Use of University of Nottingham Gas Safety Calculator

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Purpose

This document outlines the use of the in-house University of Nottingham Gas Safety calculators hosted on the University website (https://www.nottingham.ac.uk/safety/policies-and-guidance/gases/gases.aspx). The outcome of the calculation can be used as a source of information to determine the risk to users within the immediate vicinity, as well as a tool to determine whether gas detection needs to be installed.

It is noted that these calculations only form part of the risk assessment, and evidence that a calculation is carried out is not by itself considered a suitable and sufficient assessment of risk. The risk assessment process should still be carried out as normal, and the calculations should only be used to determine who can be harmed, how, and identify the necessary controls.

The calculator can be used to quantify a number of potentially hazardous scenarios related to the release of compressed or liquefied gases including:

1. Environmental oxygen depletion (asphyxiation)
2. Toxic enrichment (poisoning)
3. Flammable atmosphere creation (increased risk of fire)

In this document, a number of examples will be carried out demonstrating the use of the calculators to determine whether there is a risk associated with the release of gas within a room of given size. If the recommendation is made that gas detection is needed, such gas detection systems must be suitable for the scenario and must be installed by a competent person who will ensure appropriate location of detectors. A servicing plan must be in place, with the detection maintained in line with the manufacturer's instructions.

Assumptions:

Calculation of gas concentrations is a highly challenging task due to the number of constantly changing variables in any given scenario.

In order to carry out such calculations, a number of assumptions are made to simplify the process.

As per the BCGA guidance, these assumptions lead to a worse-case scenario situation, and it is commonplace to make recommendations based upon this calculated scenario.
The mains assumptions we make are:

1. **Compressed and Liquefied Gases behave as ideal gases:** All gas particles are the same size, all collisions are perfectly elastic, and there are no attractive/repulsive forces between the particles or cylinder walls.
2. The release of compressed/liquefied gases displaces each component of the air it expands into in equal quantities. All the existing air is replaced simultaneously, and air changes are not considered.

Preparing for Calculations:

Ahead of performing gas safety calculations, a range of information is needed up front:

1. **The properties of the gas(es)** - Some gases pose multiple threats, (Asphyxiation, Toxic and/or Flammable) so each of the potential hazards need to be considered in isolation and the hazards that present the highest risk should be considered first when identifying mitigations. For example, CO2 can create an oxygen deficient environment, but it is also toxic. Both hazards need to be evaluated separately, and the controls identified need to address both hazards if necessary. Similarly, for CO, this presents a risk of asphyxiation, enrichment as well as a flammability hazard – the enrichment is, once again, the highest risk to users.

2. **Nature of the Gas in the cylinder**: Assuming the volume of the gas in the cylinder is not known, the process to evaluate liquefied gases is different to that of compressed gases, and the variables needed to perform the calculation are different. The values you may need to know depending on the nature of the gas are given below

Compressed Gas	Liquefied Gas
Pressure of cylinder (bar)	Weight of gas in cylinder (kg)
*Cylinder water capacity (L)	**Specific volume (m^3/kg)

   Some gas cylinder suppliers will be able to provide the volume of the gas in the cylinder already. If this is the case, the above information is not required.

   *The cylinder water capacity refers to the volume of water that could be held in the cylinder. For larger cylinders, this tends to be no more than 10s of litres.

   ** The specific volume refers to the amount of space a given gas occupies per unit mass.
3. **The free air volume of the room** – This is the available volume within a room that a gas could expand into. It can be calculated by subtracting the size of all solid objects within the room (e.g. furniture and equipment) from the volume of the room itself.

Approach to Gas safety calculations:

The gas calculator works in the following way:

1. Determination of the volume of gas that could be released into a room upon release of contents.

2. Comparison of gas volume to free air volume.

   This returns either i) The percentage of contaminant in air or ii) the concentration of oxygen in the air after dilution.

