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Using Mean Oxidation Number of Organic Carbons to Count Theoretical Chemical Oxygen Demand

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Abstract

Chemical oxygen demand and mean oxidation number of organic carbons are two important concepts in redox chemistry. The former is used for counting pure or mixed organic matters in aqueous solution. The latter is a redox metric for water treatment, organic combustion, and anaerobic digestion. Currently the calculation of theoretical chemical oxygen demand of neutral organic matter is based on the number of moles of molecular oxygen (O_2). However, the calculation of theoretical chemical oxygen demand of ionic organic matter has seldom been studied. The purpose of this article is to develop a simple mathematical equation for doing so by using mean oxidation number of organic carbons. To develop the equation, relationships among chemical oxygen demand, mean oxidation number of organic carbons, number of organic carbons, and formula mass of organic matter are identified. The mathematical equations for chemical oxygen demand, total organic carbon, and the ratio of chemical oxygen demand to total organic carbon are also established for any molecule(s).

Keywords: mean oxidation number of organic carbons, structural formula, empirical formula, chemical oxygen demand, total organic carbon, ratio of chemical oxygen demand to total organic carbon

1. Introduction

Chemical oxygen demand (COD) is one of the important analytical parameters for counting pure or mixed organic matters in aqueous solution (ASTM D1252-06, 2020; ISO 15705, 2002; IUPAC, 2019; Baker et al., 1999). It is widely used in wastewater, aerobic digestion, and anaerobic digestion (Contreras et al., 2002; Brouckaert et al., 2021; Ahnert et al., 2021; Brouckaert et al., 2022; Angelidaki & Sanders, 2004; Tamis et al., 2021). The quantity of COD of organic matter is relevant to the quantitative amount of molecular oxygen (O_2). Currently the calculation of COD of neutral organic matter is based on the number of moles of molecular oxygen (nO_2) (Baker et al., 1999; Ahnert et al., 2021). However, the calculation of theoretical chemical oxygen demand of ionic organic matter has seldom been studied.

The mean oxidation number of organic carbons (ONc) of organic matter is a redox metric for environmental chemistry (Kroll et al., 2011), water treatment (Vogel et al., 2000; Li et al., 2022), organic combustion (Yuen & Lau, 2023a), and anaerobic digestion (Yuen & Lau, 2024a). Although the mathematical relationship between ONc and the ratio of COD to total organic carbon (TOC) (Vogel et al., 2000), and the relationship between ONc and nO_2 have already been established (Yuen & Lau, 2023a), the relationships among ONc, nO_2, and theoretical COD have not been explored yet.

In this article ONc is developed as a metric for determining COD of organic matter. The exploration of mathematical equations for counting COD is based on the chemical formula of organic matter. The chemical formula can be structural or empirical and the organic matter can be in molecular or ionic form. Through the integration of ONc, nO_2, and COD, the relationships among COD, ONc, number of organic carbons (nc or x), and formula mass of organic matter (μ) are identified. The relationships among ONc, COD, TOC (TCEQ, 2022), and $\frac{COD}{TOC}$ are also established. Most importantly, a mathematical equation which uses ONc to count theoretical COD is developed.

2. Methods and Materials

The methodology of the article is shown in Figure 1.

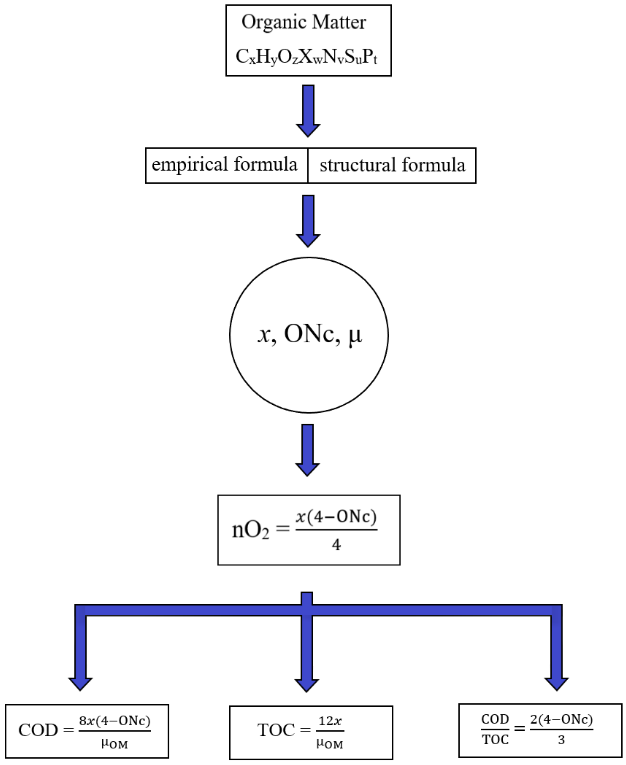


Figure 1. The methodology: from organic matter to COD, TOC, and $\frac{\text{COD}}{\text{TOC}}$

