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Modeling of the Oxidation of Lignite and Calculation of Carbon Footprint in the Gas Phase

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| Keywords | Abstract |
|------------------------|--|
| | The paper examines local coal sources and presents their physicochemical |
| coal-air system | characteristics. The Kara-Keche coal deposit has been adopted as the model system, |
| | with the following composition percentages: hydrogen (H) - 3.65%, carbon (C) - 79.03%, |
| oxidation | nitrogen (N) - 0.84%, sulfur (S) - 0.55%, and moisture content considering oxygen (H ₂ O) |
| | - 18.47%. Thermodynamic modeling of the coal oxidation process at the maximum |
| carbon footprint | entropy of the system was carried out. The concentration distribution of components |
| _ | containing H, C, N, S, and O, as well as active particles and condensed phases, was |
| thermodynamic modeling | established over a wide temperature range (298-3000 K). At the theoretical combustion |
| | temperature of coal (1998 K), the complete composition of carbon-containing |
| entropy | substances in the gas phase was determined, and the additive value of the carbon |
| | footprint was calculated for the first time, taking into account the initial mass of carbon |
| gas phase | in the solid phase. The anthropogenic carbon load in the gas phase is useful for |
| | assessing the carbon capacity per unit of industrial production obtained from the |
| | combustion of solid fuel. |

Cite

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INTRODUCTION

It is well-known that in the Kyrgyz Republic, the primary sources of energy and heat are solid fuels, namely local coals from various deposits. Consequently, the coal-fuel industry encompasses a full range of technological processes for the processing, utilization, and combustion of solid fuels. There are approximately 70 coal deposits with reserves of 2.2 billion tons, each with different characteristics (Dzhamanbaev, 1983; Solpuev, 1996; Sabyrbekov, 2019). The main coal deposits are located in four basins (Kashirin, 1951; 1990): Southern Fergana (Suluktu, Kyzyl-Kiya, Beshburhan, Abshir, Almalyk), Ozgon (Kok-Jangak, Kumbel, Zyndan); Northern Fergana (Tash-Komur, Kara-Tut, Tegenek); Kavak (Kok-Moynok, Mingkush, Kara-Keche), as well as in three coal-bearing areas (Solpuev, 1996): Alay, Alabuka-Chatyrkol, and Southern Isyk-Gol (see Fig. 1).



Fig.1. Location of coal deposits in the Kyrgyz Republic

Each year, approximately 2 million tons of coal are used during the heating season. The energy sector obtains 70% of its energy and heat from the Kara-Keche coal deposit (Sabyrbekov, 2019). Considering these circumstances, the physicochemical characteristics of the Kara-Keche coal deposit are provided in table 1 (Kashirin, 1951; Dzhamanbaev, 1983), and based on these, a thermodynamic model for this study has been developed.

MATERIALS AND METHODS

In the computational experiments, the coals of the Kara-Keche deposit were considered as the model system with the following composition percentages: hydrogen (H) - 3.65%, carbon (C) - 79.03%, nitrogen (N) - 0.84%, sulfur (S) - 0.55%, total moisture (H₂O) - 18.47%, and oxygen (O) - 15.88% (Table 1) (Mironov, 1991; Cheng, 2008; Tazhibaev, 2016; Kapakov, 2022). The oxidation processes of the solid phase were studied over a wide temperature range (298-3000 K) at the maximum entropy of the system using the "Terra" software complex (Sinyarev, 1982; Belov, 2013). The excess oxidizer (air) was set at 1.5 (alpha factor): N - 10.05; O - 2.67. The calorific value of the coal was 29.57 MJ/kg. The overall calculation matrix, considering all elements in the phases, was as follows (mol/kg): H – 49.209, C - 57.087, N - 6.745, S - 0.149, O - 10.343.

