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# Mathematical modeling of the gas phase composition during combustion of a methane-coal mixture

I A Rybenko and V N Buintsev

Siberian State Industrial University, 42 Kirova str., Novokuznetsk, 654007, Russia

E-mail: rybenkoi@mail.ru

**Abstract.** The paper presents the results of mathematical modeling of the process of combined combustion of methane and coal dust in the air in a closed reactor. The effects of the combustion reaction of a wet methane-coal dust mixture, such as temperature, pressure and the composition of the combustion products are calculated.

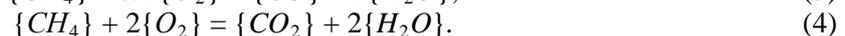
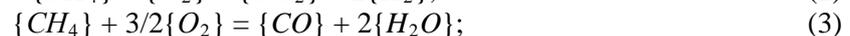
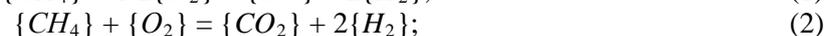
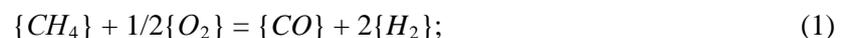
## 1. Introduction

Kuzbass is the main strategic coal basin of the country. It accounts for about 60% of the total Russian coal production, including 83% of the most valuable coking grades. Almost 70% of coal is mined by the underground method. Coal mining by the underground method is accompanied by the release of methane into the atmosphere from the face. When a certain concentration is reached methane forms an explosive mixture with atmospheric oxygen. In addition, finely dispersed coal dust is present in the atmosphere of mine workings. At certain concentrations of methane and dust a volumetric explosion is possible, accompanied by an increase in temperature and pressure in the confined space of the mine [1]. In this regard, an important task is to study the conditions for the formation of a gas phase during the combustion of a methane-coal mixture.

## 2. Development of a mathematical model

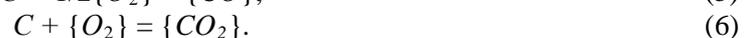
Mathematical modeling of the combined combustion of methane and coal dust at their various concentrations in the air of a confined space was carried out using the calculation method [2-6].

The process of methane combustion can be represented by the reactions [7]:



Reactions (1) – (3) are reactions of incomplete combustion or methane conversion with an excess concentration of methane in the air. Reaction (4) – the reaction of complete combustion occurs with an excess of oxygen at low concentrations of methane in the air.

The coal dust combustion, depending on its concentration in the air, can be represented by two reactions [7]:



Let us consider the formation mechanism of combustion products of a methanol-coal mixture in the reactor with a volume of  $V \text{ m}^3$  [8,9]. Suppose that in the reactor atmosphere there are  $n_{O_2}$  and  $n_{N_2}$  moles of oxygen and nitrogen. Concentrations of methane and coal dust in the air are  $k$  and  $l$  %, respectively. At this concentration, the number of methane moles, respectively, is equal to:

$$n_{CH_4, meth} = \frac{k \cdot V}{100 \cdot (100 - k) \cdot 0.0224}, \quad (7)$$

where  $V$  is the reactor volume,  $\text{m}^3$ .

The mass of coal dust at its concentration in the reactor  $l$  % is:

$$G_{dust} = \frac{l \cdot G_{air}}{(100 - l)}, \quad (8)$$

where  $G_{air} = G_{O_2} + G_{N_2}$  is the mass of air in the reactor, kg;

Coal dust consists of an organic part ( $C$ ), a mineral part ( $A$ ), moisture ( $W$ ) and volatile components ( $L$ ). The mineral part does not participate in the combustion process and remains in the form of ash. The amount of ash is determined by the formula:

$$G_{ash} = \frac{G_{dust} \cdot A}{100}, \quad (9)$$

where  $A$  – ash percentage, %.

The number of moles of water and organic carbon from coal dust, respectively, is equal to:

$$n_{H_2O_{dust}} = \frac{G_{gas} \cdot W}{100 \cdot 0.018}; \quad (10)$$

$$n_{C_{dust}} = \frac{G_{gas} \cdot C}{100 \cdot 0.012}, \quad (11)$$

where  $W$  is the moisture content of fuel, %;  $C$  – content of organic carbon in dust, %.

