## Outflow

## B outlow

The subject of this chapter is the release, or better the incidental release of hazardous materials. It is obvious that this topic is much broader than just a chapter. Nevertheless, an attempt is made to present the basic concepts, mechanisms and algorithms for the calculation of some of the most characteristic cases of incidental releases which will help to understand overall issues of outflow.

At this point it should be noted that any mention of incidental release (gas or liquid) in this chapter will be treated under the general term of "outflow." Furthermore, the outflow of compressed gases or pressurized liquefied gases can lead to the creation of a cloud. It should be noted that depending on the prevailing conditions in each outflow case (continuous or instantaneous release), the cloud would be a plume or a puff (these will be described in Section C5 on Toxic Gas Dispersion). In the present chapter, the term "cloud" will be used to describe both cases, as here we examine the outflow incident and not its consequences.

The chapter is separated into three sections:

1) The first section refers to the outflow of compressed gases. Two cases are examined. In the case of the outflow of a gas out of a vessel, the outflow itself results in reduction of density and temperature, which themselves affect the outflow rate. Hence, the procedure is basically an iterative numerical algorithm in which the gas outflow from the vessel is described in small time steps, small enough for conditions in the vessel to be considered constant during each time step.

The same algorithm is followed in the case of outflow from a hole in a pipe connected to a vessel, although in this case the calculations are a little more complicated because the outflow rate is dependent on the pressure in the vessel and on the pressure drop in the pipe

In the case of total pipe rupture, the calculation procedure adopted is based on the model of Bell [Hanna \& Drivas 1987].

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introduction

2) The second section refers to the outflow of pure liquid under pressure. Two cases are examined. In the case of liquid outflow from a vessel, the calculation depends on the difference between the pressure in the vessel and the atmospheric pressure. Thus we must account for the fact that the pressure in the vessel also decreases because of the liquid outflow. Hence, similarly to the gas case, the procedure is basically an iterative numerical procedure in which the outflow of liquid from the vessel is described in small time steps, small enough for conditions in the vessel to be considered constant during each time step.

Moreover, in the case of outflow from a hole in a pipe connected to a vessel, a similar procedure is applied although, as already stated, the calculations are a little more complicated because of the dependence of the outflow rate on the pressure in the vessel and the pressure drop in the pipe.
3) The case of a two-phase mixture outflow constitutes the hardest case to simulate as it depends on many variables. In this section, a simplified presentation of the special case of the total rupture of a vessel containing pressurized liquefied gas in a temperature above its boiling point, is shown. The rupture of the vessel results in the sudden flash of a liquid content which will expand in all directions, forming a two-phase cloud of vapor and liquid droplets (as "aerosol"), until it is cooled to a temperature below its boiling point.
The calculation algorithm is separated into three stages:

- In the first stage, the liquid flashes and expands in all directions without being mixed with the atmospheric air, forming a mixture of vapors and liquid droplets, some of which will precipitate to the ground.
- In the second stage, there is entrainment of the atmospheric air in the two-phase cloud of vapor and liquid droplets, resulting in additional mixing and further evaporation of the liquid droplets.
- In the third stage, the liquid droplets evaporate, and the homogeneous gas cloud disperses in the atmosphere.
This particular section concentrates on the first two stages, while for the third stage a dispersion model, as those described in Section C5, can be employed.

After each case, simple examples are given, in order to demonstrate the use of the algorithms and the procedures employed.

## B2 <br> Outflow of Compressed Gases

This section presents an initial study of the outflow of gas under pressure. We will first examine two cases of small releases (hole in vessel wall and hole in a pipe connected to a vessel, respectively), and then discuss the outflow resulting from a total pipe rupture.

