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A New Software Tool for Calorific Value Calculation of Solid Fuels using the Bomb Calorimeter

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Abstract
This article presents a new program for calculating the calorific value of solid fuels, using bomb calorimeter technology. Since the usual method of calculating the calorific value is complicated and time-consuming, the suggested solution facilitates this essential calculation for evaluating the efficiency of fuels. The program offers a user-friendly interface, allows for rapid evaluation of data from calorimeter experiments, and guarantees better accuracy in determining the calorific value. The results obtained are compared with traditional techniques, showing the efficiency and reliability of the solution in industrial and research applications. Compared to commercial software often offered customized for various instruments, this program can be used to calculate the calorific value of solid fuels regardless of the manufacturer of the calorimeter bomb.

Keywords
calorific value, bomb calorimeter, software tool

1. Introduction

Measuring the calorific value of solid fuels is an important process in the energy and industrial sectors. Calorific value measures the energy obtained by the total combustion of a quantity of solid fuel (usually expressed in units of energy per unit mass, such as kilocalories per kilogram (kcal/kg) or megajoules per kilogram (MJ/kg)). Knowing the calorific value of a fuel helps to improve its use, reducing energy losses and increasing the efficiency of combustion systems (e.g. furnaces, boilers, etc.). In power plants, incinerators or any type of installation that uses solid fuels, measuring the calorific value of the fuel is essential to evaluate the efficiency of the combustion process. This helps to adjust the operational parameters (temperature, pressure, fuel dosage) to obtain the best results. In the energy sector, fuels with a higher calorific value will generate more energy for the same mass, which affects the costs of energy production.

Current environmental protection requirements pose challenges for the energy industry in finding new classes of fuels that ensure the required quality. The use of biomass, pellets, and combustible waste is an alternative to the use of fossil fuels. In this regard, there are numerous studies and research that analyze the possibility of using new types of solid fuels in industry [1 - 6]. The calorific value is an attribute of the fuel quality. For example, wood, coal, pellets, or biomass have varying calorific values, and their evaluation helps to classify fuels and select the most suitable ones for various types of installations. High-quality fuels have a higher calorific value, which means more efficient combustion and reduced pollutant emissions. Also, the measurement of calorific value helps to adjust the combustion conditions to minimize the impact on the environment. The measurement of the calorific value of solid fuels is crucial for improving energy use, reducing costs, increasing efficiency and preserving the environment, having important applications in the energy, transportation and materials processing sectors. Numerous studies present the results of research in this regard, using the bomb calorimeter method as a method for determining the calorific value [7 - 10].

In addition to its use in thermal analysis, the bomb calorimeter is also used in other industries - the pharmaceutical industry for example [11].

One of the most accurate methods for determining the calorific value of a fuel is the use of a bomb calorimeter, which measures temperature changes in an isolated system. However, processing the measurement data is laborious and time-consuming. This article presents a program developed to automate the process of calculating the calorific value of solid fuels using data obtained with a bomb calorimeter. The proposed software solution significantly reduces the time required for data processing and improves the accuracy of the calculation, thus facilitating the rapid assessment of fuel characteristics for industrial and research purposes.

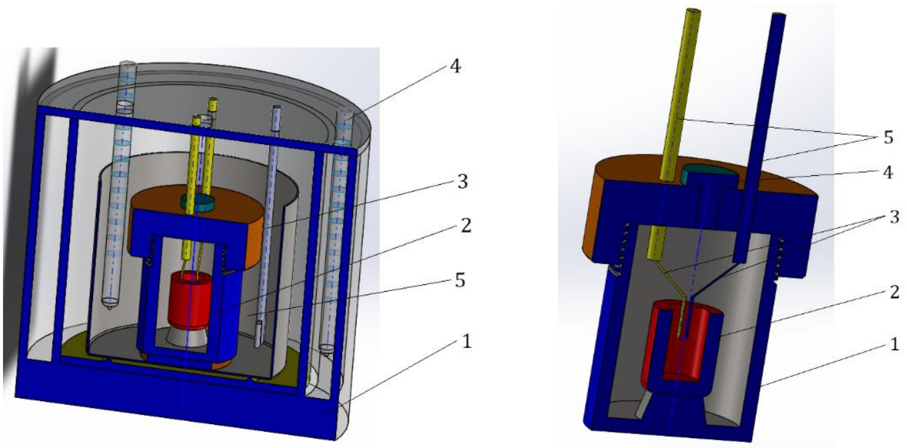
2. Methodology

2.1. Determination of calorific value

To measure the calorific value of solid fuels, there are various common methods, each with specific advantages and uses. The most relevant methods used to measure calorific value include:

- bomb calorimetry method (combustion calorimetry) – the most accurate method, which involves the complete combustion of the fuel in a sealed system and the measurement of the thermal energy released;
- indirect calorimetry method (chemical composition calculation method) – a faster and less expensive method, which estimates the calorific value based on the chemical analysis of the fuel;
- flame calorimeter method (controlled flame) – a less frequently used method, applicable to fuels that can burn at controlled temperatures and conditions;
- direct combustion calorimeter method – a simplified version of the bomb calorimeter method, where the fuel is burned directly in an isothermal enclosure, and the temperature rise in this enclosure is measured;
- water calorimeter method (water heating method) – a simplified but effective method for estimating the calorific value of solid fuels;
- gasification calorimeter method (for gaseous fuels) – this method is applicable to solid fuels that are easier to convert into gases, through gasification processes.

Each of these methods has its applications and limitations, but the bomb calorimeter remains the benchmark in measuring calorific value due to its accuracy. A bomb calorimeter (figure 1) is a device used to measure the thermal energy of a fuel by determining the amount of heat generated when the fuel is completely burned in a controlled environment. For solid fuels, this process is carried out in a bomb calorimeter, a hermetically sealed, pressure and temperature-resistant apparatus that measures the thermal energy generated by a combustion reaction.



a b

Fig. 1. Bomb calorimeter set-up

a) calorimetric system: 1 – insulated container, 2 – bomb, 3 – stirrer, 4 – thermometer, 5 – water
b) bomb (reaction chamber): 1 – bomb body, 2 – cup holding sample, 3 – fine wire in contact with sample, 4 – oxygen inlet, 5 – electrical leads for igniting the sample

The main steps of the process [10, 12, 13]:

1. The solid fuel is placed in a hermetically sealed combustion chamber of the bomb calorimeter.
2. The bomb calorimeter is filled with pure oxygen and the fuel is completely burned by an electric arc or a controlled heat source.

3. The heat created during combustion is transferred to a known medium, usually water, which is in a well-insulated container.
4. The increase in the temperature of the water is measured with a thermometer or temperature sensor. Based on this temperature increase and the mass of the water, the amount of heat (in joules or kilocalories) released as a result of the combustion of the fuel is calculated.

2.2. Calorific value calculation program

Given that a fuel pellet consisting of the fuel to be analyzed is introduced into the calorimeter bomb together with a reference fuel (whose calorific value is precisely known) and that secondary combustion products also result during combustion, the calculation of the calorific value is not simply reduced to replacing the data in a formula. Because of this, the calculation is quite laborious and time-consuming. This is also the reason why a series of programs have been developed to automate the calculation. There are several software programs that can be used to calculate the calorific value of solid fuels using the data obtained with the calorimeter bomb: Calorimeter Software (Sanyo, Parr Instrument Company), TAM Air Calorimeter Software, NETZSCH Calorimeter Software, Oxygen Bomb Calorimeter Software. These software are often customized for each type of equipment and are expensive software.

The author presents in this article a software for determining the calorific value of solid fuels (using the bomb calorimeter method) developed in Microsoft Visual Basic Express (programming environment offered free of charge by Microsoft). The program has a graphical interface (figure 2) that allows its use without special user training.

