Experimental-theoretical approach to carbon monoxide density calculation at the incipient stage of the fire indoors

S V Puzach, E V Suleykin, R G Akperov and T D Nguyen
Hydraulic and thermal physics department, State Fire Academy of EMERCOM of Russia, Moscow, Russia
puzachsv@mail.ru

Abstract. A new experimental-theoretical approach to the toxic gases concentrations assessment in case of fire indoors is offered. The analytical formulas for calculation of CO average volume density are received. These formulas do not contain the geometrical sizes of the room and surfaces dimensions of combustible materials and, therefore, are valid under conditions of as a small-scale fire as a large-scale fire. A small-scale experimental installation for modeling fire thermal and gas dynamics in the closed or open thermodynamic system has been designed. The results of the experiments on determining dependencies of CO average volume density from average volume temperature and oxygen average volume density as well as dependencies of specific coefficients of CO emission and specific mass rates of the combustible material gasification from the time of tests during the burning of wood, transformer oil and PVC cables shield are presented. The results of numerical experiments on CO density calculation in small and large scale rooms using the proposed analytical solutions, integral, zone and field models for calculation of fire thermal and gas dynamics are presented. The comparison with the experimental data obtained by the authors and given in the literature has been performed. It is shown that CO density calculation in the full-scale room at the incipient stage of the fire can be carried out taking into account only the experimental dependences of CO from temperature or O2 density, that have been obtained from small-scale experiments. Therefore the solution of the equation of carbon monoxide mass conservation law is not necessary.

1. Introduction
According to statistics, in more than 80% of cases, the cause of death of people in fires was poisoning by toxic combustion products. The quantity of released toxic gases is determined by the chemical composition and concentration of gaseous products of gasification of combustible substances and materials, as well as by the thermal and gas dynamic fire conditions [1].

At present, this problem has not been solved from the theoretical and from the experimental points of view because of the complexity of the physicochemical conditions of the gasification and combustion processes, as well as the uncertainty of the chemical composition of modern building materials. Therefore, mathematical modeling of the distribution of toxic combustion products indoors during a fire is an urgent task.

2. Mathematical model
A modified integral (one-zone) model is used [1, 2]. Equations of conservation laws of mass and energy for the gas mixture of the room, as well as the laws of conservation of the mass of oxygen and $i$-th toxic gas are respectively as:
where \( c_{pm}, c_{pm} \) – specific isobaric heat capacities of the air and gas mixture in the room, respectively, \( J \; kg^{-1}K^{-1} \); \( G_a, G_g \) – mass flow rates of incoming air and outflowing gases during natural gas exchange through the openings, respectively, \( kg \; s^{-1} \); \( k_m \) – average volume index of adiabat of the gas mixture in the room; \( L_i \) – specific mass coefficient of \( i \)-th toxic gas emission; \( L_{O2} \) – specific mass coefficient of oxygen consumption; \( \rho_{m} \) – average volume indoor pressure, \( Pa \); \( Q \) – lower working heat of combustion of combustible material, \( J \; kg^{-1} \); \( T_a \) – outside air temperature, \( K \); \( T_m \) – average volume temperature of the gas mixture in the room, \( K \); \( V \) – volume of the room, \( m^3 \); \( W_{a}, W_{m} \) – volume flow rates of supply and exhaust ventilation, respectively, \( m^3s^{-1} \); \( X_{im} \) – average volume mass concentration of the \( i \)-th toxic gas in the room; \( X_{O2a} \) – mass concentration of oxygen in outdoor air; \( X_{O2m} \) – average volume mass concentration of oxygen in the room; \( \eta \) – combustion completeness; \( \beta_{s} \) – outside air density, \( kg \; m^{-3} \); \( \rho_{m} \) – average volume density of the \( i \)-th toxic gas in the room, \( kg \; m^{-3} \); \( \rho_{m} \) – average volume density of the gas mixture in the room, \( kg \; m^{-3} \); \( \rho_{O2a} \) – density of oxygen in outdoor air, \( kg \; m^{-3} \); \( \rho_{O2m} \) – average volume density of oxygen in the room, \( kg \; m^{-3} \); \( \tau \) – time, \( s \); \( \varphi \) – the heat losses coefficient that equals to the fraction of heat released in the source of combustion and entering the enclosing constructions from the total volume of the room; \( \Psi \) – mass rate of gasification of combustible material, \( kg \; s^{-1} \).

