.

The EI of ash (EI_{Ash}) can be calculated through:

$$EI_{\text{Ash}} = \sum m_j ex_j \quad (3)$$

where

j is the ash component j

m_j and ex_j are the mass and chemical exergy of i , respectively.

The chemical exergy values of the ash components are shown in Table 1.

Table 1 Standard chemical exergy of emission gases and mineral oxides

<i>Material</i>	<i>Standard chemical exergy (kJ/mol)</i>
Emission gases	
CO ₂	19.87
NO ₂	55.60
SO ₂	313.40
Ash components	
SiO ₂	7.90
K ₂ O	413.10
CaO	110.20
P ₂ O ₅	412.65
MgO	66.80
Al ₂ O ₃	200.40
Fe ₂ O ₃	16.50
Na ₂ O	296.20
SO ₃	249.10

Source: Szargut et al. (1988)

When the fuel is completely combusted and the emissions are theoretically mainly CO₂, NO_x, SO₂, Al₂O₃, K₂O, Na₂O, MnO, SiO₂, etc. Based on these emissions, the EI of a fuel can be well obtained though using the equations presented above. However, the practical application processes (i.e., combustion, pyrolysis, gasification, etc.) are significantly varied by many factors (i.e., reaction temperature, processing time, chamber type, etc.), the products and emissions may be significantly varied accordingly. For example, if the fuel is partially combusted (actually, it is gasification), CO, CH₄ and H₂ may be produced. Then shall we calculate the chemical exergy values of CO, CH₄ and H₂ and then sum them up to assess the EI of the fuel? Actually, no! Because CO, CH₄ and H₂ are combustible gases, the chemical exergy values of CO, CH₄ and H₂ are also the energy potentials. In this case, the chemical exergy values of CO, CH₄ and H₂ indicate the energy potentials (qualities) of the CO, CH₄ and H₂ gases during the particular process, respectively. The summed (total) chemical exergy values of all the useful products (i.e., CO, CH₄, H₂ etc.) indicate the energy potential of the particular process. Still, some emissions or pollutions (i.e., CO₂, NO_x, SO₂, Al₂O₃, K₂O, Na₂O, MnO, SiO₂, etc.) may be generated during the particular process, then the summed (total) chemical exergy values of all these emissions or pollutions indicate the EI of the particular process (but not the fuel).

4 Case studies

In this section, 12 fuel samples are selected to detail the process of using exergy to reflect the environmental issues of some typical fuels, and these include three coal samples, four wheat straw samples, and five wood samples. The details are shown in Table 2. Table 3 presents the C, N, S, and ash contents of coals and biomass on as received basis. Table 4 shows the ash compositions of coals and biomass on as received basis. Based on these data, the environmental impacts of coals and biomass are compared and presented.

Table 2 Samples of coals and biomass

<i>Fuel</i>	<i>Detail</i>
Coal 1	Xiaolongtan
Coal 2	Huolinhe
Coal 3	Yangquan
Wheat straw 1	Max
Wheat straw 2	Absolvant
Wheat straw 3	Monopol
Wheat straw 4	Vuka
Wood 1	Pine
Wood 2	Cytisus
Wood 3	Christmas tree
Wood 4	Oak
Wood 5	Pepper

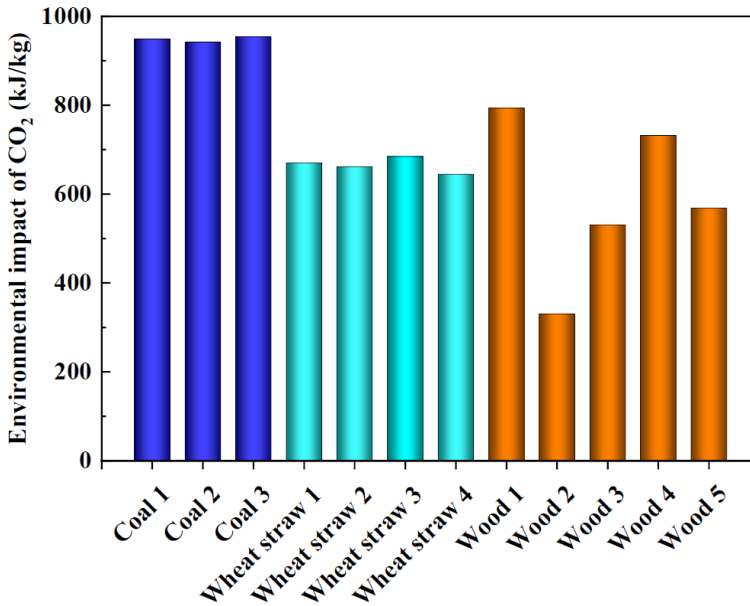
Source: Zhang et al. (2020)

