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Calculation of Gas Parameters at the Exit from a Gas Vent Stack by Means of Calculating Duration of Emptying of the Processing Equipment

Adel I. Kuptsov

Department of Industrial Safety
Kazan National Research Technological University
68 Karl Marx str.
Kazan, 420015, Russia

Roald R. Akberov

Department of Industrial Safety
Kazan National Research Technological University
68 Karl Marx str.
Kazan, 420015, Russia

Fidais M. Gimranov

Department of Industrial Safety
Kazan National Research Technological University
68 Karl Marx str.
Kazan, 420015, Russia

Abstract

Parameters and conditions of discharging a hazardous gas through a vertical gas vent stack at the critical and subcritical gas outflow conditions in the form of functions of time are described. Two methods of determining the time of emptying of the vessel (through time of loss of mass of gas in the vessel and through time of the vessel's depressurization) are proposed. Temporal dependences that can be used for CFD modeling of the process of gas release from the stack are obtained using expressions for the time of emptying of the vessel.

Keywords: boundary conditions, emptying of equipment, gas vent stack, gas efflux, efflux duration

1 Introduction

In case of emergency or during carrying out maintenance procedures, there is a need for immediate emptying of processing equipment by means of discharging gases contained inside the equipment (vessel or pipeline) to the atmosphere. For that purpose, technological gas vent stacks (vertical cylindrical pipelines), providing drain of the gas into the ambient air, are often used (see Figure 1). However, analysis of recent incidents [1-2] and results of experiments [3] showed that under certain meteorological conditions, a formed plume of the air-gas mixture is likely to spread towards locations of technological units or some other industrial facilities and, thereby, lead to air contamination by a hazardous gas in the territory of the enterprise.

At present time, for predictions of propagation of gases discharged to the atmosphere, numerical modeling methods (widely known as CFD methods) have started being used quite successfully [4], which allow obtaining a real picture of dispersion of gases at their emissions from gas vent stacks with the account of geographical relief, buildings terrain and atmospheric stability [5]. As is known, in numerical modeling it is rather difficult to impose the entire complex of boundary and initial conditions [5-8]. For adequate calculation of the subsequent propagation of an air-gas mixture in the surface layer (the lowest part of the atmospheric boundary layer), it is essential to determine correctly, in the first place, parameters and conditions of gases discharged from a gas vent stack: velocity, pressure, temperature, density and compressibility of the discharged gas at the exit from the stack. The gas draining process is non-stationary; boundary conditions change during calculation, as they are related to duration of the gas release process. Hence, it is required, at first, to determine duration time of emptying of the processing equipment, which, in itself, is an important problem for specialists of operating organizations.

Thus, the purpose of the article is determination of parameters and conditions of the gas flow at the exit from the gas vent stack, which are related to gas properties inside the equipment and, hence, vary during the emptying process. The determined temporal dependencies for the parameters can be used by the CFD community for carrying out numerical calculations using such CFD software packages as Fluent.

2 Development of Methods for Determining Duration of Emptying of Equipment

We propose to use the following two methods of determining duration of emptying the equipment:

(1) through decrease of mass of the gas (τ_m);
(2) through decrease of pressure (τ_P);

In method (1), the principle of solution is based upon solving the following equation for τ_m:

$$\frac{1}{\tau_m} = \left(\frac{1}{m}\left|\frac{dm}{dt}\right|\right)_{t=0} = \frac{1}{V}\beta^{1/k}\varphi\sqrt{2\frac{C_P T_1}{\mu}\cdot\left[1-\beta^{\frac{k-1}{k}}\right]}\cdot s\,, \tag{1}$$

where V is volume of gas contained inside the equipment, m^3; m is mass of gas contained inside the equipment, kg; t is time, s; μ is molecular viscosity, kg/(m·s); C_P is specific heat at constant pressure, W/(m·K); k is specific heat ratio; φ is hydraulic resistance coefficient (for the case of no pressure drop losses: φ=1 for the ideal gas and φ=0.8–0.9 for the real gas); β is ratio P_2/P_1; P_1 is gas pressure in the equipment, Pa; P_2 is pressure of the atmospheric air; s is cross-sectional area of the gas vent stack, m^2; T_1 is temperature in the equipment, K. For convenience of the reader, the locations corresponding to indices *1* and *2* in all the equations are denoted in Figure 1.