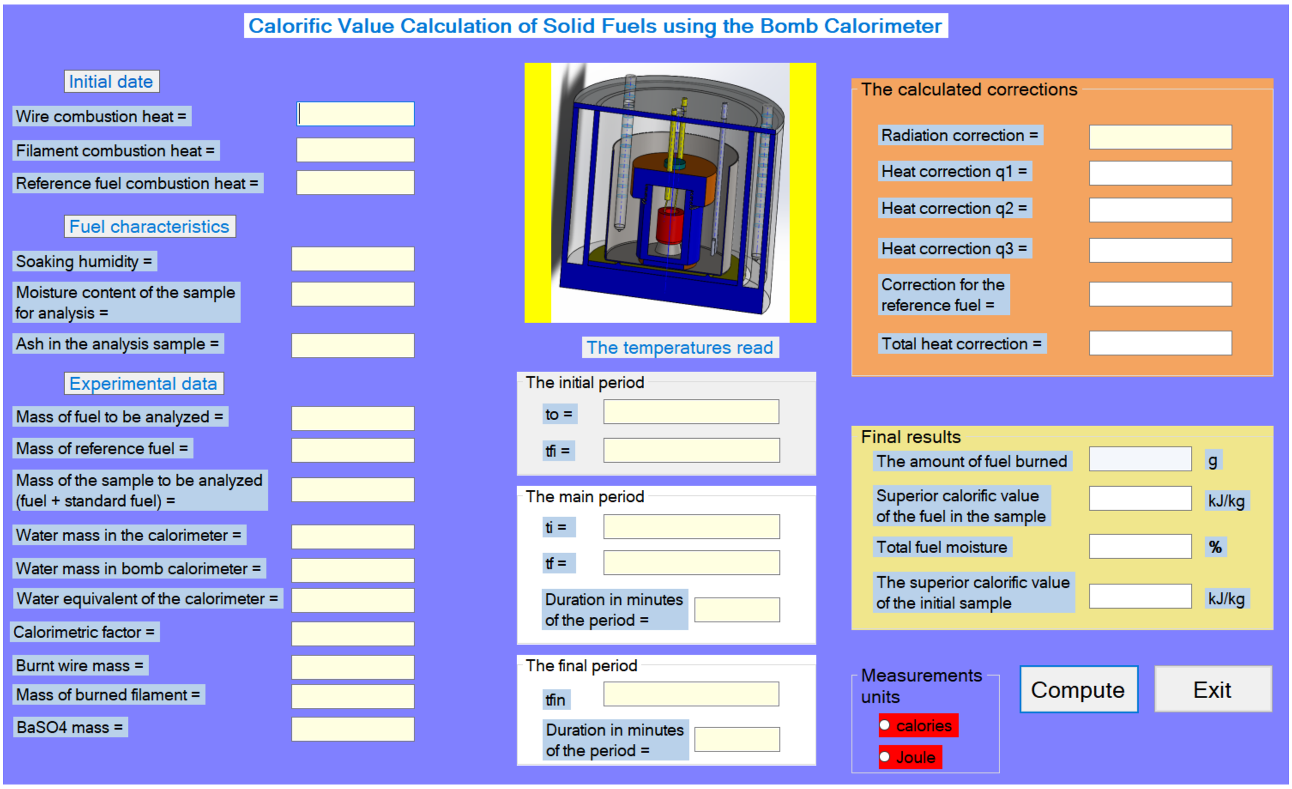


Fig. 2. The interface of the created program

The program took into account the method of determination, more precisely the reading of temperatures. The experimental procedure is divided into three periods: the initial period during which 6 readings are made (minute by minute). The first reading is denoted t_0 and the sixth (after minute 5) is denoted t_i; the main period in which the temperature is read minute by minute until the temperature continuously increases and decreases slightly (t_f). The first temperature in this period is the last in the initial period (t_i); the final period in which the temperature reading continues, minute by minute, at least as long as the main period. The last reading is t_{fin}.

Knowing the temperatures in the calorimetric system before, during and after the determination, the amount of heat developed by combustion can be calculated (it is considered that the ambient temperature is constant).

The corrections that must be made to determine the exact calorific value of the analyzed fuel are what increases the volume of the calculation. These corrections (Σq_i) refer to:

- radiation correction (α) – due to heat exchange with the environment;
- heat correction (q_1) – for the combustion of the ignition filament and the support;
- heat correction (q_2) – for the formation of sulfuric acid (sulfur in the bomb);
- heat correction (q_3) – for the formation of nitric acid;
- heat correction(q_4) – for the standard fuel.

$$\sum q_i = q_1 + q_2 + q_3 + q_4 \qquad [cal] \;\; or \;\; [J] \tag{1}$$

The superior calorific value, of the fuel in the sample to be analyzed is calculated with the formula:

$$Q_s^a = \frac{k\left(t_f - t_i + \propto\right) - \sum q_i}{m} \qquad \left[\frac{kcal}{kg}\right] \;\; or \;\; \left[\frac{kJ}{kg}\right] \tag{2}$$

where: k is the calorimetric factor; t_f – final temperature of the main period, in °C; t_i – initial temperature of the main period, in °C; α – radiation correction, due to heat exchange with the environment, in °C; Σq_i – sum of heat corrections, in cal or J; m – mass of the fuel taken for analysis, in g.