2.1 Determination of Mean Oxidation Number of Organic Carbons (ONc)

For any given structural formula of an organic matter, the ONc can be assigned by using fragmentation method (Yuen & Lau, 2022), carbon-atom method (Yuen & Lau, 2023b), or non-carbon atom method (Yuen & Lau, 2023c). Pauling's electronegativities scale [χH (hydrogen, 2.20) < χC (carbon, 2.55) < χS (sulfur, 2.58) < χI (Iodine, 2.66) < χBr (Bromine, 2.96) < χN (Nitrogen, 3.04) < χCl (Chlorine, 3.16) < χO (Oxygen, 3.44) < χF (Florine, 3.98)] is adopted to assign individual oxidation number of atoms.

For organic matters: $C_xH_yO_zX_wN_vS_uP_t^{charge}$

X = halogen atoms

charge = electrical charge of organic matter

ON_{inc} = individual oxidation number of non-carbon atom

ONc = mean oxidation number of carbons

nc = x = number of organic carbons

When charge = 0, it is a neutral organic matter, ONc = $\frac{-\Sigma ON_{inc}}{nc}$.

When charge ≠ 0, it is a charged organic matter, ONc = $\frac{charge - \Sigma ON_{inc}}{nc}$.

In the structural formula: $C_xH_yO_zX_wN_vS_uP_t^{charge}$

$C_xH_yO_zX_wN_vS_uP_t^{charge}$	C	H	O	X	N	S	P
assigned ON_{inc}	-	ON_H	ON_O	ON_X	ON_N	ON_S	ON_P
atomic coefficient (AC)	x	y	z	w	v	u	t

$\Sigma ON_{inc} = [(ON_H\ y) + (ON_O\ z) + (ON_X\ w) + (ON_N\ v) + (ON_S\ u) + (ON_P\ t)]$

The mathematical equation for calculating ONc of a structural formula is established as

$$ONc = \frac{charge-[(ON_H\ y)+(ON_O\ z)+(ON_X\ w)+(ON_N\ v)+(ON_S\ u)+(ON_P\ t)]}{x}$$

Chemical formulas of biomasses, biowastes, or unknown structures of pure and mixed organic matters are considered empirical formulas. For any given empirical formula, its ONc of an organic matter can be counted either by the molecular formula method (Yuen & Lau, 2022) or non-carbon atom method (Yuen & Lau, 2023c). All ON_{inc} in empirical formulas are assumed to be $ON_H = +1$, $ON_O = -2$, $ON_X = -1$, $ON_N = -3$, $ON_S = -2$, $ON_P = +5$ (Yuen & Lau, 2024b).

In the empirical formula: $C_xH_yO_zX_wN_vS_uP_t^{charge}$

$C_xH_yO_zX_wN_vS_uP_t^{charge}$	C	H	O	X	N	S	P
assumed ON_{inc}	-	+1	−2	−1	−3	−2	+5
atomic coefficient (AC)	x	y	z	w	v	u	t

$\Sigma ON_{inc} = (y-2z-w-3v-2u+5t)$

The mathematical equation for calculating ONc of an empirical formula is established as

$$ONc = \frac{charge-(y-2z-w-3v-2u+5t)}{x}$$

2.2 Chemical Oxygen Demand (COD)

Generally, COD is a measure of the mass of molecular oxygen that can be consumed by organic matters in a measured solution. The unit of COD is commonly expressed in grams of molecular oxygen to liters of aqueous solution or wastewater. It is represented as COD (unit, g/L) = $\frac{mO_2}{V_{solution}}$.

In the study of volatile solids in anaerobic digestion or sludges in wastewater treatment, COD is a measure of the grams of molecular oxygen that can be consumed by per gram of organic matters. It is defined as COD (unit, g/g) = $\frac{mO_2}{m_{OM}}$.

2.3 Relationship between ONc and nO_2

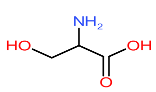
According to the general organic combustion reaction,

$$C_xH_yO_zX_wN_vS_uP_t + \frac{x(4-ONc)}{4}\ O_2 \rightarrow xCO_2 + \text{other combustion products}$$

the relationships among ONc, nO_2, and x are established as $\frac{nO_2}{n_{OM}} = \frac{x(4-ONc)}{4}$. When nOM = 1 mole, its mathematical equation will be $nO_2 = \frac{x(4-ONc)}{4}$ (Yuen & Lau, 2023a).