The system of equations (1)-(5) is solved in a general way by numerical methods. However, in a number of cases there are analytical solutions [1, 3], of which the volume average density of a toxic gas can be described by the following relationship:

\[
\rho_{im} = \rho' L_i
\]

где \( \rho' = K/Q \) – characteristic density, \( kg \; m^{-3} \); \( K \) – coefficient of proportionality, \( J \; m^3 \).

The coefficient of proportionality does not depend on the properties of the combustible material, the dimensions of the room and the area of the open surface of the combustible material and is a function of only three parameters characterizing the thermodynamic picture of the fire:

\[
K = f(T_m, T_a, \varphi)
\]

Formulas for calculating the coefficient \( K \) for different schemes of the thermal and gas dynamic picture of fire are given in table 1 (where \( f \) – variables (density, temperature and so on)).

Dependence of the average volume density of \( i \)-th toxic gas on changes of the average volume density of oxygen can be obtained from integration of equations (3) and (4) when \( G_a = G_g = W_a = W_m = 0 \):

\[
\rho_{im} = L_o \Delta \rho_{o2} \over L_{o2}
\]

где \( \Delta \rho_{o2} = \rho_{o2a} - \rho_{o2m} \) – the decrease of the average volume density of oxygen, \( kg \; m^{-3} \).

To calculate the toxic gas densities in a full-scale room, a two-zone model is used [3], the basic equations of which are (respectively) the laws of conservation of mass and energy of the gas mixture
in the ceiling layer, the law of conservation of mass of the \( i \)-th toxic gas and mass flow rate across the convective column [3]:

\[
\frac{d(\rho_i V_i)}{d\tau} = G_k
\]

(8)

\[
\frac{d(c_i \rho_i T V_i)}{d\tau} = c_i T(G_k - \rho_i \frac{dV_i}{d\tau})
\]

(9)

\[
\frac{d(\rho_i V_i)}{d\tau} = \mathcal{Q}_i
\]

(10)

when \( z > z_f \):

\[
G_k = 0.071 \left( \eta \mathcal{Q} (1 - \chi) \cdot 10^{-3} \right)^{1/3} z^{5/3} + 1.8 \cdot 10^{-6} \eta \mathcal{Q} (1 - \chi)
\]

(11)

when \( z \leq z_f \):

\[
G_k = 0.032 \left( \eta \mathcal{Q} (1 - \chi) \cdot 10^{-3} \right)^{5/3} z
\]

(12)

where \( c_i \), \( \rho_i \) – the average specific isochoric and isobaric heat capacities of the gas mixture in the ceiling layer, respectively, \( \text{J kg}^{-1}\text{K}^{-1} \); \( G_k \) – mass flow rates of gas mixture coming from the convective column to the ceiling zone, \( \text{kg s}^{-1} \); \( Q_k \) – the heat flow diverted from the ceiling gas layer into the enclosing constructions of the room, \( \text{W} \); \( Q_{\text{gas}} \) – the heat flow diverted from the convective column into the enclosing constructions of the room, \( \text{W} \); \( T_2 \) – average volume temperature of the gas mixture in the ceiling layer, \( \text{K} \); \( T_k \) – average temperature of the gas mixture in the convective column at its boundary with the ceiling layer, \( \text{K} \); \( V_2 \) – volume of the gas ceiling zone, \( \text{m}^3 \); \( z \) – the coordinate of the cross section of the convective column, measured from the open surface of the combustible material, \( \text{m} \); \( z_f = 0.166 \left( \eta \mathcal{Q} (1 - \chi) \cdot 10^{-3} \right)^{2/5} \) – height of the flame zone, \( \text{m} \); \( \rho_2 \) – average volume density of the gas mixture in the ceiling layer, \( \text{kg m}^{-3} \); \( \rho_2 \) – average volume density of the \( i \)-th toxic gas in the ceiling layer, \( \text{kg m}^{-3} \); \( \chi = Q_{\text{gas}} / (\eta \mathcal{Q}) \) – part of the heat released in the combustion zone and coming from the convective column into the enclosing structures of the room.