3. Comparison of relevant percentage to workplace exposure limits, lower explosive limits, or other relevant limits.

4. Recommendation provided based upon whether limits are exceeded.

Examples:

Example 1:

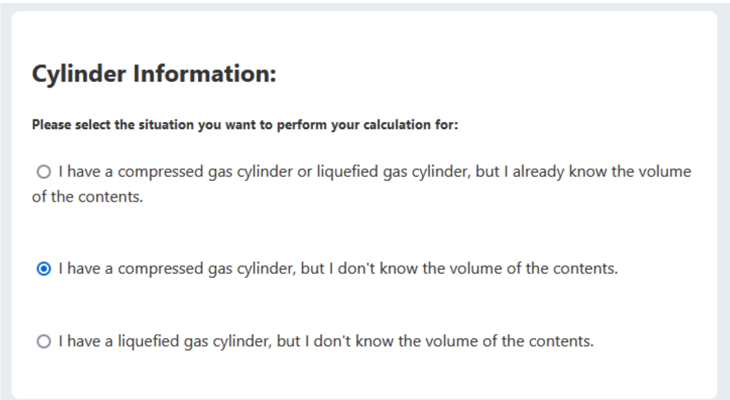
1. **A fully charged BOC Argon Cylinder is located in a lab of volume 30 m^3. The volume of all furniture in the lab has been measured to be 12 m^3. The cylinder is known to be charged to 200 bar, and the data sheet indicates a water capacity of 50L.**

   What would the concentration of oxygen be in the lab in the event of an instantaneous, accidental release?

1. In most cases, Argon comes as a compressed gas. It is not toxic or flammable, and thus the primary risk to human health will be the risk of asphyxiation. We will therefore use the Oxygen Depletion Calculator.

   https://www.boconline.co.uk/shop/en/uk/gas-a-z/argon-gas-cylinders/argon-research-grade-cylinder-293680

   Using the details in the question, we know we have a compressed gas cylinder, but we don't know the volume of the gas in the cylinder. We should therefore indicate this in the calculator – see below:



2. After this, we are then prompted to enter what we know into the calculator. As the cylinder is located in a normal lab under standard conditions, we assume that the pressure within the room is equal to atmospheric pressure. This will apply in all cases where a cylinder is located either outside or in a standard lab environment.

3. Upon clicking “Calculate” the volume of the gas in the cylinder is returned. We now need to compare this to the free air volume of the room. This can be calculated by subtracting the volume of the furniture and equipment from the volume of the room (30 m^3 – 12m^3 =18 m^3)

1. Calculate volume of gas released in worst case scenario

To use the calculator below, you must have a gas cylinder which contains a compressed gas. You must know the pressure of the gas in the cylinder (e.g., 270 bar) and the water volume of the cylinder (e.g., 50 litre).

Initial pressure of gas in cylinder [bar]:

200

Cylinder water capacity [L]:

50

Atmospheric pressure [bar]:

1.013

Calculate

Volume of gas in cylinder = **9.87m^3**

Proceed to Step 3 - your calculated value will be prepopulated into the relevant field.

4. Adding these values into the calculator and clicking “Calculate” will return the concentration of Oxygen after the release of the gas, as well as a recommendation in terms of detection.

3. Calculate Oxygen concentration after release of gas

Enter the volume of the room into the relevant box below and click "Calculate".
If you completed Sections 1 or 2, these values will be automatically populated into the relevant field below.

Volume of gas in cylinder [m^3]:

9.87

Free Air volume of room [m^3]:

18

☐ I do not know the free air volume of the area, and have entered the room volume above instead.

Calculate

% Oxygen after release = **9.46%**

Gas detection necessary

Generate Report

Conclusion:

In this instance, we can see that the % of oxygen is 9.46%. This is well below the recommended limit of 19.5%. As a result, gas detection would need to be installed, or other arrangements would need to be put in place to prevent the potential for this atmosphere to occur e.g. using a smaller gas cylinder, moving it to a bigger room, etc. In these instances, the calculations would need to be carried out again to confirm that the controls are suitable.

Example 2:

A cylinder of CO2 is located in a lab of free air volume 80m^3. The supplier has indicated that this cylinder is a liquid withdrawal cylinder that has a contents weight of 6.35kg.