2.4 Mole Relationship between $n_{organic\ matter}$ and nO_2

Two organic combustion equations are provided as examples.



$(C_3H_7O_3N,\ ONc = +\frac{2}{3}) + \frac{5}{2}\ O_2 \rightarrow 3CO_2 + 2H_2O + NH_3$

$C_{118}H_{170}O_{57}N_{17}P\ (ONc = -\frac{5}{59}) + \frac{241}{2}\ O_2 \rightarrow 118CO_2 + 58H_2O + 17NH_3 + H_3PO_4$

There is a complete reaction between 1 mole of organic matter and $\frac{x(4-ONc)}{4}$ moles of molecular oxygen. All ON_{inc} remain the same before and after any combustion reaction (Yuen & Lau, 2023a). Organic combustion equations can be used to calculate theoretical COD of any organic matter.

2.5 Mass Relationships

Based on the definitions of COD, TOC, and $\frac{COD}{TOC}$, the mathematical relationships are shown below:

$COD = \frac{mO_2}{m_{OM}}$	$TOC = \frac{m_c}{m_{OM}}$	$\frac{COD}{TOC} = \frac{mO_2}{m_{OM}} / \frac{m_c}{m_{OM}} = \frac{mO_2}{m_c}$

m = mass

OM = organic matter

C = organic carbon

μ = formula mass

2.6 Mole-Mass Relationships

When n_{OM} = 1 mole, let μc be integer 12 g/mol, let μO_2 be integer 32 g/mol, and $nO_2 = \frac{x(4-ONc)}{4}$, three mathematical equations are attained.

nO_2	Theoretical COD	Theoretical TOC	Theoretical $\frac{COD}{TOC}$
$\frac{nO_2}{n_{OM}} = \frac{x(4-ONc)}{4}$	$COD = \frac{mO_2}{m_{OM}}$	$TOC = \frac{mc}{m_{OM}}$	$\frac{COD}{TOC} = \frac{mO_2}{m_c}$
$nO_2 = \frac{n_{OM}\, x(4-ONc)}{4}$	$COD = \frac{nO_2\, \mu O_2}{n_{OM}\, \mu_{OM}}$	$TOC = \frac{nc\, \mu c}{n_{OM}\, \mu_{OM}}$	$\frac{COD}{TOC} = \frac{nO_2\, \mu O_2}{nc\, \mu c}$
$nO_2 = \frac{x(4-ONc)}{4}$	$COD = \frac{8x(4-ONc)}{\mu_{OM}}$	$TOC = \frac{12x}{\mu_{OM}}$	$\frac{COD}{TOC} = \frac{2(4-ONc)}{3}$

Since the connection between mass relationships and mole relationships has been found, the mathematical equations for theoretical COD, theoretical TOC, and theoretical $\frac{COD}{TOC}$ can be derived.

2.7 Triangular Relationships Among ONc, nO_2 and COD

Through the integration of ONc and mole-mass relationship, the triangular relationships among ONc, nO_2, and COD, and their mathematical equations are shown in Figure 2.

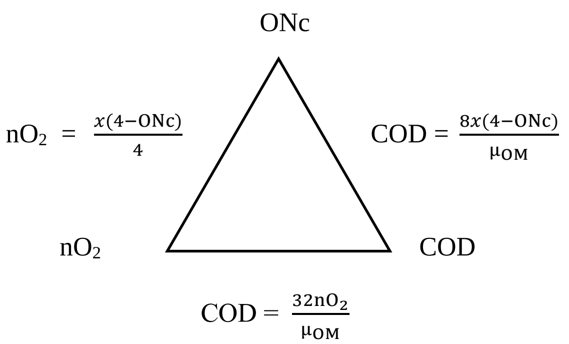


Figure 2. Mathematical relationships among ONc, nO_2 and COD

3. Procedures and Examples

The operating procedures for counting COD, TOC, and $\frac{COD}{TOC}$ are shown:

$$OM \rightarrow ONc,\ x,\ \mu OM \rightarrow COD,\ TOC,\ \frac{COD}{TOC}$$

3.1 Calculation of ONc

For any given structural formula:

$$ONc = \frac{charge-[(ON_H\ y)+(ON_O\ z)+(ON_X\ w)+(ON_N\ v)+(ON_S\ u)+(ON_P\ t)]}{x}$$

For any given empirical formula:

$$ONc = \frac{charge-(y-2z-w-3v-2u+5t)}{x}$$

3.2 Calculation of x and μ_{OM}

Both the structural and empirical formula can identify the number of organic carbon (x) and calculate the formula mass (μ_{OM}).

