

Article

Numerical Investigation of the Required Quantity of Inert Gas Agents in Fire Suppression Systems

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Abstract: Inert gas agents have the potential to be widely used in fire suppression systems due to health and safety concerns associated with active chemicals. To suppress fire while minimizing hypoxic effects in an occupied area, the discharge quantity of inert gas agents should be carefully designed to dilute the oxygen concentration to a specific threshold level. In this study, the general expressions between oxygen concentration, the discharge rate of inert gas agents, and the ventilation rate of the air-agent mixture are derived first. Then, explicit formulas to calculate the discharge/ventilation rate and the required quantity of inert gas agents are given if the discharge rate and ventilation rate both are constants. To investigate the dilution and fire extinguishing efficiencies of inert gas agents, two scenarios with a discharge of inert gas agents into an enclosure are modeled using the Fire Dynamic Simulator (FDS). The simulation results show that the average oxygen mass fraction approximately reaches the design level at the end of the discharge period. Variation in oxygen mass fraction along the enclosure height is analyzed. For the scenario with a fire source, oxygen mass fraction decreases fast as oxygen is consumed by the combustion process. Thus, the fire is extinguished a little earlier than the end of the discharge period.

Keywords: gas fire suppression; inert gas agents; agent quantity; discharge rate; ventilation rate

1. Introduction

The production of halons for fire protection was banned in most countries due to the stratospheric ozone layer depletion issue [1]. Over the last three decades, the agents used in gas fire suppression systems have therefore undergone a transition from halon agents to clean agents. The most commercialized clean agents are summarized in [2] and can be categorized into two groups, i.e., halocarbon compounds and inert gases. Halocarbon clean agents extinguish fires by a combination of chemical and physical mechanisms [3,4]. In fires, all halocarbon agents produce decomposition products which may represent a threat to the health and safety of the occupants. Inert gas agents suppress fires by diluting the oxygen concentration to a specific threshold level below which the fire flames are suppressed [5–7]. Research shows that lowering the oxygen concentration in air to below approximately 12% by volume will extinguish flaming fires [2,8]. Compared with halocarbon agents, the inert gas agents are less efficient as fire extinguishing agents in terms of required storage volume and agent weight but produce no hazardous decomposition products. Therefore, there is a potential for inert gas agents to be applied as a means of fire protection in some specific cases where health and safety related to toxicity is highly focused. Some research [9] has been carried out to investigate the application of inert gas agents in some typical buildings for disabled persons, elderly in nursing homes,

and other citizens with reduced cognitive function, etc. Inert gas agents also have great potential as inhibitors of gas explosions by reducing or possibly eliminating the risk of explosions [10–12].

The commercial inert gas agents available for fire suppression systems are Argon (IG-01), Nitrogen (IG-100), Nitrogen+Argon (IG-55), and Nitrogen + Argon + CO_2 (IG-541) [2,13,14]. The inert gas agents are stored as compressed gases and the storage volumes are much larger than that of halocarbon clean agents [2,15]. Fire suppression systems are supposed to discharge a specific amount of inert gas agents into an enclosure to achieve the desired oxygen concentration within a specified time period. If the oxygen concentration is diluted much lower than the desired level, it is called over-discharge in the present study. Over-discharge of inert gas agents results in increasing requirements in storage capacity. Over-discharge of inert agents also leads to an oxygen level that is too low, which in occupied areas, can cause severe hypoxic effects [16]. Due to health concerns, the National Fire Protection Association (NFPA) [17] limits the exposure time for clean agents to 5 min. For inert gas agents, the maximum exposure time has been intensively investigated. Research of Lambertsen and Gelfand [18] shows that cognitive performance does not drop until the inhaled oxygen level is below 14%. It does, however, decrease significantly if the oxygen level is reduced to 10%. Some tests on humans during moderate exercise (walking at a 3 mile per hour pace) were conducted by Ansul [19]. The results show that the cognitive performance returns to high scores when breathing is shifted from a 10% oxygen atmosphere to the INERGEN atmosphere (10% oxygen with 4% CO₂). The presence of CO₂ in the INERGEN agent can favorably affect the respiration, arterial blood oxygenation, and brain blood flow, which is called the "CO₂ Effect". The benefit of the "CO₂ Effect" continues for at least 10 min and undoubtedly well beyond. Laursen [9] suggests the maximum exposure time can be up to 30 min for people with COPD (chronic obstructive pulmonary disease) if they are exposed to an INERGEN atmosphere (10–12.5% O_2 with 3.5-4% CO₂). The desired oxygen concentration after discharge is expected to be no less than 10% in practice. The agent IG-541 with an 8% fraction of CO_2 , therefore, has the potential to be widely applied for fire suppression in occupied areas.