Table 3 C, N, S, and ash contents of coals and biomass on as received basis

<i>Fuel</i>	<i>C content (wt.%)</i>	<i>N content (wt.%)</i>	<i>S content (wt.%)</i>	<i>Ash content (wt.%)</i>
Coal 1	57.35	1.70	1.47	8.25
Coal 2	56.95	0.84	1.60	14.45
Coal 3	57.64	2.24	0.77	25.67
Wheat straw 1	40.52	0.73	0.07	3.17
Wheat straw 2	39.99	0.30	0.10	2.69
Wheat straw 3	41.37	0.50	0.11	3.23
Wheat straw 4	38.95	1.02	0.11	4.23
Wood 1	47.94	0.09	0	0.09
Wood 2	19.93	0.84	0.04	0.56
Wood 3	32.08	0.32	0.25	3.24
Wood 4	44.24	0.03	0.01	0.27
Wood 5	34.38	2.1	0.4	18.10

Table 4 Ash compositions of coals and biomass on as received basis

<i>Fuel</i>	<i>Composition (mol/kg)</i>								
	<i>SiO₂</i>	<i>K₂O</i>	<i>CaO</i>	<i>P₂O₅</i>	<i>MgO</i>	<i>Al₂O₃</i>	<i>Fe₂O₃</i>	<i>Na₂O</i>	<i>SO₃</i>
Coal 1	0.103	0.001	0.386	0.005	0.103	0.066	0.055	0.028	0.399
Coal 2	1.049	0.014	0.221	0.003	0.133	0.299	0.027	0.033	0.299
Coal 3	1.951	0.035	0.195	0.005	0.082	0.714	0.075	0.099	0.346
Wheat straw 1	0.214	0.081	0.064	0.013	0.043	0.003	0.001	0.004	0.006
Wheat straw 2	0.141	0.073	0.072	0.018	0.035	0.001	0.001	0.007	0.008
Wheat straw 3	0.147	0.124	0.062	0.015	0.034	0.002	0.002	0.005	0.010
Wheat straw 4	0.188	0.229	0.064	0.016	0.032	0.003	0.002	0.007	0.011
Wood 1	1.381	1.306	7.489	0	2.927	0.206	0.119	0.039	0
Wood 2	2.763	1.964	1.427	1.360	5.458	0.196	0.119	1.872	0
Wood 3	6.472	0.834	1.694	0.169	0.625	1.446	0.582	0.086	1.419
Wood 4	3.490	2.378	1.944	0.094	1.029	0.293	0.184	0.226	0.336
Wood 5	5.592	1.624	2.354	0.909	2.233	0.382	0.207	1.371	0

Figure 3 Environmental impact of CO₂ (see online version for colours)

4.1 *EI of CO₂*

Figure 3 presents the EIs of CO₂ for the 12 fuel samples. Generally, the coal samples (942.11–953.49 kJ/kg) have higher EIs of CO₂ than the biomass samples (329.73–793.15 kJ/kg). These are because when the C contents in the fuels are completely combusted or

converted, CO₂ emissions are finally produced (theoretically). The coal samples (56.95%–57.64%, Table 3) have higher C contents than the biomass samples (19.93%–47.94%, Table 3), the coal samples (942.11–953.49 kJ/kg) therefore have higher exergy values of CO₂ than the biomass samples (329.73–793.15 kJ/kg), making the coals samples have higher EIs (Zhang et al., 2020).

4.2 EI of NO₂

Figure 4 presents the EIs of NO₂ for the 12 fuel samples. The Coal 3 sample has the highest EI of NO₂ (89.08 kJ/kg) whereas the Wood 4 sample has the lowest EI of NO₂ (1.19 kJ/kg). According to the definition of the EI of gas in equation (2), the EI of gas is determined by the gas content (the chemical exergy of the gas is constant). The EI of NO₂ is therefore determined by the NO₂ content which is fundamentally determined by the N content (theoretically, the N contents in the fuels are converted to NO₂ emissions completely). The Coal 3 sample has the highest N content (2.24 %, Table 3), making it have the highest NO₂ emission and also the highest EI (exergy value) of NO₂ (89.08 kJ/kg, Figure 5) (Zhang et al., 2020). The Wood 4 sample has the lowest N content (0.03 %, Table 3), it therefore has the lowest NO₂ emission and also the lowest EI (exergy value) of NO₂ (1.19 kJ/kg, Figure 5) (Zhang et al., 2020).