**Table 1.** Formulas for calculating the proportionality coefficient (expression (6)).

| The main characteristics of the thermal and gas dynamic picture of fire | \( K \), J m\(^3\) |
|---|---|
| 1 Unsteady fire conditions, closed thermodynamic system: \( G_s = G_t = W_s = W_m = 0^s \). | \( 2.5 \cdot 10^3 \left( \frac{T_m - T_s}{1 - \phi} \right) \) |
| 2 Unsteady fire conditions; open thermodynamic system: \( W_s = W_m = 0^s \). | \( 3.5 \cdot 10^3 \left( \frac{T_m - T_s}{1 - \phi} \right) \) |
| 3 Stationary fire conditions; open thermodynamic system; mechanically induced smoke removal: \( \frac{dV_i}{d\tau} = 0^s \). | \( 3.5 \cdot 10^3 \left( \frac{T_m - T_s}{1 - \phi} \right) \) |
| 4 Stationary fire conditions; open thermodynamic system; mechanically induced smoke removal from the ceiling layer: \( \frac{dV_i}{d\tau} = 0^b \). | \( 3.5 \cdot 10^5 \left( \frac{T_2 - T_s}{1 - \phi} \right) \) |
| 5 The boundary between the convective column and ceiling zone\(^b\) | \( 1.37 \cdot 10^7 \left( \frac{1}{1 - \chi} \right) \) |

\(^a\)One-zone model (equations (1)-(4)).

\(^b\)Two-zone model (equations (8)-(12)).

Solving the system of equations (8)-(12) in the case of stationary conditions, one can obtain an analytical dependence of the average volume density of CO on the average volume temperature of the gas mixture in the ceiling layer (table 1).
A three-dimensional field model [4] is also used. The main problem of solving equations (4) and (10) is that the coefficient \( L_i \) is essentially unsteady and its average value depends essentially on the averaging period [5]. In addition, in most cases, its theoretical value cannot be calculated because of the uncertainty of the chemical composition of the combustible material and the combustion products.

3. Experimental installation and experimental procedure
An experimental small-scale installation has been developed to simulate the thermal and gas dynamics of a fire in a closed or open thermodynamic systems. The experimental setup is shown on figure 1.

![Experimental installation diagram](image)

**Figure 1.** The scheme of the experimental installation: 1 - combustion chamber; 2 - exposure chamber; 3 - transition sleeve; 4 - electrical heating radiator; 5 - sample holder; 6 - girder holes; 7 - table for scales; 8 - exposure chamber door; 9 - combustion chamber door; 10 - the fan; 11 - damper (partition) of the transition sleeve; 12 - measurement area; 13 - the fan; 14 - temperature measurement; 15 - measurement of CO, CO\(_2\) and O\(_2\) concentrations; 16 - measurement of gas flow rate.

The combustion chamber (1) is made of stainless steel sheet. Its volume equals 3\(\cdot 10^{-3}\) m\(^3\). The exposure chamber (2) is a cubic volume (0.8\(\cdot 0.8\cdot 0.8\) m\(^3\)) with a conical top part. The sample holder (5) is placed on electronic scales with an error of less than \(\pm 1\) mg, located on a special moving table.

The measurement area (12) is a steel pipe with an internal diameter of 50 mm connected to the exposure chamber (2). Behind the measurement area there is a fan (13) with an adjustable flow rate of the gas mixture to be removed from the exposure chamber (2).

Low inertial armored thermocouples were used for continuous monitoring of the temperature in the exposure chamber and in the measurement area. A multi-channel gas analyzer is used for continuous monitoring of the composition of the gas-air mixture in the exposure chamber and in the measurement area, measuring the concentration of carbon monoxide, carbon dioxide and oxygen. The velocity of
the gas mixture along the symmetry axis of the measurement area is measured using a thermo-
anemometer.

The combustible materials were tested in the flame combustion mode. The flame burning mode is provided at a test temperature of 750°C (the density of the incident heat flow equals 60 kW m$^{-2}$).

4. Initial data for experiments
The following combustible materials are used: coniferous wood, PVC cables sheath and transformer oil. Carbon monoxide is considered as a toxic gas. The CO critical density is $\rho_{\text{CO.c}}=1.16 \times 10^{-3}$ kg m$^{-3}$ [3].

There are considered the following full-scale premises:
- the power plant: cable gallery with dimensions 20-60-2.5 m$^3$, engine room – 20-60-20 m$^3$;
- the rooms with dimensions 5-5-15, 10-10-10 and 20-20-25 m$^3$.

5. Results and discussion

5.1. Conditionally hermetic thermodynamic system
The results of the experiments on determining dependencies of carbon monoxide average volume density from average volume temperature and oxygen average volume density as well as dependencies of specific coefficients of CO emission ($L_{\text{CO}}$) and specific mass rates of the combustible material gasification from the time of tests during the burning of wood, transformer oil and PVC cables shield are obtained. The experiments were carried out up to the average volume temperatures of the gas mixture inside the premises, not exceeding the critical value for a person equal to 70°C [3].