## B2.1. Gas Density

In the case of an outflow or release of gases under pressure, the knowledge of the density as a function of the pressure and the temperature is very important, because of their compressibility. For low pressures, the ideal-gas equation is valid. Hence

$$
\begin{equation*}
P=\rho_{n} R T \quad \text { or } \quad P=\left(\rho / W_{\mathrm{g}}\right) R T \tag{B2.1}
\end{equation*}
$$

where, $P(\mathrm{~Pa})$ is the pressure of a gas with molar density $\rho_{n}\left(\mathrm{~mol} / \mathrm{m}^{3}\right)$ in this pressure and temperature $T(\mathrm{~K})$. In the above equation, $R$ denotes the universal gas constant $\left(=8.314 \mathrm{Jmol}^{-1} \mathrm{~K}^{-1}\right)$. Usually, instead of the molar density it is customary to employ the mass density $\rho\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ and the molecular weight $W_{\mathrm{g}}(\mathrm{kg} / \mathrm{mol})$ of the gas. The above two expressions are widely employed because of their accuracy and ease of use.

For higher pressures, the ideal-gas equation can also be used, but with the addition of the compressibility factor $\mathrm{Z}(-)$, as

$$
\begin{equation*}
P=Z \rho_{n} R T \quad \text { or } \quad P=Z\left(\rho / W_{\mathrm{g}}\right) R T \tag{B2.2}
\end{equation*}
$$

The compressibility factor can be calculated as a function of the critical temperature and pressure [Assael, Trusler \& Tsolakis 1996].

When the pressure is considerably increased, then the Virial Equation, is recommended:

$$
\begin{equation*}
P=\rho_{n} R T\left(1+B \rho_{n}+C \rho_{n}^{2}+\ldots\right) \tag{B2.3}
\end{equation*}
$$

Outflow of Compressed Gases

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Density
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## Outflow of

 Compressed Gasesintroduction

Much of the importance of the virial equation of state lies in its rigorous theoretical foundation by which the virial coefficients appear not merely as empirical constants but with a precise relation to the intermolecular potential energy. Specifically, the second virial coefficient, $B\left(\mathrm{~m}^{3} / \mathrm{mol}\right)$, arises from the interaction between a pair of molecules, the third virial coefficient, $C\left(\mathrm{~m}^{6} / \mathrm{mol}^{2}\right)$, depends upon interactions in a cluster of three molecules, and so on. Most calculations employ either the coefficients $B$ and $C$, or only $B$.

Although there are many experimental data for the second virial coefficient, it is often necessary to estimate its value for gases that have not been studied before. Hence many different correlations have been proposed [Assael, Trusler \& Tsolakis 1996]. One of the most widely used correlations for non-polar gases is the extended scheme of corresponding states of Pitzer-Curl [Pitzer \& Curl 1958], given by Eq. (B2.4) in Table B2.1. The parameter $\omega$ shown in the equation, is the acentric factor while $T^{\mathrm{c}}(\mathrm{K})$ and $P^{\mathrm{c}}(\mathrm{Pa})$ are the critical temperature and critical pressure, respectively. Pitzer and Curl initially proposed their own expressions for the dimensionless coefficients $B_{0}$ and $B_{1}$. Here, the most recent correlations (Eq. (B2.5)-(B2.6) in Table B2.1) as a function of the reduced temperature, $T_{\mathrm{r}}=T / T^{\mathrm{C}}$, proposed by Tsonopoulos [Tsonopoulos 1974] are shown. For the third virial coefficient for non-polar gases, in Table B2.1, the correlations of Orbey and Vera [Orbey \& Vera 1983] are shown. In the case of a mixture, mixing rules of critical points are most commonly employed [Assael, Trusler \& Tsolakis 1996]. In much higher pressures, the use of equations of state like Peng-Robinson or Benedict-Webb-Rubin is unavoidable [Assael, Trusler \& Tsolakis 1996].