Over-discharge of inert agent leads to hypoxia effects for occupants while under-discharge fails to dilute oxygen concentration to suppress the fire. Therefore, the quantity of inert agents released should be carefully planned to obtain a design oxygen level at which fire can be suppressed and severe hypoxic effects can be avoided. The required quantity of inert gas agents can easily be calculated for an enclosure without ventilation [2]. However, the gas discharge usually generates an overpressure effect in a closed compartment which might lead to destructive events [2,14]. The BETTATI design manual [14] recommends a resistance value of 500 Pa as a conservative value. Therefore, it is necessary to run ventilation systems to eliminate overpressure effects in an enclosure. The operation of a ventilation system during the discharge of inert gas agents results in exhausting the discharged agent-air mixture. It then becomes difficult to estimate the oxygen level in the enclosure and also to evaluate the required quantity of inert gas agents to obtain and sustain the required oxygen level.

The present paper first derives expressions to calculate oxygen concentration as a function of ventilation mass/volume rate, oxygen level, and discharge period. Then, explicit formulas are presented to calculate the discharge rate of inert gas agents to obtain a design oxygen level when the discharge rate and ventilation rate are constant. The required quantity of inert gas agents is integral to the discharge rate over the entire discharge time period. The dilution efficiency and fire extinguishing efficiency of inert gas agents are investigated through a series of numerical simulations using computational fluid dynamics (CFD) fire dynamic simulator (FDS) software v.6.5.3 [20], which is developed by the National Institute of Standards and Technology (NIST) of the United States Department of Commerce. FDS has been widely used in numerical fire safety validations [21,22].

2. Required Quantity of Inert Gas Agents

Before discussing the discharge of inert gas agents, the limiting oxygen mass fraction, which is defined as the minimum oxygen level to support flaming combustion, is introduced first. Then the

discharge mass/volume rate to obtain a design oxygen level is discussed and finally, the calculation of the required quantity of inert gas agents is analyzed.

2.1. Limiting Oxygen Mass Fraction

Frederick [23] assumed that a combustion reaction is suppressed if the energy released from the combustion is not sufficient to raise the fuel-air-product mixture above a critical flame temperature (T_{CFT}) [24]. The amount of energy released by the combustion processes can be approximately estimated by the mass of oxygen consumed through oxygen consumption calorimetry [25]. The basis of the method is that the amount of energy (ΔH_{O_2}) released per unit mass of oxygen consumed is approximately constant. The constant is found to be around 13,100 kJ per kilogram oxygen consumed [25,26].

Under constant pressure and adiabatic conditions, the energy required to raise the bulk temperature of a unit mass at ambient temperature (T_m) to the critical flame temperature (T_{CFT}) may be expressed by:

$$Q = \overline{c}_{p}(T_{CFT} - T_{m}), \tag{1}$$

where \bar{c}_p is the average specific heat, which can be calculated based on the composition of the reacting fuel and any inert gases.

To reach the critical flame temperature (T_{CFT}), the combustion energy should be no less than the energy calculated from Equation (1). Based on the method of oxygen consumption calorimetry, the oxygen mass fraction in this volume should be no less than the limiting mass fraction:

$$\hat{Y}_{O_{2,lim}} = \frac{\bar{c}_p(T_{CFT} - T_m)}{\Delta H_{O_2}}$$
⁽²⁾

If the oxygen mass fraction Y_{m,O_2} is lower than $\hat{Y}_{O_2,\text{lim}}$, the energy released from the combustion is less than $\hat{Y}_{O_2,\text{lim}}\Delta H_{O_2}$, which is no more than the energy shown in Equation (1). Thus, the amount of energy is not sufficient to raise the fuel-air-product mixture above T_{CFT} and the combustion process will self-terminate.

Assuming an average specific heat \bar{c}_p of 1.2 kJ/(kg ·K), critical flame temperature (T_{CFT}) 1700 K for hydrocarbon diffusion flames [23,24] and ambient temperature 300 K, the limiting oxygen fraction $\hat{Y}_{O_2,lim}$ is estimated to be 12.8%. This value is in good agreement with the experiments giving volume concentrations in the range of 10.3 % to 13.9 % [24,27]. Note that these results are expressed as volume fractions.

2.2. Discharge Mass Rate of Inert Gas Agents

Inert gas agents may be discharged into an enclosure to dilute the oxygen concentration to below the design level, which results in the combustion process self-terminating. Oxygen concentration is the key factor in determining the suppression of flaming combustion. The mass fraction of oxygen in ambient air is approximately 0.23. Thus, the mass fraction of oxygen (Y_{m,O_2}) can easily be derived from the mass fraction of air $(Y_{m,air})$, i.e., $Y_{m,O_2} = 0.23Y_{m,air}$. In the following discussion, the air mass fraction in an enclosure is estimated first to derive the oxygen mass fraction. The ventilation system in the later discussion only refers to mechanical ventilation, i.e., exhaust fans. To simplify the discussion, it is assumed that air and inert gas agents are mixed instantaneously and inert gas agents and air at any time are uniformly distributed in an enclosure. Thus, the exhausted mixture from ventilation vents has the same air/agents mass fraction distribution as that remaining in the enclosure.

