5.2 Methods for calculating the technological parameters of the gasification of carboncontaining substances

The results of transformations of carbon-containing substance through their gasification are determined by the type of substance, its composition, nature, ratio of reacting components, heat transfer conditions, temperature in the reaction space, and other factors. The high value of the degree of carbon conversion of the processed substance is achieved precisely by the stoichiometric ratio of the reacting components.

The stoichiometric or theoretical ratio in the gasification of carbon-containing substance is the composition of the reacting components (oxidant/carbon), when the oxidant is supplied in an amount sufficient for the complete conversion of carbon and other gas-forming elements of the substance.

The stoichiometric oxidant consumption coefficient (α) is a specific indicator that indicates the amount of an oxidizing substance of a certain nature for the complete conversion of a unit of a carbon-containing substance with its own physical and chemical properties. Thus, the consumption coefficient of the oxidizer will be different both for carbon-containing substance with different elemental composition and for an oxidizer of different nature.

The maximum yield of thermal transformation products occurs at a concentration of the reacting components corresponding to their stoichiometric ratios, that is, the ratios of the masses involved in thermal transformation reactions.

The processes of gasification of carbon-containing substance, depending on the type of oxidizer, are divided into oxygen, steam and air [261, 262, 263]. These processes occur on the basis of such basic reactions:

$$2C + O_2 = 2CO \quad (1)$$

$$C + H_2O = CO + H_2 \quad (2)$$

$$2C + O_2 + N_2 = 2CO + N_2 \quad (3)$$

Let's rewrite reaction (1) for 1 kg of carbon:

$$1 \text{ kg } (C) + 32/24 \text{ kg } (O_2) = 56/24 \text{ kg } (CO)$$

$$1 \text{ kg } (C) + 1.333 \text{ kg } (O_2) = 2.333 \text{ kg } (CO) \quad (4)$$

That is, for the oxidation of 1 kg of carbon during gasification, 1.333 kg of oxygen is needed, while we get 2.333 kg of CO.

We write the reaction (2) in a similar way:

$$12 \text{ kg (C)} + 18 \text{ kg } (H_2O) = 28 \text{ kg (CO)} + 2 \text{ kg } (H_2)$$

$$1 \text{ kg (C)} + 18/12 \text{ kg } (H_2O) = 28/12 \text{ kg (CO)} + 2/12 \text{ kg } (H_2)$$

$$1 \text{ kg (C)} + 1.5 \text{ kg } (H_2O) = 2.333 \text{ kg (CO)} + 0.167 \text{ kg } (H_2) \qquad (5)$$

According to reaction (2), for the gasification of 1 kg of C, 1.5 kg of H_2O is needed, and in this case we will obtain 2.333 kg of CO and 0.167 kg of H_2.

With the known elemental composition of the carbon-containing substance, it is possible to determine the required stoichiometric amount of the oxidizing agent for gasification of 1 kg of the carbon-containing substance.

Indeed, according to (4) and (5), if 1 kg of carbon-containing substance contains $C^p/100$ kg of carbon, then the oxygen demand for its complete gasification will be $1.333 \cdot C^p/100$ kg, and water $1.5 \cdot C^p/100$ kg (where C^p is the carbon content in the carbon-containing substance, (% (wt.)).

However, in the composition of the carbon-containing substance there is some amount of water ($W^p/100$) and oxygen ($O^p/100$) (where W^p, O^p are the content of water and oxygen in the carbon-containing substance, respectively, (% (mass)), respectively, the need in the oxidizer will decrease. According to the chemical reaction (1), we determine how much carbon will react with oxygen, which is part of the carbon-containing substance.

Let's write reaction (1) for 1 kg of oxygen.

$$24/32 \text{ kg (C)} + 32/32 \text{ kg } (O_2) = 56/32 \text{ kg (CO)}.$$

That is, having spent 1 kg of O_2, it will undergo a transformation of 24/32 kg of carbon, and having spent $O^p/100$ - oxygen, carbon will react ($C_{O2)}$) in the amount:

$$C_{(O2)} = 24/32 \cdot O^p/100 = 0.75 \cdot O^p/100 \qquad (6)$$

Similarly, according to the chemical reaction (2), the amount of carbon ($C_{(H2O)}$), which will react with the water contained in the carbon-containing environment, will be:

$$C_{(H2O)} = 12/18 \cdot W^p/100 = 0.667 \cdot W^p/100 \quad (7)$$

Then, the amount of carbon that requires an additional oxidizer from outside ($C_м$) is determined as:

$$C_{м} = C^p/100 – (C_{(O2)} + C_{(H2O)})=$$
$$= C^p/100 – (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100) \quad (8)$$

Let us determine the consumption coefficient of the oxidizer when using pure oxygen, i.e. oxygen consumption coefficient (α_{O2}).