Table B2.1. Correlations for the Second and Third Virial Coefficients.

$$
\begin{gather*}
B=\left(R T^{\mathrm{c}} / P^{\mathrm{c}}\right)\left(B_{0}+\omega B_{1}\right)  \tag{B2.4}\\
B_{0}=0.1445-0.33 / T_{\mathrm{r}}-0.1385 / T_{\mathrm{r}}^{2}-0.0121 / T_{\mathrm{r}}^{3}-0.000607 / T_{\mathrm{r}}^{8}  \tag{B2.5}\\
B_{1}=0.0637+0.331 / T_{\mathrm{r}}^{2}-0.423 / T_{\mathrm{r}}^{3}-0.008 / T_{\mathrm{r}}^{8}  \tag{B2.6}\\
C=\left(R T^{\mathrm{c}} / P^{\mathrm{c}}\right)^{2}\left(C_{0}+\omega C_{1}\right)  \tag{B2.7}\\
C_{0}=0.01407+0.02432 / T_{\mathrm{r}}^{2.8}-0.00313 / T_{\mathrm{r}}^{10.5}  \tag{B2.8}\\
C_{1}=-0.02676+0.0177 / T_{\mathrm{r}}^{2.8}+0.040 / T_{\mathrm{r}}^{3}-0.003 / T_{\mathrm{r}}^{6}-0.00228 / T_{\mathrm{r}}^{10.5} \tag{B2.9}
\end{gather*}
$$

## B2.2. Outflow from Vessels

## B2.2.1. Small Outflow

The simulation of the dynamic behavior of a compressed gas in a vessel aims to estimate the reduction in its pressure and temperature due to gas outflow. As a part of the gas is released or leaks, the remaining gas will expand. This expansion generates cooling and decompression.

Usually this simulation takes place with an iterative numerical procedure, where the gas outflow is described in small steps in time. These steps should be small enough to consider the conditions in the vessel to be constant during one time-step. A possible algorithm will be as follows:

1) Data: vessel's volume $V\left(\mathrm{~m}^{3}\right)$, initial vessel's pressure $P_{\mathrm{o}}(\mathrm{Pa})$ and initial temperature $T_{\mathrm{o}}(\mathrm{K})$.

- From an equation of state, the density $\rho_{0}\left(\mathrm{~kg} / \mathrm{m}^{3}\right)$ is calculated.
- Then the outflow mass flow rate $\dot{m}_{0}(\mathrm{~kg} / \mathrm{s})$ is obtained (see next sections).

2) First time step $\delta t_{1}(s)$ is selected (either by experience or trial and error).

- The reduction in density (because of the mass that was released) is obtained from the equation

$$
\begin{equation*}
\delta \rho_{1}=-\frac{\dot{m}_{\mathrm{o}}}{V} \delta t_{1} . \tag{B2.10}
\end{equation*}
$$

- Then the reduction in temperature, because of the gas expansion, is calculated from the expression *

$$
\begin{equation*}
\delta T_{1}=\frac{P_{\mathrm{o}}}{\rho_{\mathrm{o}}^{2} C_{\mathrm{v}}} \delta \rho_{1} \tag{B2.11}
\end{equation*}
$$

where $C_{\mathrm{v}}\left(\mathrm{Jkg}^{-1} \mathrm{~K}^{-1}\right)$ is the specific heat capacity under constant volume.
3) New conditions are thus calculated from

$$
\begin{equation*}
\rho_{1}=\rho_{\mathrm{o}}+\delta \rho_{1}, \quad T_{1}=T_{\mathrm{o}}+\delta T_{1} \quad \text { and } \quad P_{1}=R T_{1}\left(\rho_{1} / W_{\mathrm{g}}\right) . \tag{B2.12}
\end{equation*}
$$

These conditions will be the initial conditions of the next time step. The algorithm continues until the vessel's pressure is equal to the ambient.
The algorithm is clearly demonstrated in the examples which follow immediately after the calculation of the outflow mass flow rate.