Would the instantaneous release of the contents of this cylinder into the lab be a risk to lab workers?

In this instance, there are two considerations that we need to evaluate in turn:

1. Is there a risk of Oxygen depletion?
2. Is there a risk of CO2 enrichment?

We will evaluate these separately.

1. Oxygen depletion (using the Oxygen depletion calculator):

In this instance, we have a liquid withdrawal cylinder and have been provided with the weight of the contents, so we will treat this is a liquefied gas cylinder and select that option.

Cylinder Information:

Please select the situation you want to perform your calculation for:

○ I have a compressed gas cylinder or liquefied gas cylinder, but I already know the volume of the contents.

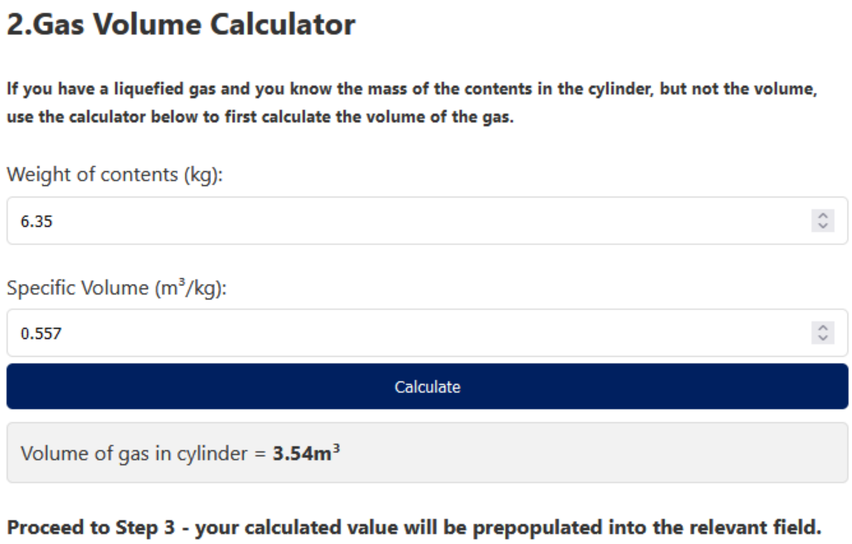
○ I have a compressed gas cylinder, but I don't know the volume of the contents.

◉ I have a liquefied gas cylinder, but I don't know the volume of the contents.

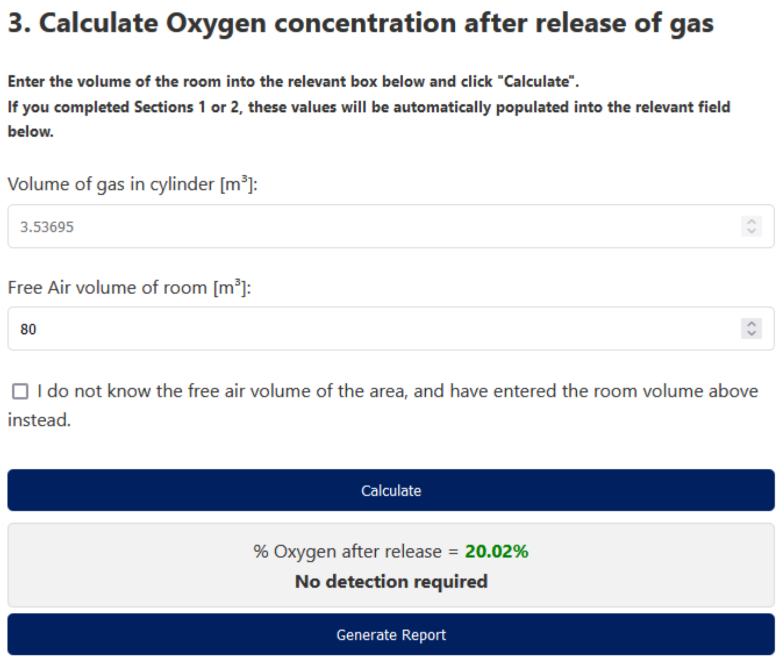
Next, we will need to calculate the volume of gas that could be released if the liquid was released and is allowed to fully expand into the environment.