Let us use reaction (1) for the gasification of a carbon-containing substance, when oxygen is used as an oxidizing agent. It follows from the reaction that 1.333 kg of oxygen is needed to oxidize 1 kg of carbon during gasification. Since 1 kg of the working composition of the carbon-containing substance contains carbon $C^p/100$, then $1.333 \cdot C^p/100$ oxygen is necessary for its gasification.

We take into account that in the composition of the carbon-containing substance there is some proportion of oxygen $O^p/100$ and water $W^p/100$, which will reduce the required amount of the introduced oxidizer. Then, for the oxidation of carbon in the amount of $C_м$, oxygen in the amount of 1.333 $C_м$ is needed, that is, the consumption coefficient of the oxidizer, in this case oxygen (α_{O2}, kg O2 / kg of substance), will be equal to:

$$\alpha_{O2} = 1.333 \cdot (C^p/100 – (C_{(O2)} + C_{(H2O)})) =$$
$$= 1.333 \cdot (C^p/100 – (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100)) \quad (9)$$

Let us determine the consumption coefficient of the oxidizer when water is used as an oxidizer, i.e. water consumption coefficient (α_{H20}).

According to equation (5), 1.5 kg of H_2O is needed to oxidize 1 kg of carbon. Then, for the oxidation of carbon in the amount of $C_м$, water is needed in the amount of 1.5 $C_м$, that is, the consumption coefficient of the oxidizer, in this case water (α_{H20}, kgH20 / kg of substance), will be equal to:

$$\alpha_{H20} =1.5 \cdot (C^p/100 – (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100)) \quad (10)$$

Let us consider reaction (3) and determine the consumption coefficient of the oxidizer when air is used as an oxidizer, i.e. airflow coefficient (α_{air}).

We proceed from the fact that the specific amount of oxygen for the gasification of a carbon-containing substance is determined by formula (9). To calculate the specific consumption of air used as an oxidizing agent during gasification, we take into account that oxygen in the air contains 23.1% (mass.). Then the air flow coefficient (α_{air}, kg air / kg substance) is equal to:

$$\alpha_{air} = 100/23.1 \cdot 1.333 \cdot (C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100) =$$
$$= 5.77 \cdot (C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100) \quad (11)$$

Given the quantity or consumption of a carbon-containing substance (G_y, kg or kg/s) with specific physical and chemical characteristics, we determine the amount or consumption of the oxidizer (in kg or kg/s):

- with oxygen gasification:

$$M_{O2} = \alpha_{O2} \cdot G_y = 1.333 \cdot (C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100)) \cdot G_y \quad (12)$$

- with steam gasification:

$$M_{H20} = \alpha_{H20} \cdot G_y = 1.5 \cdot (C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100)) \cdot G_y \quad (13)$$

- with air gasification:

$$M_{air} = \alpha_{air} \cdot G_y = 5.77 \cdot (C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100) \cdot G_y \quad (14)$$

The next step is to consider the theoretical yield of carbon-containing substance gasification products depending on their physicochemical properties and the type of oxidizer.

With oxygen gasification occurring according to the main reaction (1) and additional (2), the mass yield of H_2 ($M_{(O2)H2(p2)}$, kg or kg/s), formed during the interaction of own water with carbon according to reaction (2), will be equal to:

$$M_{(O2)H2(p2)} = 2/18 \cdot G_y \cdot W^p/100 = 0.111 \cdot G_y \cdot W^p/100 \quad (15)$$

Then the volumetric yield of H_2 under normal conditions ($V_{(O2)H2}$, m^3 or m^3/s) will be:

$$V_{(O2)H2(p2)} = M_{(O2)H2(p2)} / \rho_{H2} = M_{(O2)H2(p2)} / 0.089 = 1.247 \cdot G_y \cdot W^p/100, \quad (16)$$

where ρ_{H2} – the density of H_2 under normal conditions, ρ_{H2} = 0.089 kg/m_3.