The mass fraction of air in an enclosure at time t is assumed to be $Y_{m,air}(t)$. At the start, i.e., at t = 0, $Y_{m,air}(0) = 1$. After a small time interval Δt , the air mass fraction decreases due to the introduction of inert gas agents at t > 0. The air mass fraction at time $t + \Delta t$ is approximately given by:

$$Y_{m,air}(t + \Delta t) \approx Y_{m,air}(t) \frac{m(t)}{m(t) + R_m(t)\Delta t},$$
(3)

where $R_m(t)$ is the discharge mass rate of the inert gas agent (kg/s). $R_m(t)$ may be constant or a function of time. m(t) (kg) is the total mass of the mixture in the enclosure at time t and can be expressed as:

$$m(t) = m_0 + \int_0^t (R_m(\xi) - E_m(\xi)) d\xi,$$
(4)

where m_0 is the total mass initially present at time 0. The second term on the right represents the net increase of mass over time range [0, t] and ξ is the time variable. $E_m(t)$ is the ventilation mass rate of the mixture (kg/s). If $E_m > R_m$, the total mass of mixture in the enclosure would decrease with time. To ensure that the total mass m(t) is positive, the second term on the right of Equation (4) should be smaller than m_0 .

To deduce an explicit expression to calculate $Y_{m,air}$ at any time t, an iterative procedure is applied to Equation (3). A small time interval Δt is chosen to discretize the time, this is $t = n\Delta t$ and $t_i = i\Delta t$ ($0 \le i \le n$). Repeating the iterative procedure by the use of Equation (3) and applying the initial condition $Y_{m,air}(0) = 1$, the mass fraction of air at time t is:

$$Y_{m,air}(t) = \lim_{n \to \infty} \prod_{i=0}^{n-1} \frac{m(t_i)}{m(t_i) + R_m(t_i)\Delta t}$$
(5)

By taking the natural logarithm of both sides of the above the equation and rearranging it, Equation (5) becomes:

$$\ln\left(\frac{1}{Y_{m,air}(t)}\right) = \lim_{n \to \infty} \sum_{i=0}^{n-1} \ln\left(1 + \frac{R_m(t_i)}{m(t_i)}\Delta t\right).$$
(6)

If the time interval Δt is extremely small, the right term in Equation (6) may be approximated by:

$$\ln\left(1 + \frac{R_m(t_i)}{m(t_i)}\Delta t\right) \approx \frac{R_m(t_i)}{m(t_i)}\Delta t.$$
(7)

If $\Delta t \rightarrow 0$, that is $n \rightarrow \infty$, Equation (7) may then be written as:

$$\lim_{n \to \infty} \sum_{i=0}^{n-1} \frac{R_m(t_i)}{m(t_i)} \Delta t = \int_0^t \frac{R_m(\xi)}{m(\xi)} d\xi.$$
(8)

Substituting Equation (7) and Equation (8) into Equation (6) and rearranging it, the mass fraction of air may be expressed as:

$$Y_{m,air}(t) = e^{-\int_0^t \frac{K_m(\xi)}{m(\xi)} d\xi}.$$
(9)

If $Y_{m,O_2} = 0.23Y_{m,air}$ is applied, the mass fraction of oxygen in an enclosure at time t is given by:

$$Y_{m,O_2}(t) = 0.23e^{-\int_0^t \frac{R_m(\xi)}{m(\xi)} d\xi}.$$
(10)

Equation (10) gives an expression to calculate oxygen mass fraction as a function of ventilation mass rate, discharge mass rate, and discharge time.

To estimate the discharge quantity of inert gas agents, an explicit formula is required to calculate the discharge rate. It is easy to explicitly calculate the discharge mass rate from Equation (10) if the discharge mass rate R_m and ventilation mass rate E_m are constants. Assuming that V_0 represents the volume of the enclosure and ρ_{air} denotes the density of the ambient air, m(t) can be simplified as:

$$\mathbf{m}(\mathbf{t}) = \mathbf{V}_0 \boldsymbol{\rho}_{air} + (\mathbf{R}_m - \mathbf{E}_m)\mathbf{t},\tag{11}$$

If R_m and E_m are both constants and not equal to each other, it can be assumed that $E_m = kR_m$ ($k \neq 1$). By substituting Equation (11) into Equation (10), the required agent discharge mass rate to obtain a design oxygen fraction Y^*_{m,O_2} is given by

$$R_{m} = \frac{V_{0}\rho_{air}}{t(1-k)} \left(\left(\frac{Y_{m,O_{2}}^{*}}{0.23} \right)^{k-1} - 1 \right),$$
(12)

If the ventilation mass rate equals the discharge mass rate, that is $E_m = R_m$ (k = 1), the discharge mass rate of agents to obtain the design oxygen fraction Y^*_{m,O_2} is:

$$R_{\rm m} = \frac{V_0 \rho_{\rm air}}{t} \ln \frac{0.23}{Y_{\rm m,O_2}^*},$$
(13)

2.3. Discharge Volume Rate of Inert Gas Agents

In practice, the discharge of inert gas agents and exhaust of agent-air mixture is usually measured as volume rates. The ventilation mass rate (E_m) can not be directly converted into the volume rate (E_V) as the density of the agent-air mixture varies during the discharge period. Therefore, the discharge volume rate (R_V) can not be derived from Equation (10), Equation (12), and Equation (13) directly.