Table 1. Physico-chemical and thermo-technical characteristics of the Kara-Keche coal deposit

| Technical composition | | | | | | | | |
|---------------------------------|---------------------------------|----|----------------|---------------------|-----------|--------|--|--|
| Comple | humidity (W), % | | Ash content, | volatile substances | s bitumen | | | |
| Sample | external | aı | nalytical | A ^d , % | (V),% | (B), % | | |
| 1K | 9,68 | | 11,68 | 10,24 | 34,45 | 0,45 | | |
| 2K | 6,07 | | 16,05 | 16,85 | 38,45 | 0,64 | | |
| Physicochemical characteristics | | | | | | | | |
| Comple | humic acids (HA), density, g/cn | | m³ | functional composi | ition, % | | | |
| Sample | % | | approx. actual | | -COOH | -OH | | |

| 1K | 6, | 3 | 1,17 | 7 | 1,51 | | 0,99 | | | 5,27 |
|---------------------------|--------------------------|--------------------------------------|---------------------|---------------------------------|------------|-------|---------------|---------|--------------------|----------|
| 2K | 10,2 | 29 | 1,21 | ,21 1,58 | | | 0,78 | | | 4,61 |
| | | | | Specif | fic heat o | apaci | ity | | | |
| | | Ç | Qi | | | | | Qs | | |
| | | | | | | | | | | |
| Sample | ka | al/kg | | MJ/ | kg | | kcal/kg | | Ν | 1J/kg |
| 1K | , | 5095 | | 21,3 | 32 | | 7514 | | 31,44 | |
| 2K | | 4911 | | 20,5 | 55 | | 7730 | | 730 32,34 | |
| | | Elemental composition, % Atomic bond | | | | | | nd | | |
| Sample | С | Н | | N | S | | 0 | C/H | I | O/C |
| 1K | 77,59 | 4,1 | | 1,32 | 0,4 | 6 | 16,53 | 1,58 | | 0,16 |
| 2K | 76,13 | 4,61 | | 1,17 | 0,4 | 7 | 17,62 | 1,38 | | 0,17 |
| анализ | 79,03 | 3,65 | | 0,84 | 0,5 | 5 | 15,88 | | | |
| | | | Pet | rograph | nic comp | ositi | on, % | | | |
| | | | | | | lip | tinite + mace | erinite | M | in.sub.c |
| Sample | vitrinite V _t | semivitrii | nite S _v | S _v inertinite Y L+M | | L+M | | | es, M ₁ | |
| 1K | 35 | 7 | | 44 | 4,5 | | 5 | | | 8,5 |
| continuation of the table | | | | | | | | | | |

| The chemical composition of ash | | | | | | | | | | | | | | |
|---------------------------------|--|--------------------------|--------------------------------|------|----------|-----------------|------|--------------|---------------------|-------------------|--------------------|----|-----------------|-------------------|
| | | Macronutrients in ash, % | | | | | | | | | | | | |
| Sample | SiO | 2 | Fe ₂ O ₃ | Al | O_3 | CaO | l | MgO | | Na ₂ O | +K ₂ O | Mr | nO i | TiO ₂ |
| 1K | 22 | 2 | 12 | 1 | 25 | 17 | | 3 | | | 0,3 | 0 | ,4 | 0,12 |
| 2K | 25 | 5 | 5 | 1 | 29 | 13 | | 4 | | | 0,12 | 0 | ,5 | 0,7 |
| | | | | | The y | vield of | sem | ni-coke | e pro | ducts, | % | | | |
| Sample | Se | mi- | coke, T _s | | Tar | , S | | pyı | oge | nic wat | er, W _s | | Gas | s, G _s |
| 1K | | | 74,36 | | | 2,85 | | | | 1, | 32 | | 1 | 0,5 |
| 2K | | 73,79 | | | 3,07 | | | | - | 2 | | 5 | 8,1 | |
| | Gas composition of coal pyrolysis process, % | | | | | | | | | | | | | |
| Sample | C | O_2 + | H_2S | | C_nH_n | n | CC |) | H_2 | | $C_nH_{2n}+_2$ | | N_2 | |
| 1K | | | 40 | | - 4 | 2,7 | | 14 | 1 | 10,7 | 29,6 | | 3 | 3 |
| 2K | | | 40,2 | | 4 | 2,7 | - | 13,5 | 11 | | 29,9 | | 2 | ,7 |
| | | | | | Com | positior | 1 of | the tai | r <mark>gr</mark> o | up, % | | | | |
| Sample | С _{св.} | Ca ac | arboxylic ids | Pher | nols | prima resins | у | aspha nes | lte | parafi ns. | i neutral oils | 1 | Sol.dis CH₃O | s. in H |
| 1K | 6,2 | | 1,1 | 2 | 0 | 1,2 | | 3 | | 1 | 50 | | 10 | ,5 |
| 2K | 6,9 | | 1 | 2 | 0 | 1,2 | | 3 | | 1 | 49,9 | | 10 | ,6 |