Atomic mass	μC	μH	μO	μF	μCl	μN	μS	μP
g/mol	12.011	1.008	15.999	18.998	35.453	14.007	32.065	30.974

3.3 Calculation of COD, TOC, and $\frac{COD}{TOC}$

COD, TOC, and $\frac{COD}{TOC}$ can be calculated by using the following mathematical equations. COD is dependent on x, ONc, and μ_{OM}. TOC is related to x and μ_{OM}, but not to ONc. $\frac{COD}{TOC}$ is only dependent on ONc.

$COD = \frac{8x(4-ONc)}{\mu OM}$	$TOC = \frac{12x}{\mu OM}$	$\frac{COD}{TOC} = \frac{2(4-ONc)}{3}$

3.4 Examples

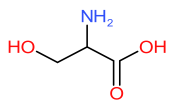
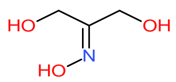
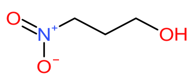
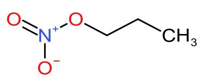
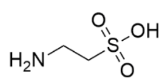
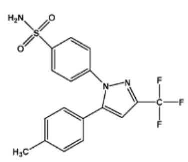
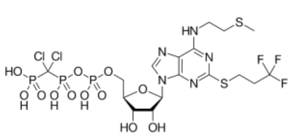
The calculated data for carbon atom, molecules, and ions are summarized in Table 2. The molecular CH_3COOH and ionic CH_3COO^- have same values of ONc and $\frac{COD}{TOC}$, but different values of COD and TOC. An organic acid and its organic salt have the same ONc, but different electrical charges and formula masses.

Table 2. ONc, COD, and parameters of simple atom, molecules, and ions

Atom / Molecule / Ion	Chemical formula	x	Formula mass	ONc	COD	TOC	$\frac{COD}{TOC}$
C	C	1	12.011	0.000	2.664	0.999	2.667
CO	CO	1	28.010	2.000	0.571	0.428	1.333
CO_2	CO_2	1	44.009	4.000	0.000	0.273	0.000
CO_3^{2-}	CO_3^{2-}	1	60.008	4.000	0.000	0.200	0.000
$HCOO^-$	HCO_2^-	1	45.017	2.000	0.355	0.267	1.333
CH_4	CH_4	1	16.043	-4.000	3.989	0.748	5.333
C_2H_5OH	C_2H_6O	2	46.069	-2.000	2.084	0.521	4.000
CH_3COOH	$C_2H_4O_2$	2	60.052	0.000	1.066	0.400	2.667
CH_3COO^-	$C_2H_3O_2^-$	2	59.044	0.000	1.084	0.406	2.667
HO_2CCO_2H	$C_2H_2O_4$	2	90.034	3.000	0.178	0.267	0.667
$HO_2CCO_2^-$	$C_2HO_4^-$	2	89.026	3.000	0.180	0.270	0.667
$^-O_2CCO_2^-$	$C_2O_4^{2-}$	2	88.018	3.000	0.182	0.273	0.667

Table 3 shows the calculated data for structural formulas of organic molecules. Isomers of HS-CH_2-CH_2-SH ($ON_S = -2$) and H_3C-S-S-CH_3 ($ON_S = -1$) have different values of ONc and $\frac{COD}{TOC}$, but same value of TOC. The same set of isomers will have the same TOC value. The more negative the value of ONc is, the greater the value of COD will become.

Table 3. ONc, COD, and parameters of structural formulas of organic molecules

Structural formula	Molecular formula	x	μ	ONc	COD	TOC	$\frac{COD}{TOC}$
HO-CH_2-CH_2-OH	$C_2H_6O_2$	2	62.068	-1.000	1.289	0.387	3.333
H_3C-O-O-CH_3	$C_2H_6O_2$	2	62.068	-2.000	1.547	0.387	4.000
HS-CH_2-CH_2-SH	$C_2H_6S_2$	2	94.200	-1.000	0.849	0.255	3.333
H_3C-S-S-CH_3	$C_2H_6S_2$	2	94.200	-2.000	1.019	0.255	4.000
	$C_3H_7O_3N$	3	105.093	0.667	0.761	0.343	2.222
	$C_3H_7O_3N$	3	105.093	0.000	0.913	0.343	2.667
	$C_3H_7O_3N$	3	105.093	-1.333	1.217	0.343	3.555
	$C_3H_7O_3N$	3	105.093	-2.000	1.370	0.343	4.000
	$C_2H_7O_3NS$	2	125.147	-1.000	0.639	0.192	3.333
	$C_{17}H_{14}O_2F_3N_3S$	17	381.377	-0.235	1.510	0.535	2.823
	$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3$	17	776.362	0.471	0.618	0.263	2.353

Based on the selected empirical formulas of organic matters (Ahnert et al., 2021), the calculated organic carbon's relevant parameters are summarized in Table 4.