To derive the discharge volume rate, a concept called standard volume (V^*) is defined as the volume at atmospheric pressure and ambient temperature. At the start, the standard volume $V^*(0)$ equals the enclosure volume V_0 . After a discharge time t, the specific volume is:

$$V^{*}(t) = V_{0} + \int_{0}^{t} (R_{V}(\xi) - E_{V}(\xi)) d\xi,$$
(14)

The volume fraction of air in an enclosure at time $t + \Delta t$ can then be approximately estimated from Equation (14) at time t:

$$Y_{V,air}(t + \Delta t) \approx Y_{V,air}(t) \frac{V^*(t)}{V^*(t) + R_V(t)\Delta t}$$
(15)

Applying the same procedure as Equation (5) to Equation (9) to the above equation, the volume percentage of oxygen is expressed as a function of discharge volume rate, ventilation volume rate, and discharge time:

$$Y_{V,O_2}(t) = 0.21 e^{-\int_0^t \frac{R_V(\xi)}{V^*(\xi)} d\xi},$$
(16)

If the discharge volume rate R_V and ventilation volume rate E_V are constants and $E_V = k R_V$ ($k \neq 1$), the required discharge volume rate of the agent to obtain a design oxygen volume fraction Y^*_{V,O_2} could be derived from Equation (16) as:

$$R_{\rm V} = \frac{V_0}{t(1-k)} \left(\left(\frac{Y_{\rm V,O_2}^*}{0.21} \right)^{k-1} - 1 \right), \tag{17}$$

If $E_V = R_V$ (k = 1), the discharge volume rate of the inert gas agent to obtain the design oxygen fraction Y^*_{V,O_2} is given by:

$$R_{\rm V} = \frac{V_0}{t} \ln \frac{0.21}{Y_{\rm V,O_2}^*},\tag{18}$$

Equation (17) with k = 0 and Equation (18) match the expressions shown in [2,14], which calculate the discharge rate from a design volume fraction of inert gas agents, not a design volume fraction of oxygen.

Equations (14) through to Equation (18) are derived by assuming that the inert gas agents are discharged at the same temperature as the air in the enclosure. The inert gas agent is, however, stored in cylinders at high pressures, i.e., 200–300 bar. When released, it expands. The energy required for this expansion results in a loss of internal energy, i.e., a temperature depletion. Therefore, inert gas agents are discharged at a lower temperature than the ambient air. When inert gas agents enter into an enclosure, the inert gas agents expand and meanwhile cool down the surrounding air. The temperature of the air-agents mixture in the enclosure is dynamic during a discharge period. The ideal gas law shows that the thermal expansion of gas agents is proportional to temperature change if the agents' mass and pressure are fixed. The ambient air is cooled down during the discharge period, which mitigates the effects of thermal expansion of inert gas agents. The effects of the thermal expansion of inert gas agents and the thermal contraction of air are very difficult to estimate and could be analyzed in future studies. In this study, the combined effect of thermal expansion of inert gas agents and thermal contraction of air is assumed to be proportional to the square root of temperature change. The discharge volume rate calculated from Equation (17) and Equation (18) is the volume rate at air temperature. To get the discharge volume rate at agents temperature, the volume rate at air temperature is simply adjusted by a proportionality coefficient c as:

$$c = \left(\frac{T_{agents}}{T_{mixture}}\right)^{0.5},$$
(19)

where T_{agents} is the discharge temperature of inert gas agents and $T_{mixture}$ is the temperature of the air-agents mixture and is calculated as:

$$T_{mixture} = \frac{c_{p,agents} Y_{m,agents} T_{agents} + c_{p,air} Y_{m,air} T_{air}}{c_{p,agents} Y_{m,agents} + c_{p,air} Y_{m,air}},$$
(20)

where c_p is the isobaric mass heat capacity. $Y_{m,agents}$ and $Y_{m,air}$ are the mass fractions of agents and mass fraction of air respectively when the oxygen level reaches the design level.