The physical properties of brown coal have been thoroughly studied and are summarized in the accompanying table 1 and fig. 2-5 (Solomon, 1992; Karabaev, 2015; Speight, 2015; Avgushevich, 2019; Niksa, 2019; Azhgaliyeva, 2021; Wilberforce, 2021; Murko, 2022; Maimekov, 2023; Ritchie, 2024).

RESULTS AND DISCUSSIONS

It was noted that the main coal deposits in the republic are located in four basins (Solpuev, 1996), of which the Kavak Valley includes sections: Kara-Keche, Donguz, Min-Kush, Kok-Moynok, Ak-Ulak, Tuura-Kavak, Kashka-Suu, Sary-Kamysh, etc. The total geological reserves of lignite in the republic are estimated at 2.5 billion tons, of which the Kara-Keche basin (Naryn region, Zhumgal district)

accounts for 437.8 million tons, and the Min-Kush - 116 million tons (Kashirin, 1951; Dzhamanbaev, 1983). The basin is 75 km long, in the western part bordered by the Kokomeren River, in the eastern part by the Lake Son-Kol, in the southern part and northern part by the foothills of Moldotoo and Kavak-Too. Coals in the Kavak basin are classified as B (brown), 3B (third brown), and 3VF (third brown fusainite). According to their quality characteristics, gas, briquettes, coal-water fuel suspensions, liquid synthetic fuel, organic acids, and activated carbon can be obtained from the coals of Kara-Keche, Min-Kush, and Kashka-Suu (Kashirin, 1951; 1990).

Figures 2–5 show comparative values of the average moisture content, ash content, volatile matter yield and specific heat of combustion of coals in the republic, including coals from the Kara-Keche deposit (designation: light brown) (Dzhamanbaev, 1983; Solpuev, 1996; Sabyrbekov, 2019).



Fig. 2. Average moisture content of coals from various deposits



Fig. 3. Ash content of coals from various deposits



Fig. 4. Volatile matter yield from coals from various deposits



Fig.5. Average specific heat capacity of combustion of coals for various deposits

The above data show that the average specific heat of combustion of Kara-Keche coals is 28.14 MJ/kg, therefore its demand in winter conditions is significant in the fuel and energy complexes of the republic. Taking into account these circumstances, the Kara-Keche coal deposit was examined and thermodynamic modeling of the coal-air system was carried out. The concentration distribution of H, C, N, S, O containing components, active particles and condensed phases in the gas phase (mol/kg) was established at 1998 K, P = 0.1 MPa (Table 2).

Table 2. Concentration distribution of H, C, N, S, O-containing components, active particles, and condensed phases formed during the oxidation of Kara-Keche coal in air (mol/kg). T=1998 K; P=0.1 MPa; U=2095.1 kJ/kg; S=10.38 kJ/(kg K); I=2637.5 kJ/kg; Lt=0.40 Bt/(m K);

| Cp=2.50 | kI/ | (kg | K). |
|---------|-------------|-----|-----|
| Cp 2.00 | L J/ | 15 | 1 |