Table 4. ONc, COD, and parameters of empirical formulas of organic matters

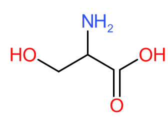
Organic matter	Empirical formula	x	Formula mass	ONc	COD	TOC	$\frac{COD}{TOC}$
Biomass (general)	$C_5H_7O_2N$	5	113.116	0.000	1.414	0.530	2.667
Biomass	$C_8H_{14}O_4N$	8	188.203	-0.375	1.488	0.510	2.917
Biomass	$C_{118}H_{170}O_{57}N_{17}P$	118	2769.694	-0.085	1.392	0.511	2.723
Pure bacterial culture	$C_6H_{10}O_3N$	6	144.150	-0.167	1.387	0.499	2.778
Escherichia coli	$CH_{1.69}O_{0.58}N_{0.2}$	1	25.795	0.070	1.219	0.465	2.620
Escherichia coli	$CH_{1.71}O_{0.37}N_{0.24}$	1	23.016	-0.250	1.477	0.521	2.833
Algal biomass	$C_{106}H_{263}O_{110}N_{16}$	106	3522.272	0.047	0.952	0.361	2.635
Picking beans (Phaseolus vulgaris)	$CH_{1.81}O_{0.81}N_{0.15}$	1	28.896	0.260	1.035	0.415	2.493
Oyster mushroom (Pleurotus ostreatus)	$CH_{1.83}O_{0.84}N_{0.26}$	1	30.937	0.630	0.871	0.388	2.247
Sawdust	$CH_{1.19}O_{0.59}N_{0.007}$	1	22.748	0.011	1.403	0.528	2.659
Rice husk	$CH_{1.7}O_{0.83}N_{0.003}$	1	27.046	-0.031	1.192	0.444	2.687
Bamboo dust	$CH_{1.66}O_{0.9}N_{0.018}$	1	28.336	0.194	1.075	0.423	2.537
Lignin	$(C_9H_{9.45}O_{2.65})_n$	9	160.022	-0.461	2.007	0.675	2.974

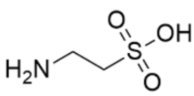
4. From Single Molecule (Organic Matter) to Multiple Molecules (Organic Matters)

Any single molecule can be represented by either a structural formula or an empirical formula. With reference to Tables 1 to 3, values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of different types of single molecules have been revealed. Table 4 shows the mathematical equations for counting total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of multiple molecules (i = number of different types of molecules; $i \geq 2$; $(n_{OM})_i > 0$).

Table 4. Mathematical equations for counting total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of multiple molecules

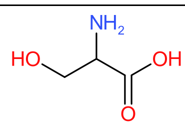
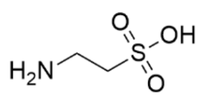
Parameter	nO_2	COD	TOC	$\frac{COD}{TOC}$
Definition	$nO_2 = \frac{n_{OM}\,x(4-ONc)}{4}$	$COD = \frac{mO_2}{m_{OM}}$	$TOC = \frac{mc}{m_{OM}}$	$\frac{COD}{TOC} = \frac{mO_2}{m_c}$
Single molecule (n_{OM} = 1 mole)	$nO_2 = \frac{x(4-ONc)}{4}$	$COD = \frac{8x(4-ONc)}{\mu OM}$	$TOC = \frac{12x}{\mu OM}$	$\frac{COD}{TOC} = \frac{2(4-ONc)}{3}$
Single molecule (n_{OM} > 0 mole)	$(nO_2)_i = \frac{(n_{OM})_i\,xi\,(4-ONci)}{4}$	$(COD)_i = \frac{8(n_{OM})_i\,x_i\,(4-ONci)}{(n_{OM})_i\,\mu_{OMi}}$	$(TOC)_i = \frac{12x_i}{(n_{OM})_i\,\mu_{OMi}}$	$(\frac{COD}{TOC})_i = \frac{2(n_{OM})_i\,x_i\,(4-ONci)}{3x_i}$
Multiple molecules ($i \geq 2$; $(n_{OM})_i > 0$)	$\text{Total } nO_2 = \Sigma(nO_2)_i = \frac{\Sigma(n_{OM})_i\,x_i\,(4-ONci)}{4}$	$\text{Total COD} = \Sigma(COD)_i = \frac{8\Sigma(n_{OM})_i\,x_i\,(4-ONci)}{\Sigma(n_{OM})_i\,\mu_{OMi}}$	$\text{Total TOC} = \Sigma(TOC)_i = \frac{12\Sigma x_i}{\Sigma(n_{OM})_i\,\mu_{OMi}}$	$\text{Total } \frac{COD}{TOC} = \Sigma(\frac{COD}{TOC})_i = \frac{2\Sigma(n_{OM})_i\,x_i\,(4-ONci)}{3\Sigma x_i}$

Example 1. Given multiple molecules which contain 3.000 mole of $H_3C\text{-}S\text{-}S\text{-}CH_3$, 2.000 moles of 

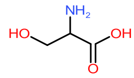
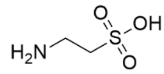
and 1.000 moles of 

, count the values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of the multiple molecules.