2.4. Required Quantity of Inert Gas Agents

If the discharge rate of inert gas agents is given, the discharge quantity of agents to obtain a design oxygen level may be calculated as:

$$m_{agents} = \int_0^t R_m(x) dx = \int_0^t R_V(\xi) \rho_{agents} d\xi,$$
(21)

If the discharge rate is constant and the density of agents is fixed during the discharge period, the discharged quantity of inert gas agents is the product of discharge mass rate and discharge period:

$$m_{agents} = R_m t = R_V \rho_{agents} t, \tag{22}$$

Substituting Equation (12) and Equation (13) into Equation (22) and assuming $V_0 = 1 \text{ m}^3$, $\rho_{air} = 1.2 \text{ kg/m}^3$ and $Y^*_{m,O_2} = 12.8\%$, the quantity of inert gas agents per unit volume becomes a function of k (k = E_m/R_m). Here k should satisfy k < $\frac{V_0\rho_{air}}{m_{agents}} + 1$ according to Equation (11). Figure 1 shows the quantity of inert gas agents as a function of k. The required inert gas quantity to obtain a design oxygen level per unit enclosure volume decreases with increasing values of k. Therefore, venting out the air-agent mixture not only removes the overpressure effect in an enclosure, it also lowers the mass requirement of inert gas agents. The explanation is that oxygen is also vented out when the mixture is vented out of an enclosure, which can accelerate the decrease of oxygen concentration and further reduce the required quantity of inert gas agents.



Figure 1. Required quantity of inert gas agents per unit volume vs. $k (k = E_m/R_m)$.

3. Numerical Investigation

In the previous section, the expressions needed for estimating oxygen fraction were derived based on the assumption that inert gas agents and air at any time are uniformly distributed within the enclosure. However, the assumption is not correct as it takes time to mix agents and air. Moreover, agents and air have different densities, which might result in an uneven distribution of oxygen along the enclosure height. The fire extinguishing efficiency of inert gas agents also needs investigation due to possible uneven distribution of oxygen and other combustion conditions. Therefore, several issues should be considered:

- Is the design oxygen level obtained at the end of the discharge period?
- What is the variation of oxygen fraction along the enclosure height?
- Would the pressure in an enclosure exceed the resistance value of 500 Pa during the discharge period?
- What about the extinguishing efficiency of the inert gas agents?

To investigate these issues, scenarios with the discharge of inert gas agents into an enclosure were numerically modeled using FDS 6.5.3. The enclosure is a studio with a bathroom, an entrance, and a main room. The size of the enclosure is the same as that of the test room built by Kraaijeveld [28] for fire suppression tests. It is 2.4 m high and its layout is shown in Figure 2. The door between the main room and the bathroom was open while the other two doors in the entrance were closed. The vent to discharge inert gas agents and the vent to exhaust the agent-air mixture were mounted at the right bottom comer of the ceiling (red square in Figure 2b) and the left bottom corner of the ceiling (green square in Figure 2b), respectively. The discharge of inert gas agents and exhaust of air-agents mixture were run in parallel. When the discharge and ventilation were not in operation, the two vents were closed.



Figure 2. (a) Test room layout (unit: mm) and (b) the corresponding simulation model.

Two kinds of inter gas agents, IG-100 and IG-541, were applied in the model separately. The necessary chemical and physical properties of the two agents are shown in Table 1. In this scenario, the temperature of inert gas agents discharged from the vent was assumed to be -5° C [29]. The agents were discharged into the enclosure for a 60 s period. The design oxygen volume fraction was set to be 11.51% for IG-100 and 12.55% for IG-54, which equals 12.8% in mass fraction for both agents. The discharge and ventilation rates were calculated from Equations (17) to (19) in volume rate since the volume flow rate is for practical reasons normally recorded. The discharge rates are listed in Table 2. The ratio of ventilation rate to discharge rate (k) varies between 0.8–1.2.

Table 1. Chemical and physical properties of inert gas agents at 1 atm and T = 293 K [2,14]. The fraction represents volume%.

| Agent | Chemical Formula | Density (kg/m ³) | Isobaric Mass Heat Capacity (kJ/kg K) |
|--------|---|------------------------------|---------------------------------------|
| IG-100 | N_2 | 1.16 | 1.04 |
| IG-541 | 52% N ₂ , 40% Ar, 8% CO ₂ | 1.42 | 0.78 |

Table 2. Summary of simulation cases. $\alpha = 0.0264 \text{ s}^{-2}$ and "-" represents no parameters are required to set up.