The mass yield of CO ($M_{(O2)CO}$, kg or kg/s), formed during the interaction of own water with carbon according to reaction (2), will be equal to:

$$M_{(O2)CO(p2)} = 28/18 \cdot G_y \cdot W^p/100 = 1.556 \cdot G_y \cdot W^p/100 \quad (17)$$

Then the volumetric yield of CO under normal conditions ($V_{(O2)CO(p2)}$, m_3 or m^3/s), formed during the interaction of own water with carbon according to reaction (2), will be:

$$V_{(O2)CO(p2)} = M_{(O2)CO(p2)} / \rho_{CO} = M_{(O2)CO(p2)} / 1.25 = 1.245 \cdot G_y \cdot W^p/100, \quad (18)$$

where ρ_{CO} – the density of CO under normal conditions, ρ_{CO} = 1.25 kg/m^3.

In this case, the amount of carbon that reacted with its own water according to reaction (2) is equal to:

$$M_{(O2)C(p2)} = 12/18 \cdot G_y \cdot W^p/100 = 0.667 \cdot G_y \cdot W^p/100 \quad (19)$$

The amount of carbon left after reaction (2) to carry out reaction (1):

$$M_{(O2)C(p1)} = G_y \cdot C^p/100 - M_{(O2)C(p2)} = G_y \cdot (C^p/100 - 0.667 \cdot W^p/100) \quad (20)$$

Then the mass yield of CO ($M_{(O2)CO(p1)}$, kg or kg/s) formed by reaction (1) will be equal to:

$$M_{(O2)CO(p1)} = 56/24 \cdot M_{(O2)C(p1)} = 2.333 \cdot G_y \cdot (C^p/100 - 0.667 \cdot W^p/100) \quad (21)$$

And the volumetric yield of CO under normal conditions ($V_{(O2)CO(p1)}$, m^3 or m^3/s) will be:

$$V_{(O2)CO(p1)} = M_{(O2)CO(p1)} / \rho_{CO} = M_{(O2)CO(p1)} / 1.25 =$$
$$= 1.866 \cdot (G_y \cdot (C^p/100 - 0.667 \cdot W^p/100)) \quad (22)$$

The total mass yield of CO ($M_{(O2)CO}$, kg or kg/s), formed during the oxygen gasification of carbon-containing substance, will be equal to:

$$M_{(O2)CO} = M_{(O2)CO(p1)} + M_{(O2)CO(p2)} =$$
$$= 2.333 \cdot G_y \cdot (C^p/100 - 0.667 \cdot W^p/100) + 1.556 \cdot W^p/10) \quad (23)$$

And the total volumetric yield of CO under normal conditions ($V_{(O2)CO}$, m^3 or m^3/s):

$$V_{(O2)CO} = V_{(O2)CO(p1)} + V_{(O2)CO(p2)} =$$
$$= 1.866 \cdot G_y \cdot (C^p/100 - 0.667 \cdot W^p/100) + 1.245 \cdot W^p/100) \quad (24)$$

Let us consider the steam gasification of carbon-containing substance, which occurs according to the main reaction (2) and additional reaction (1).

The mass yield of CO ($M_{(H20)CO(p1)}$, kg or kg/s), formed during the interaction of its own oxygen with carbon according to reaction (1), is equal to:

$$M_{(H20)CO(p1)} = 56/32 \cdot G_y \cdot O^p/100 = 1.75 \cdot G_y \cdot O^p/100 \quad (25)$$

The volumetric yield of CO under normal conditions ($V_{(H20)CO(p1)}$, m^3 or m^3/s), formed during the interaction of native oxygen with carbon according to reaction (1), will be:

$$V_{(H20)CO(p1)} = M_{(H20)CO(p1)} / \rho_{CO} = M_{(H20)CO(p1)} / 1.25 = 1.4 \cdot G_y \cdot O^p/100, \quad (26)$$

Then the amount of carbon that reacted with its own oxygen according to reaction (1) is:

$$M_{(H20)C(p1)} = 24/32 \cdot G_y \cdot O^p/100 = 0.75 \cdot G_y \cdot O^p/100 \quad (27)$$

The amount of carbon left after reaction (1) to carry out reaction (2):

$$M_{(H20)C(p2)} = G_y \cdot C^p/100 - M_{(H20)C(p1)} = G_y \cdot (C^p/100 - 0.75 \cdot O^p/100) \quad (28)$$