(i) Determine the values of n_{OM}, x, μ, and ONc of three different types of molecules

$H_3C\text{-}S\text{-}S\text{-}CH_3$ ($C_2H_6S_2$)				 ($C_3H_7O_3N$)				 ($C_2H_7O_3NS$)			
n_{OM}	x	μ	ONc	n_{OM}	x	μ	ONc	n_{OM}	x	μ	ONc
3.000	2	94.200	-2.000	2.000	3	105.093	0.667	1.000	2	125.147	-1.000

(ii) Count the values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of three different types of molecules

Single molecule	$H_3C\text{-}S\text{-}S\text{-}CH_3$ ($C_2H_6S_2$)	 ($C_3H_7O_3N$)	 ($C_2H_7O_3NS$)
$(nO_2)_i = \frac{(n_{OM})_i \text{ xi } (4-ONci)}{4}$	$= \frac{(n_{OM})_i \text{ xi } (4-ONci)}{4}$ $= \frac{(3)(2)(4-(-2))}{4}$ $= \frac{36}{4}$ = 9.000	$= \frac{(n_{OM})_i \text{ xi } (4-ONci)}{4}$ $= \frac{(2)(3)(4-(0.667))}{4}$ $= \frac{28.002}{4}$ = 7.000	$= \frac{(n_{OM})_i \text{ xi } (4-ONci)}{4}$ $= \frac{(1)(2)(4-(-1))}{4}$ $= \frac{10}{4}$ = 2.500
$(COD)_i = \frac{8(n_{OM})_i \text{ xi } (4-ONci)}{(n_{OM})_i\, \mu_{OMi}}$	$= \frac{8(n_{OM})_i \text{ xi } (4-ONci)}{(n_{OM})_i\, \mu_{Omi}}$ $= \frac{8(3)(2)(4-(-2))}{(3)(94.200)}$ $= \frac{8(36)}{282.6}$ $= \frac{288}{282.6}$ =1.019	$= \frac{8(n_{OM})_i \text{ xi } (4-ONci)}{(n_{OM})_i\, \mu_{OMi}}$ $= \frac{8(2)(3)(4-(0.667))}{(2)(105.093)}$ $= \frac{8(28.002)}{210.186}$ $= \frac{224.016}{210.186}$ = 1.066	$= \frac{8(n_{OM})_i \text{ xi } (4-ONci)}{(n_{OM})_i\, \mu_{OMi}}$ $= \frac{8(1)(2)(4-(-1))}{(1)(125.147)}$ $= \frac{8(10)}{125.147}$ $= \frac{80}{125.147}$ = 0.639
$(TOC)_i = \frac{12xi}{(n_{OM})_i\, \mu_{OMi}}$	$= \frac{12xi}{(n_{OM})_i\, \mu_{OMi}}$ $= \frac{12(2)}{(3)\ (94.200)}$ $= \frac{24}{282.6}$ = 0.085	$= \frac{12xi}{(n_{OM})_i\, \mu_{OMi}}$ $= \frac{12(3)}{(2)\ (105.093)}$ $= \frac{36}{210.186}$ = 0.171	$= \frac{12xi}{(n_{OM})_i\, \mu_{OMi}}$ $= \frac{12(2)}{(1)\ (125.147)}$ $= \frac{24}{125.147}$ = 0.192
$(\frac{COD}{TOC})_i = \frac{2(n_{OM})_i \text{ xi } (4-ONci)}{3xi}$	$= \frac{2(n_{OM})_i \text{ xi } (4-ONci)}{3xi}$ $= \frac{2(3)(2)(4-(-2))}{3(2)}$ $= \frac{2(36)}{3(2)}$ = 12.000	$= \frac{2(n_{OM})_i \text{ xi } (4-ONci)}{3xi}$ $= \frac{2(2)(3)(4-(0.667))}{3(3)}$ $= \frac{2(28.002)}{3(3)}$ = 6.247	$= \frac{2(n_{OM})_i \text{ xi } (4-ONci)}{3xi}$ $= \frac{2(1)(2)(4-(-1))}{3(2)}$ $= \frac{2(10)}{3(2)}$ = 3.333

(iii) Calculate the total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of the multiple molecules