| HRR (kW) | Y^*_{m,O_2} | Discharge Period | Inert Gas Agent | k (= E_V/R_V) | $R_V(m^3/s)$ | Case Index |
|--------------------------|---------------|------------------|-----------------|------------------|--------------|------------|
| HRR = 0 | 12.8% | 0–60 s | IG-100 | 0.8 | 0.4220 | C0_100_0.8 |
| HRR = 0 | 12.8% | 0–60 s | IG-100 | 0.9 | 0.4095 | C0_100_0.9 |
| HRR = 0 | 12.8% | 0–60 s | IG-100 | 1.0 | 0.3973 | C0_100_1.0 |
| HRR = 0 | 12.8% | 0–60 s | IG-100 | 1.1 | 0.3855 | C0_100_1.1 |
| HRR = 0 | 12.8% | 0–60 s | IG-100 | 1.2 | 0.3473 | C0_100_1.2 |
| HRR = 0 | 12.8% | 0–60 s | IG-541 | 0.8 | 0.3559 | C0_541_0.8 |
| HRR = 0 | 12.8% | 0–60 s | IG-541 | 0.9 | 0.3467 | C0_541_0.9 |
| HRR = 0 | 12.8% | 0–60 s | IG-541 | 1.0 | 0.3380 | C0_541_1.0 |
| HRR = 0 | 12.8% | 0–60 s | IG-541 | 1.1 | 0.3294 | C0_541_1.1 |
| HRR = 0 | 12.8% | 0–60 s | IG-541 | 1.2 | 0.3211 | C0_541_1.2 |
| HRR = $\alpha \cdot t^2$ | - | - | - | - | - | C1_0 |
| HRR = $\alpha \cdot t^2$ | 12.8% | 30–90 s | IG-541 | 1.0 | 0.3380 | C1_1.0 |

A new scenario with a chair fire in the room was arranged to investigate the extinguishing efficiency of inert agents. The scenario was designed similarly to the experiments conducted by Kraaijeveld [28]. A $0.5 \times 0.5 \times 0.6$ m³ chair was placed 2.0 m from the left wall and 1.1 m from the back wall, as indicated in Figure 2b. The combustion property of fabric was applied to the chair [20] and the auto-ignition temperature (T_{AIT}) was set to be 210 °C [30]. The chair was ignited by hot particles which were placed above the chair to heat the chair to above the auto-ignition temperature. The heat release rate (HRR) for the chair was set to be a t-squared fire with a 0.0264 kW/s² growth rate for the first 90 s and reached the fully developed phase in the remaining simulation time period [26]. The discharge of agents IG-541 started at t = 30 s, i.e., when the fire was well established, and ended at 90 s, i.e., a 60 s discharge period. As the oxygen level under different ratio (k) has been investigated in the first scenario, it only focused on the extinguishing efficiency of inert gas agents in this scenario. The ventilation volume rate was set to be the same as the discharge rate. In the simulation, the simple flame extinction model in FDS was applied to gauge whether or not combustion was viable based on the local oxygen concentration. The simple flame extinction model assumes that combustion does not take place if the temperature is below the auto-ignition temperature (TAIT) for fuel or if the heat released from the combustion process is not sufficient to raise the fuel-air-product mixture temperature above the empirically determined critical flame temperature (T_{CFT}). The heat released from the combustion process is limited by the availability of oxygen as shown in Section 2.1, thus the suppression of flaming combustion is based on the oxygen concentration. To observe the extinguishing efficiency of the inert gas agents, a case without a discharge of agents was also simulated. The simulation cases are summarized in Table 2.

To analyze the mesh sensitivity, four different Cartesian mesh solutions were applied to discretize the computational domain. The four solutions used cubic cells with sizes of 0.18 m, 0.15 m, 0.10 m, and 0.075 m, respectively, for the whole computational domain. The mesh sensitivity of the simulations was analyzed by comparing the temperature and oxygen mass fraction below the ceiling at the room center from the simulation case C1_1.0. Figure 3 shows the predictions of temperatures and oxygen mass fractions versus time. It is obvious that the convergence of temperature is obtained for the three finer meshes. The discrepancy of predicted temperatures from the two finest mesh solutions is no more than 9.6%. The same trend is also observed for the predicted oxygen mass fraction. Therefore, it is reasonable to assume that the mesh solution of 0.1 m is adequate to produce mesh independent simulation results. The following discussion is therefore based on the results from simulations with this mesh solution.



Figure 3. Predicted temperatures (**a**) and mass fraction versus time below the ceiling at the main room center from four mesh solutions (**b**).

4. Simulation Results and Discussion

The simulation results from scenario C0 (HRR = 0) are used to investigate the average oxygen mass fraction, oxygen distribution, and pressure within the enclosure. In a later results discussion, the predicted oxygen mass fraction, instead of the volume fraction, is given as the oxygen mass fraction used in determining the fire extinguishing efficiency in the FDS simulation models.

Figure 4 shows the average oxygen mass fraction against time for the case C0_100_1.0. The average oxygen concentration was reduced during the discharge period (first 60 s) and stayed constant for the next 40 s. The horizontal dashed line is the design oxygen mass fraction (12.8%), which corresponds to the inert gas agents' mass fraction of 44.35%. The oxygen mass fraction of the other cases displayed a similar trend as shown in Figure 4. As seen in Table 3, the average oxygen mass fraction at the end of the discharge period (60 s) did, however, vary slightly compared to case C0_100_1.0. The discrepancy between the obtained level and the design level was no more than 0.9% for case series C0_100 and 1.7% for case series C0_541. The discrepancy for the case series C0_541 is larger than that for the case series C0_100. The reason is that the density of IG-100 is close to the air density while the density of IG-541 is higher than the air density. The agent IG-541 descended to the floor during the discharge period and the air-agents mixture below the ceiling contained more oxygen than the average level. Thus, more oxygen was exhausted from the ceiling vent than expected, which resulted in the oxygen mass fraction being a little lower than the designed level. This indicates that the obtained oxygen level in an enclosure can be slightly influenced by the density of inert gas agents.