We assume that the yield of volatile components of coal dust occurs as follows: two thirds of the oxygen of volatile matter is in the form of  $CO$ , one third is in the form of  $CO_2$ . The remaining carbon is in the compound  $CH_4$ , and the remaining hydrogen is in the form of  $H_2$ . All nitrogen goes to  $N_2$ .

$$\begin{aligned} n_{CO_{vol}} &= 2/3 \cdot \left( \frac{G_{dust} \cdot L}{100} \cdot \frac{/O/_{vol}}{100} \right) / 0.016; \\ n_{CO_{2vol}} &= 1/3 \cdot \left( \frac{G_{dust} \cdot L}{100} \cdot \frac{/O/_{vol}}{100} \right) / 0.032; \\ n_{CH_4_{vol}} &= \frac{G_{dust} \cdot L}{100 \cdot 0.012} \cdot \frac{/C/_{vol}}{100} - n_{CO_{vol}} - n_{CO_{2vol}}; \\ n_{H_2_{vol}} &= \frac{G_{dust} \cdot L}{100 \cdot 0.002} \cdot \frac{/H/_{vol}}{100} - 2n_{CH_4_{vol}}; \\ n_{N_2_{vol}} &= \left( \frac{G_{dust} \cdot L}{100} \cdot \frac{/N/_{vol}}{100} \right) / 0.028. \end{aligned} \quad (12)$$

where  $L$  is the volatile content in coal dust, %;  $/O/_{vol}$ ,  $/C/_{vol}$ ,  $/H/_{vol}$ ,  $/N/_{vol}$ , – oxygen, carbon, hydrogen and nitrogen content in volatile components of dust, %.

Thus, the mixture of substances in the reactor without regard to the mineral part, which is not involved in the combustion process, has the following composition in moles:

$$\begin{aligned}
n_{O_2\text{init}} &= 1158.67; \\
n_{N_2\text{init}} &= 3305.86 + n_{N_2\text{vol}}; \\
n_{CH_4\text{init}} &= n_{CH_4\text{meth}} + n_{CH_4\text{vol}}; \\
n_{CO\text{init}} &= n_{CO\text{vol}}; \\
n_{CO_2\text{init}} &= n_{CO_2\text{vol}}; \\
n_{H_2\text{init}} &= n_{H_2\text{vol}}; \\
n_{H_2O\text{init}} &= n_{H_2O\text{dust}}; \\
n_{C\text{init}} &= n_{C\text{dust}}.
\end{aligned} \tag{13}$$

Let us calculate the composition of combustion products. We accept that initially methane burns to  $CO$  and  $H_2$  by reaction (1). If in the reactor the doubled number of oxygen moles exceeds the number of methane moles, then the moles number of  $CO$  formed as a result of methane conversion is determined by the number of methane moles, and otherwise by doubled number of oxygen moles:

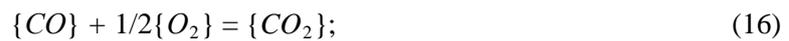
$$\text{If } 2n_{O_2\text{init}} > n_{CH_4\text{init}}, \text{ then } n_{CO\text{meth}} = n_{CH_4\text{init}}, \text{ otherwise } n_{CO\text{meth}} = 2n_{O_2\text{init}}. \tag{14}$$

For the formation of  $CO$  as a result of conversion will be consumed  $n_{CH_4\text{meth}} = n_{CH_4\text{init}} - n_{CO\text{meth}}$  methane moles and  $n_{O_2\text{meth}} = n_{CO\text{meth}}/2$  oxygen moles.

As a result of methane conversion, hydrogen is also formed. The number of hydrogen moles in the reactor is determined as follows:

$$n_{H_2\text{meth}} = 2n_{CO\text{meth}}. \tag{15}$$

If oxygen remains in the reactor after methane conversion, then part or all carbon monoxide burns to  $CO_2$ , and  $H_2$  – to  $H_2O$  according to the reactions:



If  $n_{O_2\text{init}} - n_{O_2\text{meth}} > n_{CO\text{meth}} + n_{CO\text{init}} + n_{H_2\text{meth}} + n_{H_2\text{init}}$ , then  $n_{CO\text{com}} = n_{CO\text{meth}} + n_{CO\text{init}}$  and  $n_{H_2\text{com}} = n_{H_2\text{meth}} + n_{H_2\text{init}}$ , otherwise  $n_{CO\text{com}} = 2(n_{O_2\text{init}} - n_{O_2\text{meth}})/3$  and  $n_{H_2\text{com}} = 4(n_{O_2\text{init}} - n_{O_2\text{meth}})/3$ . (18)

For the postcombustion of  $CO$  and  $H_2$  will be used  $n_{O_2\text{com}} = n_{CO\text{com}} + n_{H_2\text{com}}$  moles of oxygen.