Figure 4 Environmental impact of NO₂ (see online version for colours)

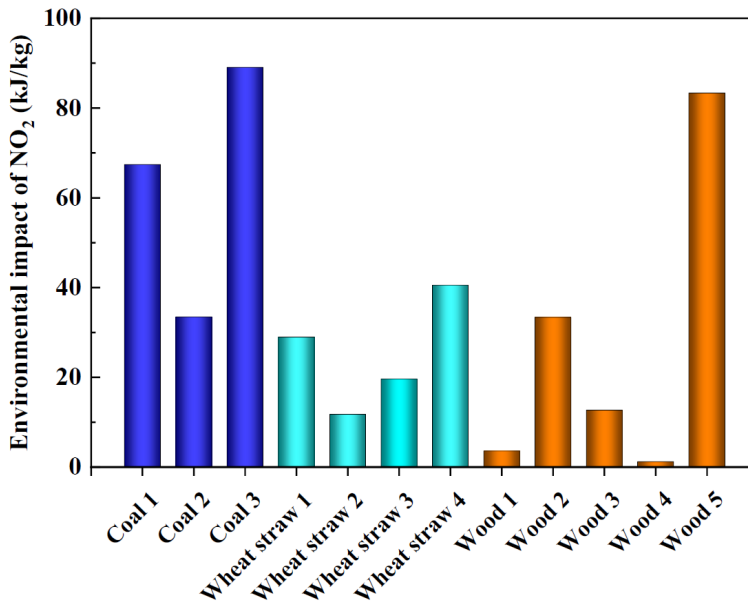


Figure 5 Environmental impact of SO₂ (see online version for colours)

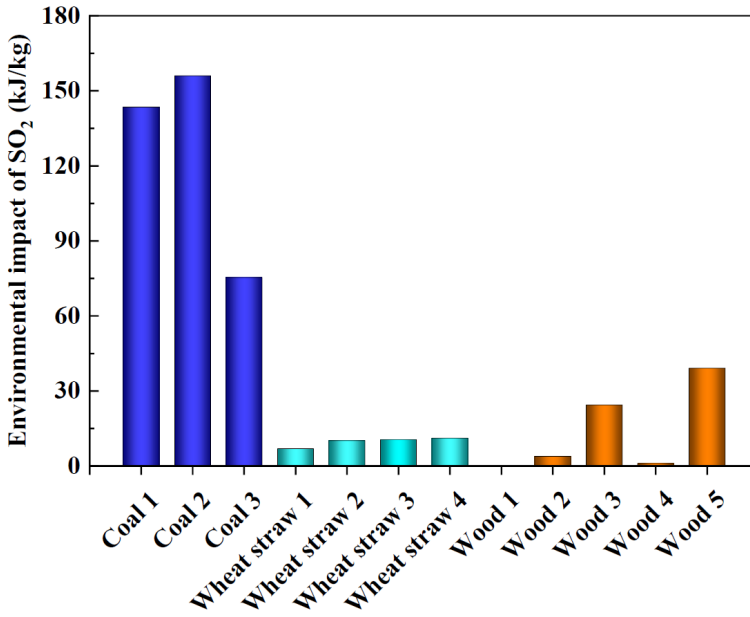
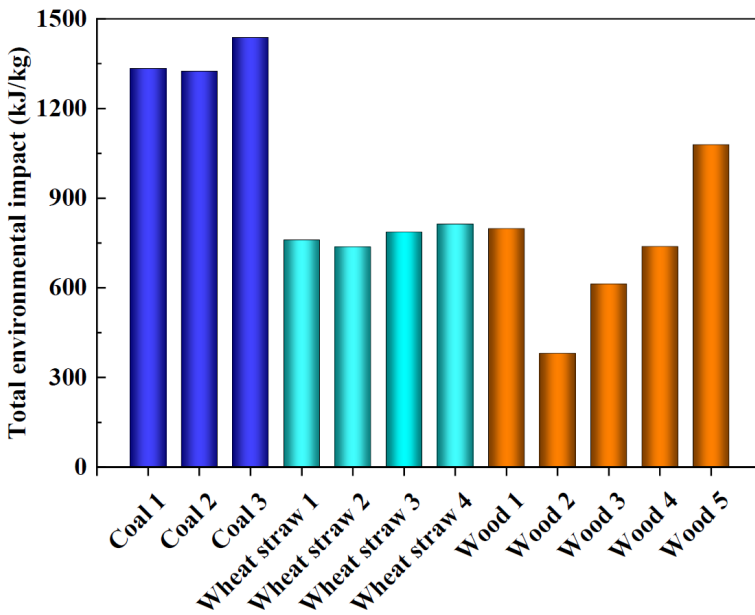


