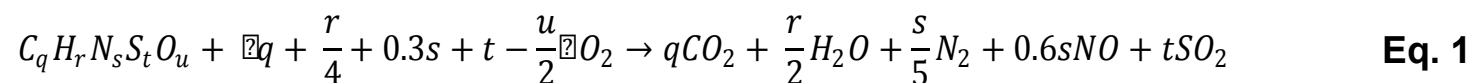


## Supporting information

- A)** Equations 1 and 2: related to the chemical composition of each sample matrix and for calculate the amount of oxygen required for sample combustion;
- B)** Equations 3: real gas equation, used to calculate the O<sub>2</sub> amount loaded in the digestion vessel;
- C)** Equation 4: Ideal gas equations, used to check the accuracy of Equation 3 in the working temperature and pressure.



$$n_s = \sum_{i=1}^N \left[ f_i \cdot \frac{m_s}{M_i} \right] \cdot \left[ q_i + \frac{r_i}{4} + 0.3s_i + t_i - \frac{u_i}{2} \right] \quad \text{Eq. 2}$$

$$P = \frac{nRT}{V} \quad \text{Eq. 3}$$

$$P = \frac{nRT}{V - nb} - a \frac{n^2}{V^2}$$

**Eq. 4**

Where:

$m_s$  is the sample mass;

$f_i$  is mass fraction and  $\dot{M}_i$  is the molar mass of an  $i$  component in the sample matrix;

$P$  is the O<sub>2</sub> pressure in the vessel;

$V$  is the headspace volume of the vessel;

$n$  is the number of O<sub>2</sub> moles present in the combustion vessel;

$R$  is the universal gas constant (0.082 atm L mol<sup>-1</sup> K<sup>-1</sup>);

$T$  is the temperature before combustion;

$n_s$  is the number of O<sub>2</sub> moles required to obtain a complete combustion;

$a$  is the van der Waals constant that provides a correction for the intermolecular forces; and

$b$  is the van der Waals constant that provides a correction for finite molecular size related to the volume of one mole of the atoms or molecules.

## D) Instructions of how to fill the left side of data sheet (system conditions) used for predicting combustion

- 1°) Complete only the yellow cells presented in the related data sheet;
- 2°) Follow the instructions, as presented below as dialog boxes;
- 3°) Final data will be presented at the right side of the data sheet.

### Stoichiometric combustion application using microwave-induced combustion



Only fill the yellow cells

System condition		Compound:	Mass fraction:	Molar weight:	Elemental ratio				
					C	H	N	S	O
Sample mass, g:	0.45	A	1.0	84.18	6	12			
O <sub>2</sub> pressure in the vessel, atm:	20	B	0.0	0					
R, (atm·L)/(mol·K):	0.082	C	0.0	0					
Temperature before combustion, K:	298	D	0.0	0					
Headspace volume of vessel, L:	0.068	Igniter (e.g. cellulose paper)							
Mass of igniter for combustion, g:	0.018				6	10			5

Data obtained by equation of ideal gas	
48.8 mmol of O <sub>2</sub> necessary to complete sample combustion	
55.7 mmol of O <sub>2</sub> present in combustion vessel	
14 % of O <sub>2</sub> excess considering stoichiometric combustion	
0.6 mmol of O from sample	
32.7 mmol of CO <sub>2</sub>	
32.6 mmol of H <sub>2</sub> O	
0.0 mmol of N <sub>2</sub> from 50% of total N present in sample	
0.0 mmol of NO from 50% of total N present in sample	
0.0 mmol of SO <sub>2</sub>	
15 atm* (final pressure) at 314 K	

\*Only for sample matrix as C<sub>q</sub>H<sub>r</sub>O<sub>u</sub> (without S and N).

In this cell, fill the sample mass, in grams.

In this cell, fill the oxygen pressure used in the vessel, in atmosphere.

In this cell, fill the room temperature, in Kelvin.

In this cell, fill the vessel headspace volume (total volume of vessel minus the volume of absorption solution minus quartz holder volume), in liter.

In this cell, fill the mass of igniter (cellulose paper) used, in grams

## E) Instructions of how to fill the central part of data sheet used for predicting combustion

### Stoichiometric combustion application using microwave-induced combustion



$$n_x = \sum_{i=1}^N \left(f_i \cdot \frac{m_x}{M_i}\right) \cdot \left(q_i + \frac{r_i}{4} + 0.3s_i + t_i - \frac{u_i}{2}\right) \quad (2)$$

$$PV = nRT \quad (3)$$

Only fill the yellow cells

System condition		Compound:	Mass fraction:	Molar weight:	Elemental ratio						
					C	H	N	S	O		
Sample mass, g:	0.45	A	1.0	84.18	6	12					
O <sub>2</sub> pressure in the vessel, atm:	20	B	0.0	0							
R, (atm·L)/(mol·K):	0.082	C	0.0	0							
Temperature before combustion, K:	298	D	0.0	0							
Headspace volume of vessel, L:	0.068	Igniter (i.g. cellulose paper)			6	10					
Mass of igniter for combustion, g:	0.018										

Data obtained by equation of ideal gas	
48.8 mmol of O <sub>2</sub> necessary to complete sample combustion	
55.7 mmol of O <sub>2</sub> present in combustion vessel	
14 % of O <sub>2</sub> excess considering stoichiometric combustion	
0.6 mmol of O from sample	
32.7 mmol of CO <sub>2</sub>	
32.6 mmol of H <sub>2</sub> O	
0.0 mmol of N <sub>2</sub> from 50% of total N present in sample	
0.0 mmol of NO from 50% of total N present in sample	
0.0 mmol of SO <sub>2</sub>	
15 atm* (final pressure) at 314 K	

\*Only for sample matrix as C<sub>q</sub>H<sub>r</sub>O<sub>u</sub> (without S and N).

In these lines, fill each cell according to the elemental ratio presented in sample composition.

In these lines, fill each cell according to the elemental ratio of igniter (example already filled for cellulose paper).

The stoichiometric amount of oxygen, available for combustion, will be presented in this cell (in percentage). It is important to notice that a minimum excess oxygen must be used to ensure complete sample combustion