Figure 4. Oxygen mass fraction vs. time for the case C0_100_1.0.

Table 3. Predicted average oxygen mass fraction and pressure difference for case series C0.

| Case Index | $\mathbf{Y}_{\mathbf{O}_2}$ | Pressure Difference (Pa) |
|------------|-----------------------------|--------------------------|
| C0_100_0.8 | 11.9% | 1.79×10^{4} |
| C0_100_0.9 | 12.1% | 8.30×10^{3} |
| C0_100_1.0 | 12.5% | 23.3 |
| C0_100_1.1 | 12.8% | -7.14×10^{3} |
| C0_100_1.2 | 13.0% | -1.33×10^{4} |
| C0_541_0.8 | 11.1% | 1.50×10^{4} |
| C0_541_0.9 | 11.3% | 7.11×10^{4} |
| C0_541_1.0 | 11.4% | 25.1 |
| C0_541_1.1 | 11.6% | -6.7×10^{3} |
| C0_541_1.2 | 11.8% | -1.17×10^{4} |

Table 3 also gives the pressure difference from standard atmospheric pressure within the enclosure. There is a very small pressure difference if the ventilation rate equals the discharge rate. However, if the ventilation rate varies from 10% to 20% up or down of the discharge rate, the pressure difference varies from about 10^3 to 10^4 Pa. This means that the enclosure structure may be exposed to damaging pressures if the ventilation rate is smaller than the discharge rate.

To investigate the oxygen distribution within the enclosure, the modeled oxygen mass fraction was analyzed at floor level (height 0.1 m), at 1.2 m height and at ceiling level (height 2.3 m) at three locations (see Figure 2). Figures 5 and 6 show the oxygen mass fraction at these heights and at the three locations (I, II, and III) for the case C0_100_1.0 and C0_541_1.0 respectively. At each height or location, the lowest, median, and highest values are shown as short horizontal dashes. The horizontal line is the average oxygen mass fraction in the enclosure. Figure 5 shows that the obtained oxygen level varied slightly around the average level at three heights and three locations for the case C0_100_1.0. The oxygen mass fraction varied between 11.6 and 14.4 % within the enclosure. The slight variation is partly a result of the similar density between IG-100 and air and thermal expansion of inert gas agents. Figure 6 shows the oxygen level for case C0_541_1.0. At the floor level, the oxygen mass fraction was always lower than the average level at the three other locations. At height 1.2 m above the floor, the oxygen mass fraction was slightly lower than the average level at three locations. At ceiling height, the oxygen mass fraction was always higher than the design level and varied between 16.7 and 20.4%. Therefore, it can be concluded that the oxygen mass fraction decreased with decreasing enclosure height and the value was normally no more than the design level at the middle height of the enclosure for IG-541. This is partly a result of the density difference between the IG-541 at -5 °C and the ambient air.



Figure 5. The lowest, median, and highest oxygen mass fraction at height 0.1, 1.2, and 2.3 m above the floor (**a**), and at locations I, II, and III at 100 s for case C0_100_1.0 (**b**).



Figure 6. The lowest, median, and highest oxygen mass fraction at height 0.1, 1.2, and 2.3 m above the floor (**a**), and at locations I, II, and III at 100 s for case series C0_541_1.0 (**b**).

The extinguishing efficiency of inert gas agents was investigated through the case series C1, which set HRR as a t-square fire. In the case C1_0, no inert gas agents were discharged into the enclosure and the HRR grows approximately as the square of time (Figure 7). The oxygen was consumed by the combustion processes and its mass fraction dropped from 23.1% to 21.6% at the end of the 100 s simulation period. For the case C1_1.0, inert gas agent IG-541 was released into the enclosure between 30 s and 90 s. The HRR of case C1_1.0 increased during the first 70 s and then dropped to 0 at 76 s. The simple flame extinction model adopted in FDS models terminates combustion due to oxygen starvation. It might not match the reality as smoldering combustion may continue at a very low rate even at oxygen concentrations insufficient to sustain flaming combustion. The oxygen mass fraction around the fire source decreased from 12.8% to 11.4% between 72 s and 76 s. Two phenomena were observed from the case C1_1.0. The oxygen mass fraction dropped faster than the case C0_541_1.0, which runs without a fire source. The reason for this is that oxygen was consumed during the combustion, which accelerated the decrease in oxygen concentration. The second phenomenon is that HRR reached 0 at an oxygen level of 11.4%, which is lower than the design level. The design oxygen mass fraction 12.8% is derived from Equation (2) with an ambient temperature of 300 K, air specific heat c_p of 1.2 kJ/(kg·K), and critical flame temperature (T_{CFT}) of 1700 K. However, the real ambient temperature around the chair reached 340 K. The specific heat of IG-541 is 0.82 kJ/(kg·K) at this temperature, which means the specific heat of air-agents mixture is lower than 1.2 kJ/(kg-K). The critical flame temperature (T_{CFT}) adopted in FDS is 1600 K [23], which is lower than the value suggested in Section 2.1. The limiting oxygen concentration estimates are based on the heat required to heat the combustion products from the ambient temperature to the critical flame temperature (T_{CFT}). When experiencing a locally increased "ambient temperature", less heat is required to reach the critical flame temperature, i.e., more inert gases are needed to prevent combustion taking place. Therefore, the real oxygen limit level should be lower than 12.8% according to Equation (2) in the case C1_1.0. After the fire was extinguished at 80 s, the IG-541 was discharged