As a result of postcombustion,  $CO_2$  and  $H_2O$  are formed:

$$n_{CO_2\text{com}} = n_{CO\text{com}} \text{ and } n_{H_2O\text{com}} = n_{H_2\text{com}}. \tag{19}$$

Let us check the condition  $n_{O_2\text{init}} - n_{O_2\text{meth}} - n_{O_2\text{com}} > 0$ . If this condition is fulfilled, and the oxygen in the reactor still remains,  $CO$  is formed from the combustion of organic carbon of coal dust by reaction (5). If no oxygen remains, then  $n_{CO\text{dust}} = 0$ .

If oxygen remains, the amount of  $CO$  generated from dust combustion is determined as follows: if

$$\begin{aligned}
2(n_{O_2\text{init}} - n_{O_2\text{meth}} - n_{O_2\text{com}}) > n_{C\text{init}}, \text{ then } n_{CO\text{dust}} &= n_{C\text{init}}, \\
\text{otherwise } n_{CO\text{dust}} &= 2(n_{O_2\text{init}} - n_{O_2\text{meth}} - n_{O_2\text{com}}).
\end{aligned} \tag{20}$$

For the combustion of carbon moles  $n_{C\ dust} = n_{CO\ dust}$  of will be used  $n_{O_2\ dust} = n_{CO\ dust}/2$  of oxygen. If there is still oxygen in the reactor, postcombustion of  $CO$  to  $CO_2$  will take place by reaction (16).

$$\text{If } n_{O_2\ init} - n_{O_2\ meth} - n_{O_2\ com} - n_{O_2\ dust} > n_{CO\ init} + n_{CO\ meth} + n_{CO\ dust} - n_{CO\ com}, \text{ then} \\ n_{CO\ post} = n_{CO\ init} + n_{CO\ meth} + n_{CO\ dust} - n_{CO\ com}, \text{ otherwise } n_{CO\ post} = 2(n_{O_2\ init} - n_{O_2\ meth} - n_{O_2\ com} - n_{O_2\ dust}). \quad (21)$$

At the same time  $n_{CO_2\ post} = n_{CO\ post}$  of  $CO_2$  moles is formed, and  $n_{O_2\ post} = n_{CO\ post}/2$  of moles of oxygen will be used.

As a result of the combustion reactions, the following substances will be present in the reactor:  $CO$ ,  $CO_2$ ,  $N_2$ ,  $H_2$ ,  $H_2O$ ,  $CH_4$ ,  $O_2$ ,  $C$  and ash.

The composition of the combustion products is determined by equations (22):

$$\begin{aligned} n_{CO} &= n_{CO\ init} + n_{CO\ meth} + n_{CO\ dust} - n_{CO\ com} - n_{CO\ post}; \\ n_{CO_2} &= n_{CO_2\ init} + n_{CO_2\ com} + n_{CO_2\ post}; \\ n_{N_2} &= n_{N_2\ init}; \\ n_{H_2} &= n_{H_2\ init} + n_{H_2\ meth} - n_{H_2\ com}; \\ n_{H_2O} &= n_{H_2O\ init} + n_{H_2O\ com}; \\ n_{CH_4} &= n_{CH_4\ init} - n_{CH_4\ meth}; \\ n_{O_2} &= n_{O_2\ init} - n_{O_2\ meth} - n_{O_2\ com} - n_{O_2\ dust} - n_{O_2\ post}; \\ n_C &= n_{C\ init} - n_{C\ dust}. \end{aligned} \quad (22)$$

The mass and volume of the  $i$ -th component of the mixture are determined in accordance with the formulas:

$$G_i = n_i \cdot M_i; \quad (23)$$

$$V_i = \frac{n_i}{\sum_{j=1}^N n_j} \cdot V_p. \quad (24)$$

where  $M_i$  – the molar mass of the  $i$ -th component, kg/mol;  $V_p$  – reactor volume, m<sup>3</sup>;  $N$  – the number of gas phase components.