Then the mass yield of CO ($M_{(H20)CO(p2)}$, kg or kg/s) formed by reaction (2) will be equal to:

$$M_{(H20)CO(p2)} = 28/12 \cdot M_{(H20)C(p2)} = 2.333 \cdot G_y \cdot (C^p/100 - 0.75 \cdot O^p/100) \quad (29)$$

And the volumetric yield of CO under normal conditions ($V_{(H202)CO(p2)}$, m^3 or m^3/s) will be:

$$V_{(H20)CO(p2)} = M_{(H20)CO(p2)} / \rho_{CO} = M_{(H20)CO(p2)} / 1.25 =$$
$$= 1.866 \cdot (G_y \cdot (C^p/100 - 0.75 \cdot O^p/100)) \quad (30)$$

The total mass yield of CO ($M_{(H20)CO}$, kg or kg/s), formed during the steam gasification of carbon-containing substance, will be equal to:

$$M_{(H20)CO} = M_{(H20)CO(p1)} + M_{(H20)CO(p2)} =$$
$$= 1.75 \cdot G_y \cdot O^p/100 + 2.333 \cdot G_y \cdot (C^p/100 - 0.75 \cdot O^p/100)=$$
$$= G_y (1.75 \cdot O^p/100 + 2.333 \cdot (C^p/100 - 0.75 \cdot O^p/100) , \quad (31)$$

And the total volumetric yield of CO under normal conditions ($V_{(H20)CO}$, m^3 or m^3/s):

$$V_{(H20)CO} = V_{(H20)CO(p1)} + V_{(H20)CO(p2)} =$$
$$= G_y (1.4 \cdot O^p/100 + 1.866 \cdot (C^p/100 - 0.75 \cdot O^p/100) \quad (32)$$

During steam gasification, the mass yield of H_2 ($M_{(O2)H2(p2)}$, kg or kg/s) formed during the interaction of water with carbon according to reaction (2) will be equal to:

$$M_{(H20)H2(p2)} = 2/12 \cdot M_{(H20)C(p2)} = 0.167 \cdot G_y \cdot (C^p/100 - 0.75 \cdot O^p/100) \quad (33)$$

Then the volume output of H_2 under normal conditions ($V_{(H20)H2}$, m^3 or m^3/s) will be:

$$V_{(H20)H2(p2)} = M_{(H20)H2(p2)} / \rho_{H2} = M_{(O2)H2(p2)} / 0.089 =$$
$$= 1.876 \cdot G_y \cdot (C^p/100 - 0.75 \cdot O^p/100) \quad (34)$$

Let us consider the air gasification of carbon-containing substance, which occurs according to the main reaction (3) and additional reactions (1) and (2).

The mass yield of CO ($M_{(air)CO(p1)}$, kg or kg/s), formed during the interaction of its own oxygen with carbon according to reaction (1), is equal to:

$$M_{(air)CO(p1)} = 56/32 \cdot G_y \cdot O^p/100 = 1.75 \cdot G_y \cdot O^p/100 \quad (35)$$

The volumetric yield of CO under normal conditions ($V_{(H20)CO(p1)}$, m^3 or m^3/s), formed during the interaction of native oxygen with carbon according to reaction (1), will be:

$$V_{(air)CO(p1)} = M_{(air)CO(p1)} / \rho_{CO} = M_{(H20)CO(p1)} / 1.25 = 1.4 \cdot G_y \cdot O^p/100, \quad (36)$$

Then the amount of carbon that reacted with its own oxygen according to reaction (1) is:

$$M_{(air)C(p1)} = 24/32 \cdot G_y \cdot O^p/100 = 0.75 \cdot G_y \cdot O^p/100 \quad (37)$$

The mass yield of H2 ($M_{(air)H2(p2)}$, kg or kg/s), formed during the interaction of own water with carbon according to reaction (2), will be equal to:

$$M_{(air)H2(p2)} = 2/18 \cdot G_y \cdot W^p/100 = 0.111 \cdot G_y \cdot W^p/100 \quad (38)$$

Then the volumetric yield of H2 under normal conditions ($V_{(O2)H2}$, m_3 or m^3/s) will be:

$$V_{(air)H2(p2)} = M_{(air)H2(p2)} / \rho_{H2} =$$
$$= M_{(air)H2(p2)} / 0.089 = 1.247 \cdot G_y \cdot W^p/100 \quad (39)$$