[^0]
## Outflow of Gases <br> from Vessel

calculation<br>procedure



## Outflow of Gases from Vessel

calculation procedure

Initial Conditions

Selection of Time Step

| $\downarrow$ |
| :---: |
| Outflow |
| Mass Flow Rate |
| (from vessel or |
| pipe and vessel) |
| $\downarrow$ |
| Reduction of |
| density and |
| temperature |
| $\downarrow$ |
| New |
| Conditions |
| $\downarrow$ |
| Next |
| Time Step |

Mass Flow Rate (from vessel or pipe and vessel)

Reduction of density and temperature

New Conditions Next Time Step

## a) Outflow through Hole in Vessel's Wall

The calculation of the outflow mass flow rate, $\dot{m}(\mathrm{~kg} / \mathrm{s})$, of a gas under pressure through a hole in a vessel, Figure B2.1, can be accomplished with the following expression

$$
\begin{equation*}
\dot{m}=C_{\mathrm{d}} A_{\mathrm{h}} P_{\mathrm{o}} K \sqrt{\frac{W_{\mathrm{g}}}{\gamma R T}} . \tag{B2.13}
\end{equation*}
$$

In this relation, $C_{\mathrm{d}}(-)$ is the discharge coefficient, $A_{\mathrm{h}}\left(\mathrm{m}^{2}\right)$ the hole's cross-sectional area, $P_{\mathrm{o}}(\mathrm{Pa})$ the initial gas pressure in the vessel (for each time step), and $W_{\mathrm{g}}$ $(\mathrm{kg} / \mathrm{mol})$ the molecular weight of the gas. Also, $\gamma(-)$ denotes the Poisson ratio, i.e., the ratio of specific heat capacity at constant pressure, $C_{\mathrm{p}}\left(\mathrm{Jkg}^{-1} \mathrm{~K}^{-1}\right)$, over the specific heat capacity at constant volume $C_{\mathrm{v}}\left(\mathrm{Jkg}^{-1} \mathrm{~K}^{-1}\right)$, while $R$ is the universal gas constant $\left(=\left(C_{\mathrm{p}}-C_{\mathrm{v}}\right) W_{\mathrm{g}}=8.314 \mathrm{Jmol}^{-1} \mathrm{~K}^{-1}\right)$, and $T(\mathrm{~K})$ the temperature of the gas.

The coefficient $K(-)$ depends upon whether the outflow is
a) subsonic (unchoked) : the gas exit velocity is smaller than the speed of sound. That is, the Mach number, $M_{\mathrm{j}}<1$.
b) sonic or supersonic (chocked): the gas exit velocity is equal or larger than the speed of sound. That is, the Mach number, $M_{\mathrm{j}} \geq 1$.

The following expression can be considered as a criterion, as it declares that a flow can be considered as supersonic (or sonic) flow when

$$
\begin{equation*}
\frac{P_{\mathrm{o}}}{P_{\mathrm{a}}} \geq\left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}}, \tag{B2.14}
\end{equation*}
$$

where $P_{\mathrm{a}}(\mathrm{Pa})$ is the ambient pressure.

The coefficient $K(-)$ is calculated from the following expressions
for subsonic flow

$$
\begin{equation*}
K=\sqrt{\frac{2 \gamma^{2}}{\gamma-1}\left(\frac{P_{\mathrm{a}}}{P_{\mathrm{o}}}\right)^{\frac{2}{\gamma}}\left[1-\left(\frac{P_{\mathrm{a}}}{P_{\mathrm{o}}}\right)^{\frac{\gamma-1}{\gamma}}\right]}, \tag{B2.15}
\end{equation*}
$$

for supersonic (or sonic) flow

$$
\begin{equation*}
K=\gamma\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} \tag{B2.16}
\end{equation*}
$$



Figure B2.1. Outflow of compressed gas from a hole in a vessel.

The discharge coefficient, $C_{d}(-)$ is a function of the type of the hole/orifice in the vessel and the gas velocity at the hole. For sharp orifices the discharge coefficient usually is taken equal to 0.62 , while for rounded orifices it usually takes a value between 0.95 and 0.99 [Beek \& Mutzall 1975].