Next, let us calculate the heat balance of the process.

The heat input consists of thermal effects of independent reactions of the system transition from the initial to the final state, which include the methane conversion reaction (1), incomplete combustion of carbon (5) and postcombustion of  $CO$  (16) and  $H_2$  (17). The total thermal effect of exothermic reactions can be calculated as follows:

$$\begin{aligned} \Delta H_{ch.r.} &= \Delta H_{CH_4} (n_{CH_4\ init} - n_{CH_4}) + \Delta H_C (n_{C\ init} - n_C) + \\ &+ \Delta H_{CO} (n_{CO_2} - n_{CO_2\ init}) + \Delta H_{H_2} (n_{H_2O} - n_{H_2O\ init}), \end{aligned} \quad (25)$$

where  $\Delta H_{ch.r.}$  – total heat effect of chemical reactions;  $\Delta H_{CH_4}$ ,  $\Delta H_C$ ,  $\Delta H_{CO}$ ,  $\Delta H_{H_2}$  are the standard thermal effects of methane conversion reactions, carbon combustion,  $CO$  and  $H_2$  postcombustion, respectively, kJ/mol.

Taking into account the standard thermal effects

$$\begin{aligned} \Delta H_{ch.r.} = & 149 \cdot (n_{CH_4^{init}} - n_{CH_4}) + 115 \cdot (n_{C^{init}} - n_C) + \\ & + 283 \cdot (n_{CO_2} - n_{CO_2^{init}}) + 252 \cdot (n_{H_2O} - n_{H_2O^{init}}). \end{aligned} \quad (26)$$

The heat of exothermic reactions is consumed for the products heating. The heating enthalpy of an arbitrary substance is determined as follows:

$$\Delta H_T^0 = \Delta H_{298}^0 + \int_{298}^{T_{ph.t.1}} \Delta C_{p1} dT + \Delta H_{ph.t.1} + \dots + \int_{T_{ph.t.k}}^T \Delta C_{pk} dT, \quad (27)$$

where  $\Delta C_{p1}, \dots, \Delta C_{pk}$  is the change in isobaric heat capacity before the first and after the  $k$ -th phase transition of the substance, kJ/mol·K;

$T_{ph.t.1}, \dots, T_{ph.t.k}$  – temperature of the 1, ...,  $k$ -th phase transitions, respectively, K;

$T$  – final temperature, K;

$\Delta H_{ph.t.1}, \dots, \Delta H_{ph.t.k}$  – change in enthalpy as a result of the corresponding phase transition, kJ/mol;

The enthalpy of products heating is determined by:

$$\begin{aligned} \Delta H_{heat} = & \Delta H_{CH_4}^0 n_{CH_4} + \Delta H_{CO}^0 n_{CO} + \Delta H_{CO_2}^0 n_{CO_2} + \Delta H_{H_2}^0 n_{H_2} + \\ & + \Delta H_{H_2O}^0 n_{H_2O} + \Delta H_{O_2}^0 n_{O_2} + \Delta H_{N_2}^0 n_{N_2} + \Delta H_C^0 n_C + \Delta H_A^0 n_A. \end{aligned} \quad (28)$$

The calculation of the enthalpy of heating is determined at an arbitrary temperature. Then, the objective function of the heat balance residual is formed  $\varepsilon = \Delta H_{inc} - \Delta H_{cons} = \Delta H_{ch.r.} - \Delta H_{heat}$ , and the temperature at which the residual is zero is determined using the built-in optimizer of the Excel spreadsheet processor.

Next, we calculate the pressure in the reactor:

$$P = \frac{\sum_{j=1}^N n_j \cdot RT}{1000 \cdot V}, \quad (29)$$

where  $R$  is the universal gas constant, kJ/kg·K.

### 3. An example of calculation of the combined combustion of methane and coal dust in a confined space

Let us take the concentration of methane in the reactor 5% and dust 3%. The volume of the reactor is 100 m<sup>3</sup>. With a standard air composition of 21% O<sub>2</sub> and 79% N<sub>2</sub> in a given volume and normal conditions 25.95 m<sup>3</sup> (37.08 kg) of oxygen and 74.05 m<sup>3</sup> (92.56 kg) of nitrogen will be present, which is = 1158.67 and  $n_{N_2} = 3305.86$  moles of oxygen and nitrogen, respectively.