| O=0.22×10-9 | H=0.04 | H ₂ =24.36 | OH=0.15 ×10- |
|--|--|--|--|
| H ₂ O=0.7 ×10 ⁻³ | S=0.73 ×10-3 | S ₂ =0.001 | S3=0.47 ×10-7 |
| SO=0.14 ×10-6 | SO ₂ =0.84 ×10 ⁻¹¹ | S ₂ O=0.20 ×10 ⁻⁹ | SH=0.01 |
| $H_2S=0.09$ | HSO=0.19 ×10-10 | SOH=0.27 ×10-9 | H ₂ SO=0.29 ×10-11 |
| N=0.98 ×10-8 | N ₂ =3.29 | NO=0.19 ×10-8 | NH=0.13 ×10-6 |
| NH ₂ =0.79 ×10 ⁻⁶ | NH ₃ =0.11 ×10 ⁻³ | N ₂ H ₂ =0.60 ×10 ⁻¹¹ | NS=0.16 ×10 ⁻⁵ |
| C(c)=46.49 | C=0.11 ×10 ⁻⁸ | C ₂ =0.81 ×10 ⁻¹⁰ | C ₃ =0.10 ×10 ⁻⁸ |
| CO=10.34 | CO ₂ =0.72 ×10-4 | C ₂ O=0.20 ×10-7 | C ₃ O ₂ =0.66 ×10-9 |
| CH=0.48 ×10-8 | CH ₂ =0.69 ×10 ⁻⁶ | CH ₃ =0.27 ×10 ⁻³ | CH ₄ =0.006 |
| C ₂ H=0.26 ×10 ⁻⁵ | C ₂ H ₂ =0.019 | C ₂ H ₃ =0.85 ×10 ⁻⁵ | C ₂ H ₄ =0.81 ×10 ⁻⁴ |
| C ₂ H ₅ =0.15 ×10 ⁻⁷ | C ₂ H ₆ =0.26 ×10 ⁻⁷ | C ₃ H=0.21 ×10 ⁻⁴ | C ₃ H ₄ =0.13 ×10 ⁻⁸ |
| C ₃ H ₆ =0.10 ×10 ⁻¹⁰ | C ₄ H=0.70 ×10 ⁻⁹ | C ₄ H ₂ =0.10 ×10 ⁻³ | C ₄ H ₄ =0.27 ×10 ⁻¹¹ |
| C ₅ H ₆ =0.27 ×10 ⁻¹¹ | $C_6H_6=0.10 \times 10^{-10}$ | CHO=0.47 ×10-5 | CHO ₂ =0.25 ×10 ⁻¹⁰ |
| CH ₂ O=0.27 ×10 ⁻⁵ | CH ₂ O ₂ =0.8 ×10 ⁻¹⁰ | CH ₃ O=0.15 ×10 ⁻¹¹ | CS=0.026 |

| CS ₂ =0.005 | COS=0.001 | CN=0.61 ×10-5 | CN2=0.10 ×10-7 |
|--|---|---|--|
| C ₂ N=0.12 ×10-7 | C ₂ N ₂ =0.58 ×10 ⁻⁵ | NCO=0.83 ×10 ⁻¹⁰ | HCN=0.15 |
| HNC=0.11 ×10-4 | C ₂ HN=0.43 ×10-7 | C ₃ HN=0.001 | C ₅ HN=0.81 ×10 ⁻³ |
| C ₇ HN=0.18 ×10 ⁻³ | C9HN=0.33 ×10-4 | N ₂ C=0.32 ×10 ⁻⁵ | - |
| SH-=0.14 ×10-11 | NH4+=0.91 ×10-11 | CHO+=0.30 ×10-11 | CN-=0.78 ×10-11 |

Based on Table 2, the concentration distribution of carbon-containing components, active particles, and condensed phases in the gas phase was established (Fig. 6, Table 3).



Fig. 6. Concentration distribution of H, C, N, S, O - containing components, active particles, and condensed phases in the gas phase (mol/kg). T = 298 - 3000 K, P = 0.1 MPa.