The superior calorific value of the initial sample is then calculated taking into account the moisture content of the fuel (in the delivered state).

$$Q_s^i = Q_s^a \frac{100 - W_t^i}{100 - W_a^a} \qquad \left[\frac{kcal}{kg}\right] \;\; or \;\; \left[\frac{kJ}{kg}\right] \tag{3}$$

where: W_a^a is the moisture content of the sample for analysis, in %; W_t^i is the total moisture content, in %.

$$W_t^i = W_i^i + W_a^a \frac{100 - W_i^i}{100} \qquad [\%] \tag{4}$$

where W_i^i is the soaking humidity, in %.

The input data that must be entered into the program can be divided into four categories:

- known initial data about the standard fuel and the system for producing ignition in the bomb;
- characteristics of the fuel - moisture and ash content;
- data from the bomb calorimeter determination;
- temperatures read and duration of the determination periods.

All these calculations (including the calculation of corrections) are performed manually, which involves a certain amount of time to obtain the final result. By using the presented software, the working time is substantially reduced and the accuracy is greatly increased.

2.3. Example of use

The determination of calorific value using the bomb calorimeter can be applied for a number of solid fuels: coal of different types (brown coal, anthracite coal, lignite coal) which is a solid fuel frequently used for determining calorific value, as it has a varied composition and a significant calorific value; wood (oak, beech, fir, etc.), used both for heating and in the energy industry, can be tested to determine its calorific value; solid biomass, such as plant residues, straw, nut shells or other organic materials used as biofuels, can be analyzed using the bomb calorimeter to determine the calorific value; wood pellets which are processed forms of biomass, frequently used in thermal power plants, and can be tested for calorific value; coke which is a by-product obtained from coal processing and is mainly used in the metallurgical industry; Lignite is another type of coal, with a lower calorific value than anthracite coal, but still usable for energy generation.

For the entire range of fuels mentioned, the calculation of the calorific value can be done with the designed software (in the case of using the calorific bomb for the determination). The great advantage lies in the very high calculation speed, which translates into results obtained almost instantly and with very high precision. The way in which fuels are stored and transported certainly influences their quality.

If storage or transportation is done improperly, the moisture content of the fuel can increase, which has the effect of decreasing the calorific value for the same mass of fuel. Another advantage of the developed software is that simulations of the variation of the calorific value (for a determination performed) can be made depending on the moisture content of the fuel.

For example, the software was used to calculate the calorific value of a solid fuel using data from the literature [13] of an analysis performed with a bomb calorimeter. After running the program, its validity was found – the results coincided with those in the literature but with increased precision and in an infinitely shorter time than through classical processing.

In the figure 3 the data of the analyzed sample, the results of the bomb determination as well as the temperatures read during the experiment are presented. In the figure 4 the results obtained with the help of the created software are presented.