Equation (1) was obtained from equations (2), (3) and (4) by means of consideration of loss of total mass of gas m with time t caused by gas effluence through the gas vent stack having the cross-sectional area s:

$$\frac{dm}{dt} = -\rho_2 \cdot w_t \cdot s \tag{2}$$

where ρ_2 is gas density at the exit section of the gas vent stack, kg/m^3, which can be represented through gas density in the equipment ρ_1, kg/m^3, as follows:

$$\rho_2 = \rho_1 \beta^{1/k}\,, \tag{3}$$

w_t is gas velocity at the exit from the gas vent stack, m/s; in case of s being much smaller than the equipment size, w_t is determined through the following expression (which is called the Saint-Venant-Ventsel equation):

$$w_t = \varphi\sqrt{2\frac{C_P T_1}{\mu}\cdot\left[1-\beta^{\frac{k-1}{k}}\right]}\,. \tag{4}$$

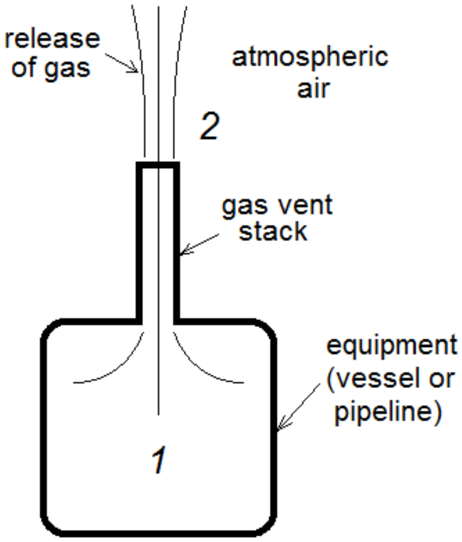

Fig. 1. Schematic of release of gas from equipment (depressurization) to the ambient atmospheric air through a vertical cylindrical gas vent stack. *1* stands for the interior volume of equipment; *2* stands for the atmospheric air near the exit from the gas vent stack

When the pressure ratio β increases, gas velocity w_t can increase only up to a certain maximum value, which is roughly equal to the local sound speed. The critical pressure ratio β_{crit}, corresponding to the maximum velocity of gas effluence from the stack, is determined via the following expression:

$$\beta_{crit} = \left(\frac{P_2}{P_1}\right)_{crit} = \left(\frac{2}{k+1}\right)^{\frac{k}{k-1}}. \tag{5}$$

When pressure P_1 increases above the value corresponding to β_{crit}, the actual speed of gas efflux will not increase any further. Hence, in case of $\beta \le \beta_{crit}$ (subcritical efflux), the following expression is substituted to equation (1):

$$\beta = \left(\frac{2}{k+1}\right)^{\frac{k}{k-1}}, \tag{6}$$

and in case of $\beta > \beta_{crit}$ (supercritical efflux), the following expression is substituted to equation (1):

$$\beta = \frac{P_2}{P_1}. \tag{7}$$

Thus, the critical efflux velocity at the exit from the stack roughly equals to the local speed of sound, and it can be represented as follows:

$$w_t = w_{crit} = \varphi\sqrt{\frac{2k}{k+1}\cdot\frac{P_1}{\rho_1}} = \varphi\sqrt{\frac{2k}{k+1}\cdot\frac{RT_1}{\mu}} = \varphi\sqrt{2\frac{C_P T_1}{\mu}\cdot\frac{k-1}{k+1}}. \tag{8}$$

In method (2), determining duration of pressure relieving or depressurization, τ_P, is based upon using the following expression:

$$\frac{1}{\tau_P}=\left(\frac{1}{P_1}\left|\frac{dP}{dt}\right|\right)_{t=0}=\frac{s\cdot w_{vac}}{V}\beta^{1/k}\left(\varphi^2 k\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]+\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right)\cdot\varphi\sqrt{\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]}\,, \tag{9}$$

where w_{vac} is velocity of gas efflux into vacuum, m/s.