Table 3. Concentration distribution of carbon-containing components, active particles, and condensed phases in the gas phase (mol/kg). T = 1998 K, P = 0.1 MPa.

| $C(\lambda)$ | C | C | C | C | C |
|---------------------------------|-------------------|-------------------|-------------------------------|-------------------------------|------------------------|
| C(c) | C | C_2 | C3 | C4 | C5 |
| 46,49 | 1,1×10-9 | 8,1×10-11 | 1,0 ×10-9 | 5,1×10 ⁻¹⁴ | 1,9 ×10 ⁻¹³ |
| СО | CO ₂ | C ₂ O | C_3O_2 | CH | CH ₂ |
| 10,34 | 7,2 ×10-5 | 2,0 ×10-8 | 6,6×10-10 | 4,8 ×10-9 | 6,9 ×10-7 |
| CH ₃ | CH ₄ | C ₂ H | C_2H_2 | C_2H_3 | C_2H_4 |
| 2,0 ×10-4 | 6,0 ×10-3 | 2,7 ×10-6 | 1,9 ×10-2 | 8,5 ×10-6 | 8,1 ×10 ⁻⁵ |
| C_2H_5 | C_2H_6 | C ₃ H | C ₃ H ₄ | C_3H_6 | C_3H_8 |
| 1,5 ×10-8 | 2,6 ×10-8 | 2,1 ×10-5 | 1,3 ×10-9 | 1,0×10-11 | 2,4 ×10-13 |
| C ₄ H | C_4H_2 | C_4H_4 | C_4H_6 | C ₅ H ₆ | C_6H_6 |
| 7 ×10 ⁻¹⁰ | 1 ×10-4 | 2,7×10-12 | 2 ×10-13 | 2,7×10-12 | 1,0 ×10-11 |
| СНО | CHO ₂ | CH ₂ O | CH_2O_2 | CH ₃ O | $C_2H_4O_2$ |
| 4,7 ×10-6 | 2,5 ×10-11 | 2,7 ×10-6 | 8 ×10-11 | 1,5×10-12 | 1,8 ×10 ⁻¹⁵ |
| C ₃ H ₆ O | C_2H_4O | CS | CS ₂ | COS | CN |
| 4,6 ×10-15 | 2,7 ×10-14 | 2 ×10-2 | 5 ×10-3 | 1 ×10-3 | 6,1 ×10-6 |
| CN ₂ | C ₂ N | C_2N_2 | NCO | HCN | HNC |
| 1,0 ×10-8 | 1, ×10-8 | 5,8 ×10-6 | 8,3×10-11 | 1,5 ×10-1 | 1 ×10-5 |
| C ₂ HN | C ₃ HN | C5HN | C7HN | C ₉ HN | N ₂ C |

| 4,4 ×10-8 | 1 ×10-3 | 8 ×10-4 | 1 ×10-4 | 3,3 ×10-5 | 3,2 ×10-6 |
|----------------------|------------------------|-----------|-----------|-----------------|-----------|
| C ²⁻ | CO+ | CH+ | C+ | C ²⁺ | |
| 1,9 ×10-17 | 1,3 ×10-19 | 2,6×10-21 | 1,9×10-22 | 1,93 ×10-22 | |
| CHO+ | CN- | - | - | - | |
| 3 ×10 ⁻¹² | 7,8 ×10 ⁻¹² | - | - | - | |

It has been noted that when calculating the carbon footprint, it is necessary to consider not only the masses of carbon oxides (CO, CO_2), methane, and condensed carbon C(s) (Magacho et al., 2024), but also all carbon-containing components, active particles, and condensed phases in the gas phase (Table 4) (Durojaye, 2020).