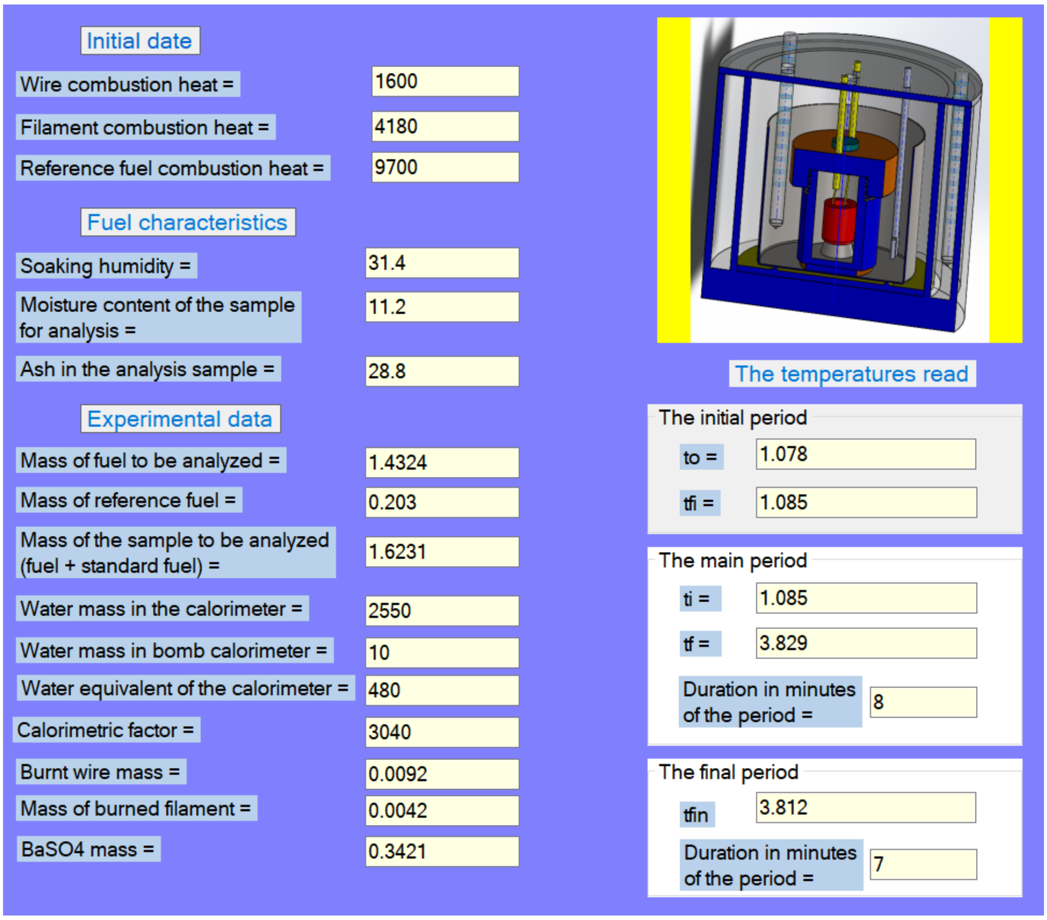


Fig. 3. Experimental determination data taken into account

A simulation was performed on the same determination data regarding the influence of the humidity content on the calorific value of the same fuel. Its clear negative influence is observed: the same amount of fuel, with different humidity contents, provides different values of the heat developed by combustion (figure 5).

3. Conclusions

The software developed can be used very easily to calculate the calorific value of solid fuels using the bomb calorimeter. It is very suitable for use in research laboratories that do not have an instrument-centered software. It can also be used by students in laboratory work that includes determining the calorific value. Regardless of whether the initial data is in tolerated units of measurement (cal), the program converts the result into units from the international system of units (J) The calculation program was created using Microsoft Visual Basic Express and the program is original.

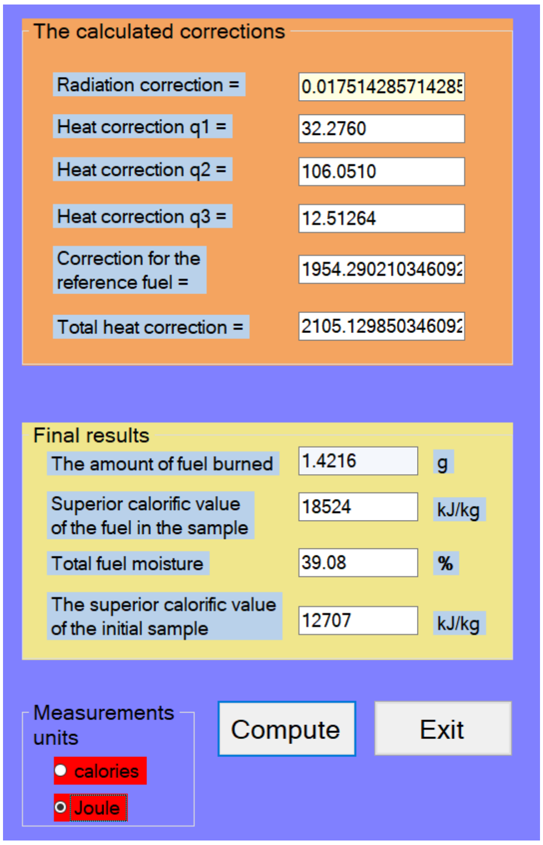


Fig. 4. The results obtained after running the created calculation program

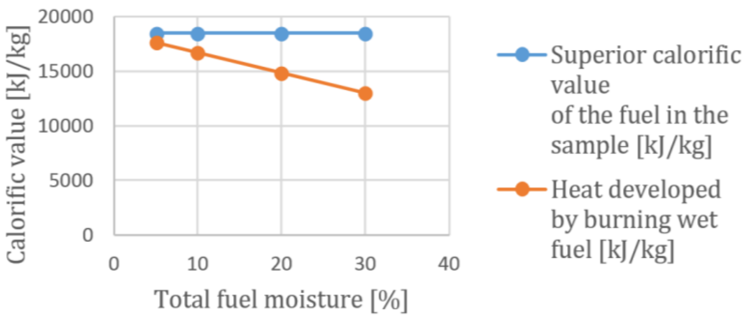


Fig. 5. Influence of fuel humidity on calorific value

In the future, the software can be developed for automatic measurement acquisition by creating an electronic interface to connect with the experimental instrument.

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