The outflow mass flow rate calculated by Eq. (B2.13), as well as the equivalent mass flow rate from a pipe (that will be discussed in the next section), refer to initial pressure, $P_{\mathrm{o}}(\mathrm{Pa})$, in the vessel which remains stable during a time step. Hence, in essence it is valid for the time step in which the vessel's pressure $P_{\mathrm{o}}$ can be considered stable.

The above discussion refers solely to cases where there is no condensation of the exit gas, that is the gas pressure will not, under any means, be higher than the saturation pressure at the temperature of the process.


Propane fire erupted as a result of a ruptured one-ton chlorine container on February 16, 2007, at the Valero McKee Refinery in Sunray, TX, U.S.A. (Reproduced by kind permission of the U.S. Chemical Safety Board.)


Outflow of Gases from Vessel example


EXAMPLE B2.1.
Hole in Vessel's Wall
Calculate the outflow mass flow rate of compressed hydrogen release from a hole in a vessel wall. The following data are available:

| - | Vessel's volume, $V$ | $:$ | 50 |
| :--- | :--- | :---: | :--- |
| $\mathrm{~m}^{3}$ |  |  |  |
| Initial vessel's pressure, $P_{\mathrm{o}}$ | $:$ | 5 | MPa |
| Initial vessel's temperature, $T_{\mathrm{o}}$ | $:$ | 288.15 | K |
| - | Hole's diameter, $d_{\mathrm{h}}$ | $:$ | 0.1 |
| m |  |  |  |
| Discharge coefficient, $C_{\mathrm{d}}$ | $:$ | 0.62 | - |
| - | Molecular weight of Hydrogen, $W_{\mathrm{g}}$ | $:$ | 0.002 |
| Spg/mol |  |  |  |
| Specific heat at constant volume, $C_{\mathrm{v}}$ | $:$ | 10.24 | $\mathrm{kJkg} \mathrm{kg}^{-1}$ |
| Poisson ratio, $\gamma$ | $:$ | 1.4 | - |

We follow the steps described in Section B2.2.1.

1) Data: vessel's volume $V\left(\mathrm{~m}^{3}\right)$, initial pressure $P_{\mathrm{o}}(\mathrm{Pa})$, temperature $T_{\mathrm{o}}(\mathrm{K})$.

- The density is calculated from the ideal-gas equation,

$$
\rho_{\mathrm{o}}=P W_{\mathrm{g}} /(R T)=5 \times 10^{6} \times 0.002 /(8.314 \times 288.15)=4.17 \mathrm{~kg} / \mathrm{m}^{3} .
$$

- From Eq. (B2.13) the initial outflow mass flow rate $\dot{m}_{0}(\mathrm{~kg} / \mathrm{s})$ is obtained. The flow is supersonic $\left(P_{\mathrm{o}} / P_{\mathrm{a}}=50>1.9=((\gamma+1) / 2)^{\gamma /(\gamma-1)}\right)$ and $K=0.81$, independent of the pressure. From Eq. (B2.13), $\dot{m}_{\mathrm{o}}=15.23 \mathrm{~kg} / \mathrm{s}$.

2) The first time step $\delta t_{1}(\mathrm{~s})=1 \mathrm{~s}$, is selected.