Figure 6 Environmental impact of ash (see online version for colours)



4.3 *EI of SO₂*

Figure 5 presents the EIs of SO₂ for the 12 fuel samples. The Coal 2 sample has the highest EI of SO₂ (156.00 kJ/kg) whereas the Wood 1 sample has the lowest EI of SO₂ (0 kJ/kg). Being similar to the EI of NO₂ as shown in Figure 4, these are due to the facts that the Coal 2 sample has the highest S content (1.60 %, Table 3) whereas the Wood 1 sample has the lowest S content (0%, Table 3). Generally, the coal samples (75.36–156.00 kJ/kg) have higher EIs (exergy values) of SO₂ than the biomass samples (0–39.09 kJ/kg).

4.4 *EI of ash*

Figure 6 shows the EIs of ash for the 12 fuel samples. The Wood 5 sample has the highest EI of ash (387.58 kJ/kg) whereas the Wood 1 sample has the lowest EI of ash (1.46 kJ/kg). According to the definition of EI of ash in equation (3), the EI of ash is calculated based on the ash content and ash compositions (Zhang et al., 2020). The Wood 5 sample has the highest EI (exergy value) of ash (387.58 kJ/kg) is due to the facts that:

- a it has the second highest ash content (18.10 wt.% in Table 3, the highest one is the Wood 3 sample with an ash content of 25.6 wt.%)
- b it has higher ash compositions of K₂O and P₂O₅ (than the Wood 3 sample) which have very high chemical exergy values (in Table 1, K₂O and P₂O₅ have the highest and second highest chemical exergy values, respectively).

However, the Wood 1 sample has the lowest EI (exergy value) of ash (1.46 kJ/kg) is mainly due to its lowest ash content (0.09 wt.% in Table 3).

4.5 *Total EI*

Figure 7 shows the total EIs of the 12 fuel samples. The Coal 3 sample has the highest total EI (1,437.47 kJ/kg) whereas the Wood 2 sample has the lowest total EI (381.02 kJ/kg). According to the definition of total EI of a fuel in equation (1), the total EI of a fuel is determined by the EIs of the emissions of both gases and ashes (Zhang et al., 2020). Generally, the coal samples (1,324.99–1437.47 kJ/kg) have higher exergy values of released gas emissions and ash components than the biomass samples (381.02–1078.81 kJ/kg), the coal samples therefore have higher total EIs than the biomass samples, indicating that biomass fuels are more environmentally friendly.

Because the exergy method is based on a uniform basis, the EIs of all the emissions are also on the same basis. Consequently, the EIs of the different emissions (gas pollutants and ash compositions) can be added and summed. Then, the EIs of different fuels can be obtained and compared.

4.6 *Distribution of EI*

Figure 8 shows the distributions of EI for the 12 fuel samples. The distribution of EI is defined as the EI of a particular emission (CO₂, SO₂, NO₂, or ash) divided by the total EI of the fuel. Generally, the EIs of the 12 fuel samples are mainly contributed by CO₂

(52.72%–99.37%), followed by ash (0.18%–35.93%), SO₂ (0%–11.77%) and NO₂ (0.16%–8.75%).