The composition of the coal dust is given in table 1. Table 2 presents the composition of the volatile components of the dust, table 3 presents the composition of the initial mixture in the reactor.

**Table 1.** The composition of coal dust.

Dust composition	W	A	C	L	Total
%	1	10	77	12	100
kg	0.040	0.401	3.087	0.481	4.0095

**Table 2.** The composition of the volatile components of coal dust.

Substance	$CO$	$CO_2$	$CH_4$	$N_2$	$H_2$	Total
kg	0.081	0.032	0.311	0.034	0.023	0.481
%	16.85	6.62	64.66	7.07	4.81	100.00
$m^3$	0.0648	0.0162	0.4356	0.0272	0.2589	0.8028

**Table 3.** The composition of the initial mixture in the reactor.

Substance	$O_2$	$N_2$	$CH_4$	$CO$	$CO_2$	$H_2$	$H_2O$	$C$	$A$	Total
$M_i$ , kg/mol	0.032	0.028	0.016	0.028	0.044	0.002	0.018	0.012		
$G_i$ , kg	37.1	92.6	4.07	0.08	0.03	0.02	0.04	3.09	0.40	137.41
% by weight	26.98	67.39	2.96	0.06	0.02	0.02	0.03	2.25	0.29	100.00
$V_i$ , $nm^3$	24.5	69.8	5.4	0.1	0.0	0.2	0.0			100.00
% by volume	24.46	69.81	5.37	0.06	0.02	0.24	0.05			100.00
$n_i$ , mol	1158.7	3307.1	254.4	2.9	0.7	11.6	2.2	257.3		4994.9

As a result of the calculation, the following results were obtained (table 4).

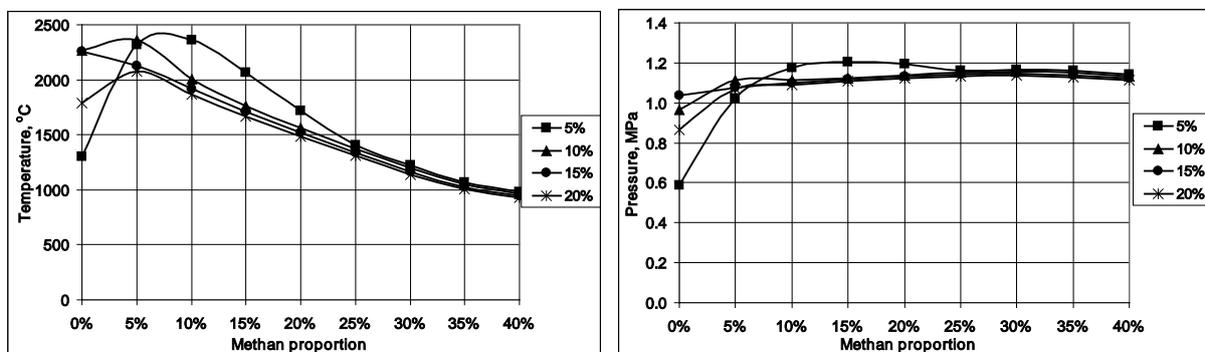
**Table 4.** The composition of combustion products.