We know the weight of the contents (6.35kg), but we will need to locate the specific volume for CO2. This can be found in online datasheets, and the value for CO2 is 0.557 m^3/kg.

Entering these values into the calculator yields a gas volume of 3.54 m^3.



Knowing this, we can proceed to the final step of the calculation. We enter the free air volume and click “Calculate”



In this instance, we can see that the % of oxygen isn’t significantly perturbed compared to normal (20.9%), thus O2 detection **would not** be a requirement.

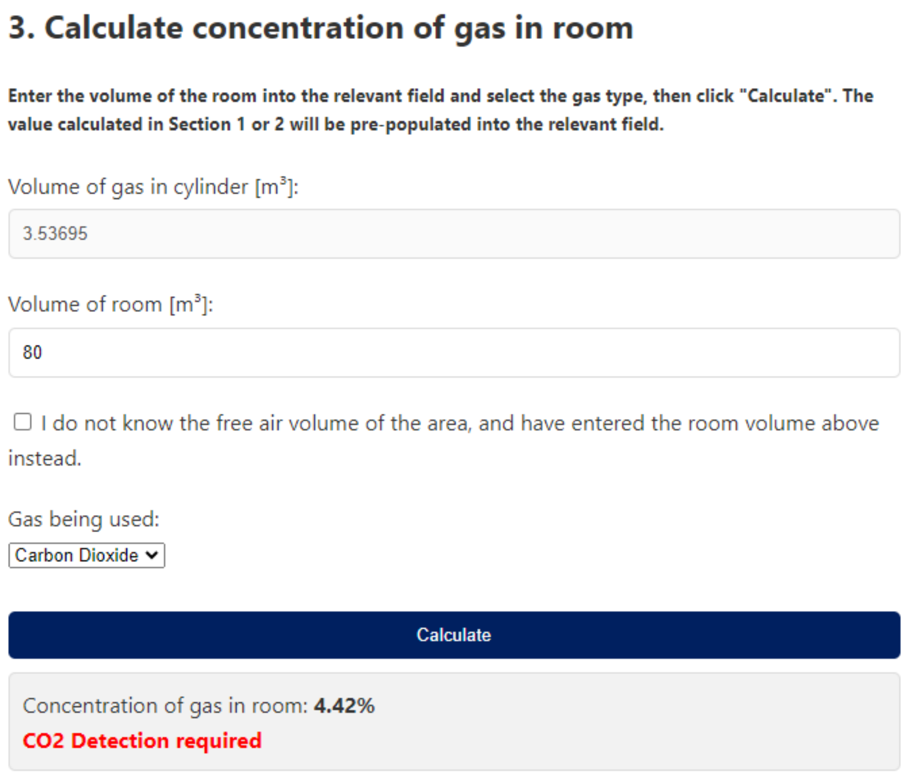
We now move on to evaluate the risk of CO2 enrichment.

2. CO2 enrichment (using the Toxic, Flammable/Enrichment calculator):

This calculation starts off similarly to the last one, and we follow the same steps until we calculate the volume of the gas in the cylinder (3.54 m^3).

Once we know the volume of the gas, we can enter this into the calculator alongside the free air volume. We can select “Carbon Dioxide” under “Gas being used”, and this will ensure that we calculate the correct air composition.

Clicking calculate will return the percentage composition of CO2 in the air, as well as the recommendation.



What we can see here is that the concentration of CO2 in the air would be 4.42%. This is more than both the short- and long-term exposure limits (1.5% and 0.5% respectively).

Conclusion:

In this instance, we can see that the concentration of oxygen after equilibration is still within the accepted tolerance, and therefore we don’t need to consider detection for the oxygen depletion risk.

For CO2, the percentage is well above the 0.5% limit, and therefore the enrichment risk is much higher and, therefore, **CO2 detection <u>would</u> be required**.