Figure 7 Total environmental impact (see online version for colours)

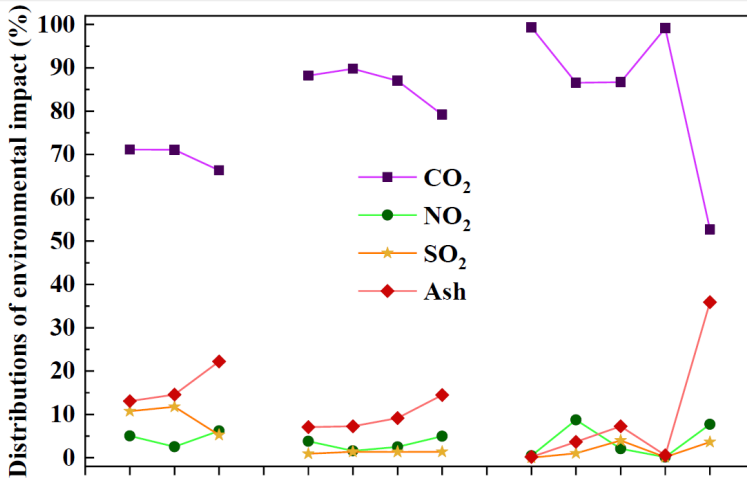
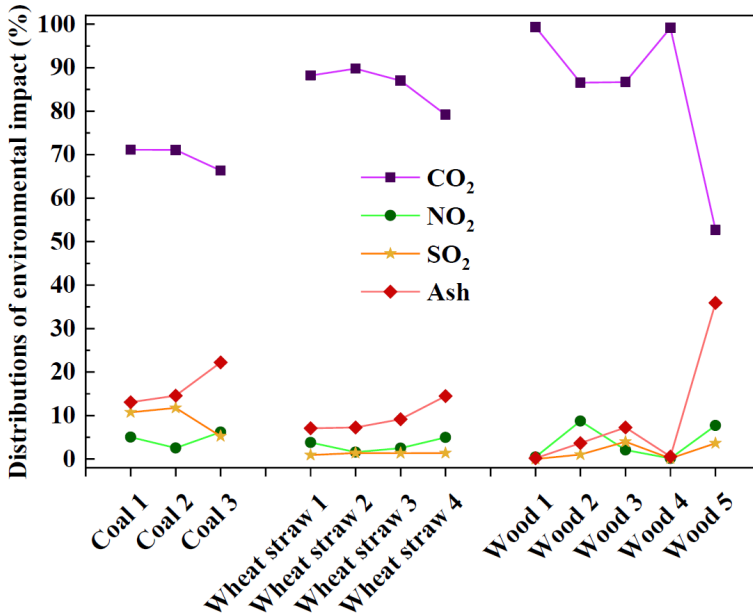


Figure 8 Distribution of environmental impact (see online version for colours)



Because the exergy method is based on a uniform basis, the EIs of the different emissions (gas pollutants and ash compositions) can be obtained and compared. This section further demonstrates how to determine the contributions of the specific factors (i.e., CO₂, SO₂, NO₂, and ash) to the (total) EI of a fuel.

5 Validation of the method

A universal exergy method is proposed in this study to measure the EI of a fuel based on the exergy values of the released gas emissions and ash components. The exergy values of the released gas emissions and ash components have the same exergy basis, validating well the method.

Based on the exergy method proposed in this study, the EIs of different pollutions or emissions can be compared and added, and also the EIs of different fuels can be estimated and assessed. The results of case studies show that the coal samples have higher EIs (1,324.99–1,437.47 kJ/kg) than the biomass samples (381.02–1078.81 kJ/kg), indicating that biomass fuels are more environmentally friendly. These are also validated by the GHG technology results (Williams et al., 2001; Yang et al., 2021).

If the data (i.e., components, concentrations, etc.) of released gas emissions and ash components of the fuels in practical processes and systems are detailed, this method can be further used to assess or evaluate the EIs of the actual processes and systems.

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6 Conclusions

This study elaborates if exergy can be used to reflect the environmental issues of a fuel. The environmental issues of 12 fuel samples including three coal samples, four wheat straw samples, and five wood samples are detailed, and these include the EIs of CO₂, SO₂, NO₂, and ash. Some conclusions are obtained.

- 1 The coal samples (1,324.99–1,437.47 kJ/kg) have higher total EIs than the biomass samples (381.02–1,078.81 kJ/kg).
- 2 For both coal samples and biomass samples, the EIs are mainly contributed by CO₂ (52.72%–99.37%), followed by ash (0.18%–35.93%), SO₂ (0%–11.77%) and NO₂ (0.16%–8.75%).
- 3 Actual processes and products should be taken into account to further complete the method proposed in this study.

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