Equation (9) was obtained via the following equation for change in the total energy of gas inside the considered volume of equipment:

$$\frac{dE}{dt}=-\left(\frac{\rho_2 w_t^2}{2}+\frac{\rho_2 C_V T_2}{\mu}\right)\cdot w_t\cdot s \tag{10}$$

In this expression, the sum $\left(\rho_2 w_t^2/2+\rho_2 C_V T_2/\mu\right)$ represents volume density of gas (energy per volume) near the exit from the stack. The first term in the sum is volume kinetic energy associated with movement of gas, and the second term is volume internal energy of gas.

The total energy E of discharged gases from the considered volume of equipment is connected with gas pressure P (which is time-dependent) and volume V (which is constant) via the expression:

$$E=\frac{C_V}{R}PV \tag{11}$$

from which it follows that

$$dE/dt=\left(C_V/R\right)V\,dP/dt$$

and expression for the pressure change becomes:

$$\frac{C_V}{R}V\frac{dP}{dt}=-\rho_2\left(\varphi^2\frac{C_P T_1}{\mu}\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]+\frac{C_V T_2}{\mu}\right)\cdot\varphi\sqrt{2\frac{C_P T_1}{\mu}\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]}\cdot s\,. \tag{12}$$

Then, taking into account the equation for density (3) and the fact that T_2 is temperature at the exit from the stack determined by the equation:

$$T_2=T_1\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\,, \tag{13}$$

we obtain that:

$$\frac{C_V}{R}V\frac{dP}{dt}=-\rho_1\beta^{1/k}\left(\varphi^2\frac{C_P T_1}{\mu}\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]+\frac{C_V T_1}{\mu}\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right)\cdot\varphi\sqrt{2\frac{C_P T_1}{\mu}\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]}\cdot s\,\cdot \tag{14}$$

Introducing the term “gas efflux into vacuum” determined by the expression $w_{vac}=\sqrt{2C_P T_1/\mu}$ and using the Mendeleev-Clapeyron equation, one can obtain the equation:

$$\frac{1}{P_1}\frac{dP}{dt}=-\frac{s\cdot w_{vac}}{C_V\cdot V}\beta^{1/k}\left(\varphi^2 C_P\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]+C_V\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right)\cdot\varphi\sqrt{\left[1-\beta^{\frac{\mathrm{k}-1}{\mathrm{k}}}\right]}\,. \tag{15}$$

Such parameters of gas as density, velocity, pressure and temperature at the exit from the stack at a subcritical speed of gas efflux can be determined via expressions (3), (4), (7) and (13). For determining boundary conditions at the exit from the stack in case of reaching of critical velocity of efflux, we return to consideration of determination of the critical pressure ratio β_{crit} given in equation (5). In this case, parameters of gas at the exit from the stack can be expressed through so-called parameters of "stagnated flow", i.e. through parameters in the equipment, which, indeed, represent some functions of time. Velocity of gas motion in the equipment towards the stack is small in comparison with gas velocity at the exit from the stack determined via equation (8). By neglecting it, we obtain the required boundary conditions:

$$\rho_{crit} = \rho_1(t)\left(\frac{2}{\kappa+1}\right)^{1/(k-1)} , \tag{16}$$

$$T_{crit} = T_1(t)\left(\frac{2}{\kappa+1}\right), \tag{17}$$

$$P_{crit} = P_1(t)\left(\frac{2}{\kappa+1}\right)^{k/(k-1)} > P_2 \tag{18}$$

Taking into account formulas (1), (8), (9) and (16)-(18), we obtain the following estimations of time of emptying of the equipment:

$$\frac{1}{\tau_m} = \left(\frac{1}{m}\left|\frac{dm}{dt}\right|\right)_{t=0} = \frac{1}{V}\left(\frac{2}{\kappa+1}\right)^{1/(k-1)} \varphi\sqrt{2\frac{C_P T_1}{\mu}\cdot\frac{k-1}{k+1}}\cdot s\,, \tag{19}$$