Example 3:

A cylinder containing $10m^3$ of a mixture of gases is located in a room of free air volume $12m^3$. The cylinder contains a mixture of 4% CO2, 16% O2, 4% CH4 (Methane gas) and 76% N2.

Evaluate the potential hazards in the event of an instantaneous release of these contents into the lab.

Here, we have a large number of considerations to make. We have a mixture of gases, all of which present different hazards that need to be evaluated. We should break these down into specific hazard groups and tackle them individually. **Note**: For toxic and flammable gases, if there are multiple of these, the percentage of each needs to be calculated and treated individually as each gas will have its own LEL and WEL.

1. O2 Depletion: CO2, CH4 and N2 (Total volume = 4% + 4% + 76% = **84%** of cylinder contents)
2. Flammable environment: CH4 (**4%** of cylinder contents)
3. Toxic Enrichment: CO2 (**4%** of cylinder contents)
4. Oxygen enrichment: O2 (**16%** of cylinder contents)

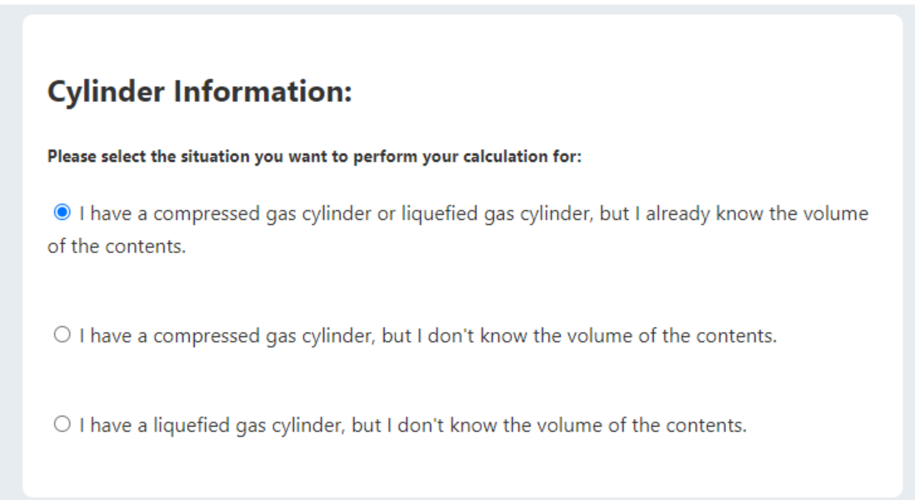
Each of these gases will be compressed gases, so will all be treated as such.

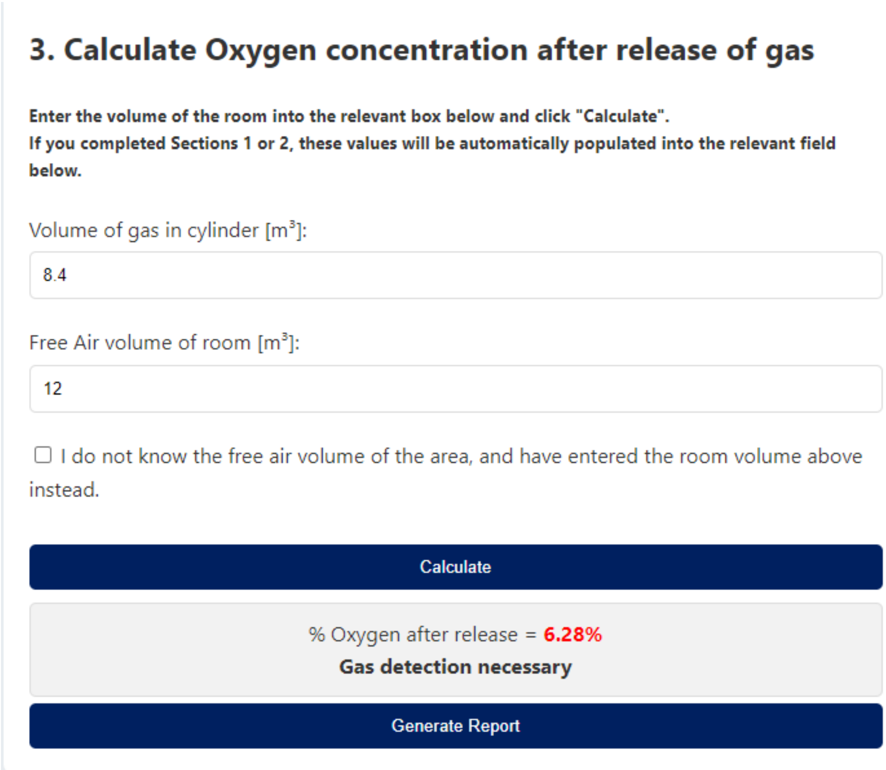
We are assuming that all the gases in the cylinder behave as ideal gases, therefore the volume of each gas will be the total volume of gas in the cylinder multiplied by the percentage of each component.