Total nO_2 $= \frac{\Sigma(n_{OM})_i\, xi\,(4-ONci)}{4}$	Total COD $= \frac{8\Sigma(n_{OM})_i xi\,(4-ONci)}{\Sigma(n_{OM})_i\, \mu_{OMi}}$	Total TOC $= \frac{12\Sigma xi}{\Sigma(n_{OM})_i\, \mu_{OMi}}$	Total $\frac{COD}{TOC}$ $= \frac{2\Sigma(n_{OM})_i\, xi\,(4-ONci)}{3\Sigma xi}$
$= \frac{\Sigma(n_{OM})_i\, xi\,(4-ONci)}{4}$ $= \frac{(36+28.002+10)}{4}$ $= \frac{74.002}{4}$ = 18.505	$= \frac{8\Sigma(n_{OM})_i\, xi\,(4-ONci)}{\Sigma(n_{OM})_i\, \mu_{OMi}}$ $= \frac{8(36+28.002+10)}{(3)\,(94.200)+(2)\,(105.093)+(1)\,(125.147)}$ $= \frac{8(74.002)}{617.933}$ = 0.958	$= \frac{12\Sigma xi}{\Sigma(n_{OM})_i\, \mu_{OMi}}$ $= \frac{12(2+3+2)}{(3)\,(94.200)+(2)\,(105.093)+(1)\,(125.147)}$ $= \frac{12(7)}{617.933}$ = 0.136	$= \frac{2\Sigma(n_{OM})_i\, xi\,(4-ONci)}{3\Sigma xi}$ $= \frac{2(36+28.002+10)}{3(2+3+2)}$ $= \frac{2(74.002)}{3(7)}$ = 7.048

With reference to Table 4, any biomass, biowaste, or biomaterial can be represented by an empirical formula. Any complicated biomass is considered a single molecule or an organic matter. The calculation of the total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of multiple molecules or organic matters is demonstrated in Example 2.

Example 2. Given three different biomass molecules which contain 1.000 mole of $C_5H_7O_2N$, 2.000 moles of $C_8H_{14}O_4N$, and 3.000 moles of $C_{118}H_{170}O_{57}N_{17}P$, count the total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of the multiple molecules.

(i) Determine the values of n_{OM}, x, μ, and ONc of different types of molecules

$C_5H_7O_2N$				$C_8H_{14}O_4N$				$C_{118}H_{170}O_{57}N_{17}P$			
n_{OM}	x	μ	ONc	n_{OM}	x	μ	ONc	n_{OM}	x	μ	ONc
1.000	5	113.116	0.000	2.000	8	188.203	-0.375	3.000	118	2769.694	-0.085

(ii) Count the values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of different types of molecules

Single molecule	$C_5H_7O_2N$	$C_8H_{14}O_4N$	$C_{118}H_{170}O_{57}N_{17}P$
$(nO_2)_i = \frac{(n_{OM})_i\ xi\ (4-ONci)}{4}$	$= \frac{(n_{OM})_i\ xi\ (4-ONci)}{4}$ $= \frac{(1)(5)(4-(0))}{4}$ $= \frac{20}{4}$ = 5.000	$= \frac{(n_{OM})_i\ xi\ (4-ONci)}{4}$ $= \frac{(2)(8)(4-(-0.375))}{4}$ $= \frac{70}{4}$ = 17.500	$= \frac{(n_{OM})_i\ xi\ (4-ONci)}{4}$ $= \frac{(3)(118)(4-(-0.085))}{4}$ $= \frac{1146.09}{4}$ = 286.500
$(COD)_i = \frac{8(n_{OM})_i\ xi\ (4-ONci)}{n_{OMi}\ \mu_{OMi}}$	$= \frac{8(n_{OM})_i\ xi\ (4-ONci)}{n_{Omi}\ \mu_{Omi}}$ $= \frac{8(1)(5)(4-(0))}{(1)(113.116)}$ $= \frac{8(20)}{113.116}$ $= \frac{160}{113.116}$ = 1.414	$= \frac{8(n_{OM})_i\ xi\ (4-ONci)}{n_{OMi}\ \mu_{OMi}}$ $= \frac{8(2)(8)(4-(-0.375))}{(2)(188.203)}$ $= \frac{8(70)}{376.406}$ $= \frac{560}{376.406}$ = 1.488	$= \frac{8(n_{OM})_i\ xi\ (4-ONci)}{n_{OMi}\ \mu_{OMi}}$ $= \frac{8(3)(118)(4-(-0.085))}{(3)(2769.694)}$ $= \frac{8(1146.09)}{8309.082}$ $= \frac{11568.72}{8309.082}$ = 1.392
$(TOC)_i = \frac{12xi}{(n_{OM})_i\ \mu_{OMi}}$	$= \frac{12xi}{(n_{OM})_i\ \mu_{OMi}}$ $= \frac{12(5)}{(1)\ (113.116)}$ $= \frac{60}{113.116}$ = 0.530	$= \frac{12xi}{(n_{OM})_i\ \mu_{OMi}}$ $= \frac{12(8)}{(2)\ (188.203)}$ $= \frac{96}{376.406}$ = 0.255	$= \frac{12xi}{(n_{OM})_i\ \mu_{OMi}}$ $= \frac{12(118)}{(3)\ (2769.694)}$ $= \frac{1416}{8309.082}$ = 0.170
$(\frac{COD}{TOC})_i = \frac{2(n_{OM})_i\ xi\ (4-ONci)}{3xi}$	$= \frac{2(n_{OM})_i\ xi\ (4-ONci)}{3xi}$ $= \frac{2(1)(5)(4-(0))}{3(5)}$ $= \frac{2(20)}{3(5)}$ = 2.667	$= \frac{2(n_{OM})_i\ xi\ (4-ONci)}{3xi}$ $= \frac{2(2)(8)(4-(-0.375))}{3(8)}$ $= \frac{2(70)}{3(8)}$ = 5.833	$= \frac{2(n_{OM})_i\ xi\ (4-ONci)}{3xi}$ $= \frac{2(3)(118)(4-(-0.085))}{3(118)}$ $= \frac{2(1446.09)}{3(118)}$ = 8.170