Table 4. Oxidation of Kara-Keche coal and calculation of additive carbon footprint in
the gas phase (g/kg)

| components and particles in the gas phase | content, mol/kg | content, grams | carbon in the gas phase, g/kg |
|--|-------------------------|------------------------|----------------------------------|
| C(c) | 4,65 ×101 | 557,98 | 557,98 |
| С | 1,12 ×10-9 | 1,34 ×10-8 | 1,34 ×10-8 |
| C ₂ | 8,19 ×10-11 | 1,97 ×10-9 | 1,97 ×10-9 |
| C ₃ | 1,01 ×10-9 | 3,64 ×10 ⁻⁸ | 3,64 ×10-8 |
| C ₄ | 5,12 ×10-14 | 2,46 ×10-12 | 2,46 ×10-12 |
| C ₅ | 1,96 ×10-13 | 1,18 ×10-11 | 1,18 ×10-11 |
| СО | 1,03 ×101 | 289,52 | 1,24 ×10 ² |
| CO ₂ | 7,22 ×10 ⁻⁵ | 3,18 ×10-3 | 8,66 ×10-4 |
| C ₂ O | 2,05 ×10-8 | 8,20 ×10-7 | 4,92 ×10-7 |
| C ₃ O ₂ | 6,63 ×10-10 | 4,51 ×10-8 | 1,62 ×10-6 |
| СН | 4,83 ×10-9 | 6,28 ×10-8 | 5,80 ×10-8 |
| CH ₂ | 6,92 ×10-7 | 9,69 ×10-6 | 8,30 ×10-6 |
| CH ₃ | 2,73 ×10-4 | 4,10 ×10-3 | 3,28 ×10-3 |
| CH ₄ | 6,78 ×10-3 | 1,08 ×10-1 | 8,13 ×10-2 |
| C ₂ H | 2,70 ×10-6 | 6,75 ×10-5 | 6,48 ×10-5 |
| C_2H_2 | 1,96 ×10-2 | 5,09 ×10-1 | 4,70 ×10-1 |
| C_2H_3 | 8,52 ×10-6 | 2,30 ×10-4 | 2,04 ×10-4 |
| C_2H_4 | 8,18 ×10-5 | 2,29 ×10-3 | 1,96 ×10-3 |
| C_2H_5 | 1,58 ×10-8 | 4,52 ×10-7 | 3,79 ×10-7 |
| C_2H_6 | 2,66 ×10-8 | 7,98 ×10-7 | 6,38 ×10-7 |
| C ₃ H | 2,16 ×10 ⁻⁵ | 7,99 ×10-4 | 7,78 ×10-4 |
| C_3H_4 | 1,37 ×10-9 | 5,48 ×10-8 | 4,93 ×10-8 |
| C_3H_6 | 1,05 ×10-11 | 4,41 ×10-10 | 3,78 ×10-10 |
| C_3H_8 | 2,48 ×10 ⁻¹³ | 1,09 ×10-11 | 8,93 ×10 ⁻¹² |
| C ₄ H | 7,00 ×10-10 | 3,43 ×10-8 | 3,36 ×10-8 |
| C ₄ H ₂ | 1,01 ×10-4 | 5,05 ×10-3 | 4,48 ×10-3 |
| C_4H_4 | 2,73 ×10 ⁻¹² | 1,50 ×10-11 | 1,31 ×10-10 |
| C ₄ H ₆ | 2,06 ×10-13 | 1,11 ×10-11 | 9,89 ×10-12 |
| C ₅ H ₆ | 2,76 ×10-12 | 1,82 ×10-10 | 1,6 ×10-10 |