Starting with the asphyxiation risk:

1. The combined volume of CO2, CH4 and N2 is 84%, therefore the volume of these is $10m^3$ $*0.84 = 8.4m^3$

Entering this into the calculator alongside the free air volume ($12m^3$)





Here, we see that the % Oxygen concentration (in terms of depletion) is well below 19.5%, so therefore O2 detection would be necessary.

In reality, the oxygen in the cylinder would also mix back into the air. The volume of oxygen in this cylinder here would not be nearly high enough to replace what the asphyxiant gases have displaced, but in the event that the % Oxygen was closer to 19.5%, a more detailed risk assessment may be needed to confirm whether detection would be necessary.

2. Flammable Environment:

Here we've identified one of the gases in the mixture as a flammable, and we calculate the volume of this by multiplying the total volume of the cylinder by the % concentration of the relevant gas in the cylinder ($10m^3 * 0.04 = 0.4\ m^3$ of CH_4)

We can then enter this value (and the Free air volume) into the calculator once again, select "Flammable" and then click Calculate (see image overleaf)

Here, we see that the concentration of this gas would be 3.33% upon release into the lab.
The LEL for Methane gas is 5%, so we need to compare our concentration to 25% of the LEL (1.25%).
As can be seen, the concentration of the gas is 3.33% and 25% of the LEL is 1.25%, and therefore detection would need to be considered.

A reasonable question to ask would be: why do we need detection if the equilibrated concentration of the gas is below the LEL? Despite the equilibrated concentration being below the limit, in the immediate instance in which the gas is released, the surrounding environment will more than likely exceed the LEL, and therefore an explosive atmosphere will be created temporarily. At this point, the DSEAR regulations would apply and there may be need to ensure that a DSEAR risk assessment is carried out.

3. Calculate concentration of gas in room

Enter the volume of the room into the relevant field and select the gas type, then click "Calculate". The value calculated in Section 1 or 2 will be pre-populated into the relevant field.

Volume of gas in cylinder [m^3]:

0.4

Volume of room [m^3]:

12

☐ I do not know the free air volume of the area, and have entered the room volume above instead.

Gas being used:

Flammable

Calculate

Concentration of gas in room: **3.33%**

Please compare this to the LEL for your gas to confirm whether detection is required.
Note: Detection is required if the calculated percentage is 25% or over the LEL for the gas.