(iii) Calculate the total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of the multiple molecules

Total nO_2	Total COD	Total TOC	Total $\frac{COD}{TOC}$
$=\frac{\Sigma(n_{OM})_i\ xi\ (4-ONci)}{4}$	$=\frac{8\Sigma n_{OMi}\ xi\ (4-ONci)}{\Sigma n_{OMi}\ \mu_{OMi}}$	$=\frac{12\Sigma xi}{\Sigma n_{OMi}\ \mu_{OMi}}$	$=\frac{2\Sigma n_{OMi}\ xi\ (4-ONci)}{3\Sigma xi}$
$=\frac{\Sigma(n_{OM})_i\ xi\ (4-ONci)}{4}$	$=\frac{8\Sigma(n_{OM})_i\ xi\ (4-ONci)}{\Sigma(n_{OM})_i\ \mu_{OMi}}$	$=\frac{12\Sigma xi}{\Sigma(n_{OM})_i\ \mu_{OMi}}$	$=\frac{2\Sigma(n_{OM})_i\ xi\ (4-ONci)}{3\Sigma xi}$
$=\frac{(20+70+1146.09)}{4}$	$=\frac{8(20+70+1146.09)}{(1)\ (113.116)+(2)\ (188.203)+(3)\ (2769.694)}$	$=\frac{12(5+8+118)}{(1)\ (113.116)+(2)\ (188.203)+(3)\ (2769.694)}$	$=\frac{2(20+70+1146.09)}{3(5+8+118)}$
$=\frac{1236.09}{4}$	$=\frac{8(1236.09)}{8798.604}$	$=\frac{12(131)}{8798.604}$	$=\frac{2(1236.09)}{3(131)}$
= 309.023	= 1.124	= 0.179	= 6.291

5. Conclusion

ONc and theoretical COD of organic matter are two important redox parameters. In this article, ONc is developed as a metric for quantifying theoretical COD. Based on any given formula, empirical or structural, of an organic matter which can either be in molecular or ionic form, the relationships among ONc, x, μOM, COD, TOC, and $\frac{COD}{TOC}$ are established. By using $nO_2 = \frac{x(4-ONc)}{4}$ as a medium, the mathematical equations of COD = $\frac{8x(4-ONc)}{\mu_{OM}}$, TOC = $\frac{12x}{\mu OM}$, and $\frac{COD}{TOC} = \frac{2(4-ONc)}{3}$ are formulated for any single organic matter when n_{OM} = 1 mole. Furthermore, the total values of nO_2, COD, TOC, and $\frac{COD}{TOC}$ of multiple organic matters are developed as $\frac{\Sigma(n_{OM})_i\ xi\ (4-ONci)}{4}$, $\frac{8\Sigma(n_{OM})_i\ xi\ (4-ONci)}{\Sigma n_{OMi}\ \mu_{OMi}}$, $\frac{12\Sigma xi}{\Sigma n_{OMi}\ \mu_{OMi}}$, and $\frac{2\Sigma(n_{OM})_i\ xi\ (4-ONci)}{3\Sigma xi}$ respectively.

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Authors contributions

Dr. Pong Kau Yuen was responsible for designing the study, drafting, and revising the manuscript. Dr. Cheng Man Diana Lau was responsible for revising the manuscript. All authors read and approved the final manuscript.

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Data sharing statement

No additional data are available.

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