Experimental dependences of the average volume density of carbon monoxide ($\rho_{\text{CO.m}}$) on changes of the average volume temperature and average volume density of oxygen in the case of burning of PVC cable sheath are presented in figure 2 and figure 3, where $F$ – surface area of the sample, m$^2$; $\Delta T_m=T_m-T_a$ – the increase of average volume temperature, K.

Experiments have shown that the values of the specific coefficients of CO emission vary significantly with time since the onset of combustion and their average values essentially depend on the averaging period of test time.

![Figure 2](image_url)

**Figure 2.** Dependences of the average volume density of carbon monoxide on the change of the average volume temperature during burning of PVC cables sheath: experimental values: 1 – $\varphi=0.97$, $F=0.0067$ m$^2$; 2 – $\varphi=0.97$, $F=0.0059$ m$^2$; 3 – $\varphi=0.98$, $F=0.012$ m$^2$; equation (5): 4 – $F=0.0067$ m$^2$; 5 – $F=0.0059$ m$^2$; 6 – $F=0.012$ m$^2$; 7 – $\rho_{\text{CO.c}}$. 
A comparison of the calculation results obtained with the proposed expression (5) and three-dimensional field model [4] during fire in power plant is shown on figure 4.

It is clear from figure 4 that when values of $\Psi$, $Q$, $L_{CO}$, $L_{O2}$ are constants, the dependences of CO average volume density on the average volume temperature obtained with the help of the proposed formula (5) and the field model [4] practically coincide each other.

**Figure 3.** Dependences of the average volume density of CO on the change of the average volume density of $O_2$ during burning of the PVC cable sheath: the experimental values: $1 - F=0.0067$ m$^2$; $2 - F=0.0122$ m$^2$; equation (7): $3 - F=0.0067$ m$^2$; $4 - F=0.0122$ m$^2$; $5 - \rho_{CO,c}$

**Figure 4.** Dependences of the average volume density of carbon monoxide on the average volume temperature: cable gallery (PVC cable sheath): $1$ – equation (5); $2$ – field model [4]; power plant hall (transformer oil): $3$ – equation (5); $4$ – field model [4].
5.2. The open thermodynamic system

Experimental dependences of the average volume density of carbon monoxide on the increase of the mean volume temperature in the case of burning of coniferous wood are presented on figure 5.

Figure 5. Dependences of the average volume density of carbon monoxide on the change of the average volume temperature during burning of coniferous wood: 1 – one-zone model (equation (5), $\varphi=0.9$); two-zone model: 2 – the room 20-20-25 m$^3$, $\varphi=0.6$; 3 – 5-5-15 m$^3$, $\varphi=0.6$; 4 – 10-10-10 m$^3$, $\varphi=0.6$; experimental values: 5 – $W_m=0.007-0.0133$ m$^3$s$^{-1}$, $\varphi=0.9$; 6 – $W_m=0.005-0.009$ m$^3$s$^{-1}$, $\varphi=0.97$; 7 – natural smoke removal, $\varphi=0.92$.

It is clear from figure 5 that when values of $\Psi$, $Q$, $L_{CO}$, $L_{O2}$ are constants, the dependences of CO average volume density on the average volume temperature obtained with the help of the proposed formula (5) and the two-zone model practically coincide each other.

6. Conclusion

Carbon monoxide density calculation in the full-scale room at the incipient stage of the fire can be carried out taking into account only the experimental dependences of average volume density of CO on average volume temperature or average volume density of $O_2$ and experimental values of the heat losses coefficient $\varphi$, that have been obtained from small-scale experiments. Therefore the solution of carbon monoxide mass conservation law (the equations (4) and (10)) is not necessary.

References
[1] Puzach S V 2005 Methods for calculating the heat and mass transfer in a fire at the premises and their application in solving practical problems of fire safety (Moscow: State Fire Academy of Emercom of Russia Publ.)
[2] Puzach S V, Puzachs V G and Kazennov V M 2005 Certain regularities of heat and mass transfer through an open aperture in fire in the compartment Heat Transfer Research J. 7 p. 615
[3] Koshmarov Y A 2000 Prediction of fire dynamics factors in the room (Moscow, State Fire Academy of Emercom of Russia Publ.)
[4] Puzach S V and Puzachs V G 2005 Mathematical modeling of heat and mass transfer in fire in a compartment of complex geometry Heat Transfer Research J. 7 p. 585
[5] Puzach S V and Akperov R G 2016 Experimental determination of the specific coefficient of release of carbon monoxide during a fire in the room Fire and Explosion Safety J. 5 (25) p. 18