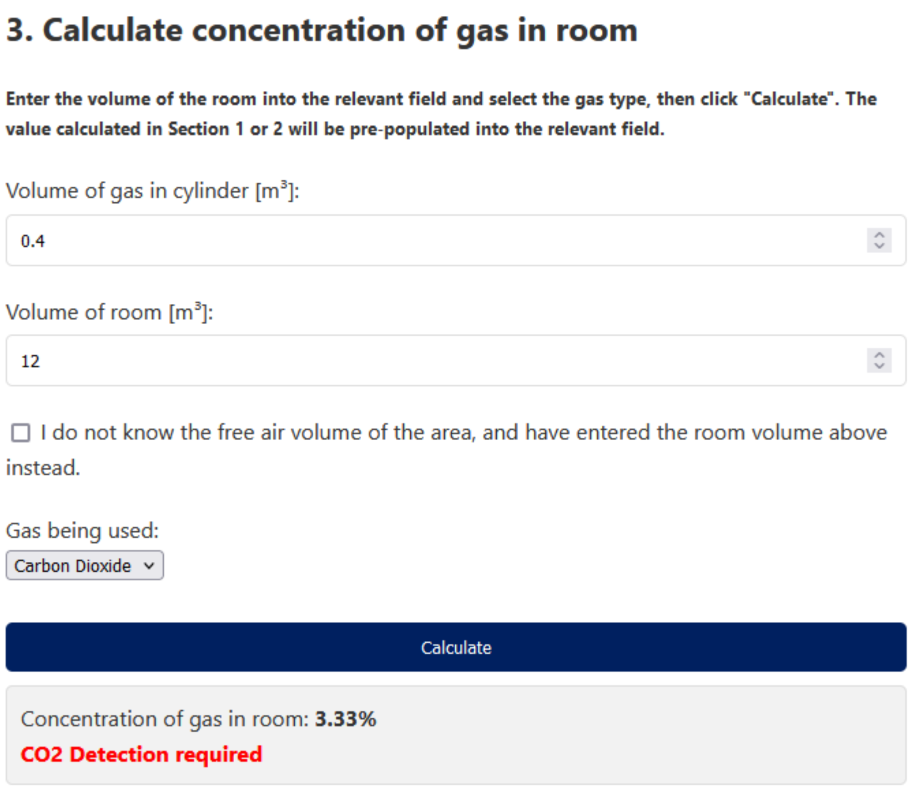
Common example of LELs include:

- Acetylene: 2%
- Hydrogen: 4%
- Methane: 5%

3. Toxic Enrichment

Once again, we've identified that CO2 is a potential toxic risk within the mixture of gases.
We will calculate the volume of CO2 by multiplying the %concentration by the total volume of gas in the cylinder ($10m^3 * 0.04 = 0.4m^3$)

Knowing this, we can then enter this into the calculation. We enter the volume of the gas and the free air volume, and we then select "Carbon Dioxide" as the gas being used (For other toxic gases, you would select "Toxic").
Click "Calculate", and this will indicate that the concentration of CO2 is 3.33% which is over the long-term exposure limit of 0.5%, and therefore detection would need to be considered.



4. Oxygen Enrichment

Once again, the calculation starts in a very similar way.
We need to identify the volume of O2 in the cylinder, and we do this my multiplying the %concentration of O2 in the cylinder by the volume of the gas in the cylinder.
($10m^3 * 0.16 = 1.6m^3$)

Similar, we enter this into the calculator alongside the free air volume. We select “Oxygen” as the gas being used, and click “Calculate” (see overleaf)

We see that the concentration of O2 in the room is 31.53% which is over the recommended limit of 23.5%, and therefore the use of O2 detection would need to be considered.

Conclusion:

In this instance, the calculations would indicate that multiple different types of detected would be needed, However, for a scenario like this, it may not be wholly necessary. In the event of, for example, a bursting disc for this cylinder breaking, and with the concentration of each gas in the cylinder being different, it may be expected that different sensors would alert at different times. Similarly, different gases can have different onsets for the risks associated with them.

The selection of detection should bear this in mind and be subject to risk assessment. Given the complexity related to the use of mixed gases, it would be pertinent to get competent advice from a professional gas detection and installation before deciding on and installing any detection.

3. Calculate concentration of gas in room

Enter the volume of the room into the relevant field and select the gas type, then click "Calculate". The value calculated in Section 1 or 2 will be pre-populated into the relevant field.

Volume of gas in cylinder [m^3]:

1.6

Volume of room [m^3]:

12

☐ I do not know the free air volume of the area, and have entered the room volume above instead.

Gas being used:

Oxygen

Calculate

Concentration of gas in room: **31.53%**

O2 Detection required