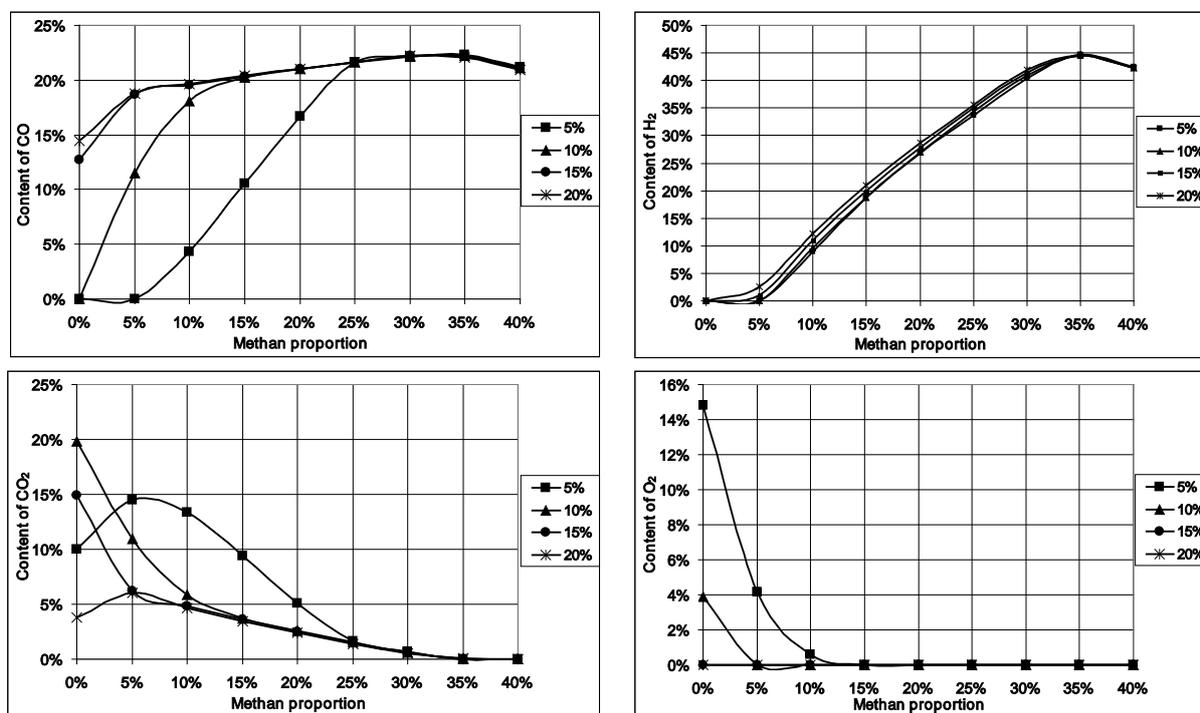
Substance	$CO$	$CO_2$	$N_2$	$H_2$	$H_2O$	$CH_4$	$O_2$	$C$	$A$	Total
$G_i$ , kg	0.00	22.67	92.60	0.00	9.41	0.00	12.33	0.0	0.40	137.41
% by weight	0.00	16.50	67.39	0.00	6.85	0.00	8.97	0.0	0.29	100.00
$V_i$ , $nm^3$	0.00	10.89	69.92	0.00	11.05	0.00	8.15			100.00
% by volume	0.00	10.89	69.91	0.00	11.05	0.00	8.15			100.00
$n_i$ , mol	0.00	515.32	3307.08	0.00	522.63	0.00	385.33	0.0		4730.35

The calculated temperature inside the reactor was 2257 K (1984 °C), pressure – 0.8873 MPa (8.87 atm).

Using the developed model, we studied the effect of methane and coal dust concentrations on the combustion product parameters – temperature, pressure (figure 1) and gas phase composition (figure 2). The ratio of methane concentrations and coal dust were determined, with which temperatures of combustion products and pressure in the reactor were maximal.

The maximum temperature of the combustion products and the pressure correspond to a methane concentration of 7% with a dust content in the atmosphere of 5%.

**Figure 1.** Dependencies of the parameters of the joint methane and coal dust combustion on the methane proportion at different coal dust concentrations in the reactor.



**Figure 2.** Dependence of the gas phase composition during the methane and coal dust combustion on the methane proportion at different coal dust concentrations in the reactor.

#### 4. Conclusion

Thus, this paper confirms the well-known fact that the dangerous factors for people in the mine workings, in which the explosion of the air-methane-coal dust mixture occurred, are high temperature and pressure. In addition, analyzing the graphs in Figure 2, we can conclude that the atmosphere in the mine workings after the methane-coal dust explosion is not suitable for breathing even with a filtering gas mask, since there is practically no oxygen. It can be also seen from the graphs that the atmosphere after the explosion contains a sufficiently large amount of  $CO$  and  $H_2$ , therefore, gas clearing is likely to lead to the formation of a new explosive gas mixture and to a new repeated explosion. In general, analyzing the results of modeling, it is possible to conclude that the work in the coal face is best to be done at the highest possible methane content. This, in principle, will eliminate explosions, but at the same time the presence of working personnel, at least without oxygen breathing apparatuses.

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