| components and particles in the gas phase | content, mol/kg | content, grams | carbon in the gas phase, g/kg |
|--|-------------------------|-----------------------|----------------------------------|
| C ₆ H ₆ | 1,09 ×10-11 | 8,50 ×10-10 | 7,85 ×10-10 |
| CS | 2,64 ×10-2 | 1,16 ×100 | 3,17 ×10-1 |
| CS ₂ | 5,98 ×10-3 | 4,55 ×10-1 | 7,18 ×10-2 |
| COS | 1,67 ×10-3 | 1,00 ×10-1 | 2,01 ×10-2 |
| CN | 6,12 ×10-6 | 1,61 ×10-4 | 7,42 ×10-5 |
| CN ₂ | 1,03 ×10-8 | 4,12 ×10-7 | 1,24 ×10-7 |
| C ₂ N | 1,27 ×10-8 | 4,83 ×10-7 | 3,05 ×10-7 |
| C_2N_2 | 5,86 ×10-6 | 3,05 ×10-4 | 1,41 ×10-4 |
| NCO | 8,39 ×10-11 | 3,52 ×10-9 | 1,01 ×10-9 |
| HCN | 1,5 ×10-1 | 4,26 ×10 ⁰ | 1,89 ×100 |
| HNC | 1,20 ×10-4 | 3,24 ×10-3 | 1,44 ×10-3 |
| C ₂ HN | 4,40 ×10-8 | 1,72 ×10-6 | 1,06 ×10-6 |
| C ₃ HN | 1,11 ×10-3 | 5,65 ×10-2 | 3,99 ×10-2 |
| C ₅ HN | 8,17 ×10-4 | 6,13 ×10-2 | 4,90 ×10-2 |
| C7HN | 1,81 ×10-4 | 1,79 ×10-2 | 1,52 ×10-2 |
| C ₉ HN | 3,32 ×10-5 | 4,08 ×10-3 | 3,59 ×10-3 |
| N ₂ C | 3,2 ×10-6 | 1,32 ×10-4 | 3,95 ×10-5 |
| C+ | 1,93 ×10-22 | 2,32 ×10-21 | 2,32 ×10-21 |
| C ²⁺ | 1,93 ×10-22 | 4,63 ×10-21 | 4,63 ×10-21 |
| C ²⁻ | 1,95 ×10 ⁻¹⁷ | 4,68 ×10-16 | 4,68 ×10-16 |
| CO+ | 1,38 ×10-19 | 3,86 ×10-18 | 1,66 ×10-18 |
| CH+ | 2,63 ×10 ⁻²¹ | 3,42 ×10-20 | 3,16 ×10-20 |
| CHO+ | 3,00 ×10-12 | 8,70 ×10-11 | 3,60 ×10-11 |
| CN- | 7,85 ×10 ⁻¹² | 2,04 ×10-10 | 9,42 ×10-11 |

According to Table 4, the total mass of carbon in the gas phase was 685.04 g C, of which condensed carbon - 557.98 g, carbon monoxide - 124 g, acetylene - 0.47 g, hydrocyanic acid - 1.89 g, and the remaining carbon-containing particles account for approximately 0.7 % carbon. At the same time, the carbon content in the original coal was 67.98 mol/kg, i.e. 815.76 g C. Hence, the additive carbon footprint at the theoretical temperature of coal combustion (T = 1998 K) is 685.04/81.76 = 0.84, which is useful in assessing the carbon capacity per unit of product produced by burning coal from the Kara-Keche deposit.

From the data obtained, it is clear that 130.72 g or 16 % of carbon is lost due to the exergy of the flow, i.e. due to the dissipation of particles inside and outside the system when it interacts with the environment. It should be noted here that during the oxidation of coal in an oxidizing agent (T = 1998 K), the additive carbon footprint in the gas phase is mainly due to CO and $C_{(c)}$. However, when calculating the carbon footprint, it is necessary to take into account not only the mass of carbon oxides (CO, CO₂), acetylene, methane, and condensed carbon $C_{(c)}$, and all carbon-containing additive components, active particles, and condensed phases in the gas phase.

CONCLUSION

A model system of coal-air was considered with the overall calculation matrix (mol/kg): H – 49.209, C – 57.087, N – 6.745, S – 0.149, O – 10.343, and thermodynamic modeling of the oxidation process of the solid phase was conducted at the maximum entropy of the system. Concentration distributions of H, C, N, S, O-containing components, active particles, and condensed phases were determined over a wide temperature range (298-3000 K). At the theoretical combustion temperature of coal (1998 K), the complete composition of carbon-containing substances in the gas phase was identified, and for the first time, the additive value of the carbon footprint was calculated, taking into account the initial mass of carbon in the solid phase. The anthropogenic carbon load in the gas phase is valuable for assessing the carbon capacity per unit of industrial production obtained from the combustion of solid fuel.

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