$$\frac{1}{\tau_P} = \left(\frac{1}{P_1}\left|\frac{dP}{dt}\right|\right)_{t=0} = \frac{s\cdot w_{vac}(T_1)}{V}\left(\frac{2}{\kappa+1}\right)^{1/(k-1)}\left(\frac{\varphi^2 k\cdot(k-1)+2}{k+1}\right)\cdot\varphi\sqrt{\frac{k-1}{k+1}} \tag{20}$$

Equations (19) and (20), derived by us, utilize the assumption that the amount of time corresponding to transition from critical efflux to subcritical efflux ($P_2/P_1>\beta_{crit}$) is much greater than the amount of time starting from the moment of transition to the subcritical efflux until the end of the discharge.

3 Results and Discussions

Using equations (1), (9), (19) and (20), we carried out calculations and subsequent analysis of discharge of acetylene, methane and air at the subcritical and critical efflux. Results of calculations are presented in Table 1.

It follows from the table that values of the time of emptying determined via decrease of mass of gas (τ_m) and via pressure decrease in the equipment (τ_P) are approximately equal to each other; the difference makes approximately 1-2%, which is considered acceptable. The reason for the divergence is in the fact that gas temperature in the equipment also changes with time; thus, the assumption that gas temperature always manages to get equal to the ambient temperature is implausible in this case, as duration of the process of gas discharge can be rather small. It is clear that for such a small time, gas temperature in the volume of the equipment does not manage to get equal to the ambient temperature due to heat exchange with the ambient air through the equipment walls. And, nevertheless, values of time can be determined if, for example, the equations (1), (9), (19) and (20) are solved numerically [9]. The error of calculations will decrease with decrease in the Mach number at a subcritical velocity, as in described in [10].

Table 1. Calculated data at the subcritical and critical pressure ratios

Gas	P_1, MPa	φ	V_1, m^3	T_1, K	d, diameter of stack, m	τ_m , s	τ_P , s
At subcritical pressure ratio							
Acetylene	0.14	0.9	100	293	0.3	8.23	8.18
Methane	0.14	0.9	100	293	0.3	6.46	6.42
Air	0.14	0.9	100	293	0.3	8.62	8.51
At critical pressure ratio							
Acetylene	4	0.9	200	273	0.3	15.82	15.64
Methane	4	0.9	200	273	0.3	12.41	12.27
Air	4	0.9	200	273	0.3	16.42	16.06

Our analysis also showed that a difference between values of the time of emptying determined through reduction of mass of gas and the time of emptying determined through pressure decrease does not change with changes in the stack's diameter, temperature in the equipment and volume of the equipment. Thus, it is possible to use different dependences of time of emptying depending on the problem statement. During numerical modeling (CFD calculations) of gas discharge through the stack, there is a possibility of choosing the type of an initial boundary condition at the exit from the stack by setting the pressure, mass flowrate or gas velocity in the form of some functions of time.

4 Conclusions

The proposed mathematical description of the key parameters and conditions of the processes of emptying of the processing equipment by means of releasing hazardous gases from the equipment to the atmosphere with the account of nonstationarity of the processes allowed to obtain equations for determination of duration of the gas efflux from the equipment before its complete emptying in cases of subcritical and critical efflux velocities.

The proposed two methods of determining the time of emptying of the equipment, through decrease of mass of gas (τ_m) and through gas pressure decrease (τ_P), produce results differing from each other by approximately 1–2%.

The obtained analytical dependences allow determining flow parameters at the stack's tip (pressure, mass flowrate, temperature, density and velocity) as functions of time. Use of the dependences for setting time-dependent boundary conditions in calculation of gas releases [5], allows to adequately calculate, using such CFD software packages as Fluent, the process of propagation of the air-gas mixture in the atmospheric surface layer at releasing hazardous gases from the industrial vessels in cases of shutdowns of technological systems for repairs or during emergencies.

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