The mass yield of CO ($M_{(air)CO}$, kg or kg/s), formed during the interaction of own water with carbon according to reaction (2), will be equal to:

$$M_{(air)CO(p2)} = 28/18 \cdot G_y \cdot W^p/100 = 1.556 \cdot G_y \cdot W^p/100 \quad (40)$$

Then the volumetric yield of CO under normal conditions ($V_{(air)CO(p2)}$, m^3 or m^3/s), formed during the interaction of own water with carbon according to reaction (2), will be:

$$V_{(air)CO(p2)} = M_{(air)CO(p2)} / \rho_{CO} = M_{(air)CO(p2)} / 1.25 = 1.245 \cdot G_y \cdot W^p/100 \quad (41)$$

In this case, the amount of carbon that reacted with its own water according to reaction (2) is equal to:

$$M_{(air)C(p2)} = 12/18 \cdot G_y \cdot W^p/100 = 0.667 \cdot G_y \cdot W^p/100 \quad (42)$$

The amount of carbon that will remain after reactions (1) and (2) to carry out reaction (3):

$$M_{(air)C(p3)} = G_y \cdot C^p/100 - M_{(air)C(p1)} - M_{(air)C(p2)} =$$
$$= G_y \cdot C^p/100 - 0.75 \cdot G_y \cdot O^p/100_{)} - 0.667 \cdot G_y \cdot W^p/100 \quad (43)$$

The mass yield of CO ($M_{(O2)CO(p1)}$, kg or kg/s), formed by reaction (3), will be equal to:

$$M_{(air)CO(p3)} = 56/24 \cdot M_{(O2)C(p3)} =$$
$$= 2.333 \cdot G_y \cdot (C^p/100 - 0.75 \cdot O^p/100) - 0.667 \cdot W^p/100) \quad (44)$$

And the volumetric yield of CO under normal conditions ($V_{(air)CO(p3)}$, m^3 or m^3/s) will be:

$$V_{(air)CO(p3)} = M_{(air)CO(p3)} / \rho_{CO} = M_{(air)CO(p3)} / 1.25 =$$
$$= 1.866 \cdot G_y \cdot (C^p/100 - 0.75 \cdot O^p/100) - 0.667 \cdot W^p/100) \quad (45)$$

The total mass yield of CO ($M_{(air)CO}$, kg or kg/s), formed during air gasification of carbon-containing substance, will be equal to:

$$M_{(air)CO} = M_{(air)CO(p1)} + M_{(air)CO(p2)} + M_{(air)CO(p3)} =$$
$$= G_y (1.75 \cdot O^p/100 + 1.556 \cdot W^p/100 +$$
$$+ 2.333 \cdot (C^p/100 - 0.75 \cdot O^p/100) - 0.667 \cdot W^p/100), \quad (46)$$

And the volumetric yield of CO under normal conditions ($V_{(air)CO(p3)}$, m^3 or m^3/s) will be:

$$V_{(air)CO} = M_{(air)CO} / \rho_{CO} =$$
$$= 0.8 \cdot G_y (1.75 \cdot O^p/100 + 1.556 \cdot W^p/100 +$$
$$+ 2.333 \cdot (C^p/100 - 0.75 \cdot O^p/100) - 0.667 \cdot W^p/100) \quad (47)$$

Since the air contains nitrogen and during air gasification, it does not take part in chemical reactions, i.e. is actually neutral, then its amount at the outlet will be equal to the amount of nitrogen introduced with air.

Using formula (14) and taking into account that the mass content of nitrogen in the air is 76.9%, we determine the mass yield of N2 ($M_{(air)N2}$, kg or kg/s), with air gasification:

$$M_{(air)N2} = 0.769 \cdot M_{air} =$$

$$= 4.473\ G_y \cdot (C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100) \quad (48)$$

And the volumetric output of N_2 under normal conditions ($V_{(air)N2}$, m^3 or m^3/s) will be:

$$V_{(air)N2} = M_{(air)N2} / \rho_{N2} = M_{(air)N2} / 1.25 =$$

$$= 3.578 \cdot G_y(C^p/100 - (0.75 \cdot O^p/100 + 0.667 \cdot W^p/100), \quad (49)$$

where ρ_{N2} – the density of N_2 under normal conditions, $\rho_{N2} = 1.25$ kg/m^3.

Thus, the above method for calculating technological parameters makes it possible to determine the consumption coefficients of oxidizers and the amount of oxidizer, as well as the amount of products formed during the gasification of carbon-containing substance, depending on their physicochemical properties.