continuously until 90 s and the oxygen mass fraction reached 10.2%. The oxygen level of 10.2 % is an acceptable value in an occupied area considering the benefit of the "CO₂ Effect".



Figure 7. Heat release rates (HRRs) versus time for series case C1.

5. Conclusions and Suggestions for Future Studies

This paper proposes general expressions between oxygen level, discharge rate, and ventilation rate. Explicit equations are given to calculate the discharge rate and the required quantity of inert gas agents to obtain a design oxygen level when the discharge rate and ventilation rate are both constants.

The proposed expressions in the present study are derived based on the assumption that inert gas agents and air at any time are uniformly distributed in an enclosure. The assumption simplifies the gas discharge phenomenon. To investigate the discharge efficiency and extinguishing efficiency of inert gas agents, several simulation scenarios with and without a fire source were run using the CFD simulation tool—FDS. The simulation results show that:

- The design oxygen level could be approximately obtained at the end of the discharge period if the discharge rate and ventilation rate are calculated from the suggested equations. The obtained oxygen level in an enclosure can be slightly influenced by the density of inert gas agents.
- Oxygen fraction varies with height as a result of density differences between air and inert gas agents. The oxygen mass fraction was normally below the design level at the lower half of the enclosure.
- To avoid enclosure over-pressure effects, the discharge volume rate should be close to the ventilation volume rate.
- For the case with a chair fire, the HRR dropped to zero before the end of the discharge period partly due to the oxygen consumed in combustion.

This study demonstrates that ventilation systems not only play an important role in mitigating the possible released inert gas agent overpressure effect but also reduce the required quantity of inert gas agents to obtain a design oxygen level. The oxygen mass fraction increased with the height of the enclosure if the density of an inert gas agent is higher than the density of the air. This ensures that inert gas fire suppression systems perform better in the low elevation in an enclosure as most inert gas agents have a higher density than that of air. In the case with a fire, the oxygen consumed in combustion during discharge time accelerated the fire extinguishing. In future work, the inert gas agents extinguishing efficiency for different fire sizes, and the thermal pressure caused by fires in an enclosure should be investigated. In addition to the mechanical ventilation system, the natural ventilation system, e.g., open doors, windows, and leaks [31,32] in reality also alters the ventilation flow rate and should be taken into consideration in future studies. Moreover, experimental validations are needed for the practical applications of this study as variation in the agents' discharge rate may be expected.

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Nomenclature

| c p | average specific heat (kJ/(kg·K)) |
|-----------------------------|--|
| Em | ventilation mass rate of mixture (kg/s) |
| E _V | ventilation volume rate of mixture (m ³ /s) |
| ΔH_{O_2} | energy released per unit mass of oxygen consumed (kJ/kg) |
| HRR | heat release rate (kW) |
| k | ratio of ventilation rate to discharge rate |
| m | total mass of gases in the enclosure (kg) |
| m ₀ | total mass in the enclosure at start (kg) |
| m _{agents} | discharge quantity of agents (kg) |
| Q | energy (kJ) |
| R _m | discharge mass rate of agents (kg/s) |
| R _V | discharge volume rate of agents (m ³ /s) |
| t | time (s) |
| T _{CFT} | critical flame temperature (K) |
| T _m | ambient temperature (K) |
| V_0 | volume of an enclosure (m ³) |
| V^* | standard volume (m ³) |
| Ym | mass fraction |
| Y _{m,air} | air mass fraction in mixture |
| Y _{m,O2} | oxygen mass fraction in mixture |
| Y^*_{m,O_2} | design oxygen mass fraction |
| Y _{V,air} | air volume fraction in mixture |
| Y_{V,O_2} | oxygen volume fraction in mixture |
| Y^*_{V,O_2} | design oxygen fraction |
| Y _V | volume fraction |
| $\hat{Y}_{O_{2,\prime}lim}$ | limiting oxygen fraction to sustain a flame |
| ρ | density (kg/m ³) |

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