- The reduction in density and temperature, because of the released mass, is calculated from Eqs. (B2.10) and (B2.11), respectively

$$
\begin{gathered}
\delta \rho_{1}=-\frac{\dot{m}_{\mathrm{o}}}{V} \delta t_{1}=-0.30 \mathrm{~kg} / \mathrm{s} \\
\delta T_{1}=\frac{P_{\mathrm{o}}}{\rho_{\mathrm{o}}^{2} C_{\mathrm{v}}} \delta \rho_{1}=-8.54 \mathrm{~K}
\end{gathered}
$$

3) New conditions are calculated from Eq. (B2.12), as
$\rho_{1}=\rho_{0}+\delta \rho_{1}=3.87 \mathrm{~kg} / \mathrm{m}^{3}$,
$T_{1}=T_{\mathrm{o}}+\delta T_{1}=279.6 \mathrm{~K}$,
and $\quad P_{1}=R T_{1}\left(\rho_{1} / W_{\mathrm{g}}\right)=4.50 \mathrm{MPa}$.
These conditions will be the new initial conditions of the immediate next time step.

The results for the next 30 time steps ( 30 s ) are shown in Table B2.2, while Figure B2.2 shows the reduction in temperature, pressure and outflow mass flow rate, respectively. In Table B2.2 the change in the mass $M(\mathrm{~kg})$ remaining in the vessel is also shown. Iterations stop when the vessel's pressure becomes equal to the ambient pressure, or the outflow mass flow rate drops below a specified value.

Finally, the reader can check that even if the selection of the time step was essentially arbitrary, the results are not significantly influenced by it.


Figure B2.2. Reduction in temperature, pressure and outflow mass flow rate as a function of time.

## Outflow of Gases

 from Vesselexample



| $M$ <br> $(\mathrm{~kg})$ | $t$ <br> $(\mathrm{~s})$ | $T$ <br> $(\mathrm{~K})$ | $\rho$ <br> $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ | $P$ <br> $(\mathrm{MPa})$ | $P_{\mathrm{o}} / P_{\mathrm{a}}$ <br> $(-)$ | $\dot{m}$ <br> $(\mathrm{~kg} / \mathrm{s})$ | $\delta \rho$ <br> $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ | $\delta T$ <br> $(\mathrm{~K})$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 209 | 0 | 288.2 | 4.17 | 5.00 | 50.0 | 15.23 | -0.30 | -8.54 |
| 193 | 1 | 279.6 | 3.87 | 4.50 | 45.0 | 13.91 | -0.28 | -8.16 |
| 180 | 2 | 271.5 | 3.59 | 4.05 | 40.5 | 12.72 | -0.25 | -7.80 |
| 167 | 3 | 263.6 | 3.34 | 3.66 | 36.6 | 11.65 | -0.23 | -7.47 |
| 155 | 4 | 256.2 | 3.10 | 3.31 | 33.1 | 10.68 | -0.21 | -7.16 |
| 145 | 5 | 249.0 | 2.89 | 2.99 | 29.9 | 9.80 | -0.20 | -6.86 |
| 135 | 6 | 242.2 | 2.69 | 2.71 | 27.1 | 9.01 | -0.18 | -6.58 |
| 126 | 7 | 235.6 | 2.51 | 2.46 | 24.6 | 8.29 | -0.17 | -6.31 |
| 117 | 8 | 229.3 | 2.35 | 2.24 | 22.4 | 7.64 | -0.15 | -6.06 |
| 110 | 9 | 223.2 | 2.20 | 2.04 | 20.4 | 7.05 | -0.14 | -5.82 |
| 103 | 10 | 217.4 | 2.05 | 1.86 | 18.6 | 6.51 | -0.13 | -5.59 |
| 96 | 11 | 211.8 | 1.92 | 1.69 | 16.9 | 6.02 | -0.12 | -5.38 |
| 90 | 12 | 206.4 | 1.80 | 1.55 | 15.5 | 5.57 | -0.11 | -5.18 |
| 85 | 13 | 201.3 | 1.69 | 1.42 | 14.2 | 5.16 | -0.10 | -4.98 |
| 79 | 14 | 196.3 | 1.59 | 1.30 | 13.0 | 4.79 | -0.10 | -4.80 |
| 75 | 15 | 191.5 | 1.49 | 1.19 | 11.9 | 4.44 | -0.09 | -4.62 |
| 70 | 16 | 186.8 | 1.40 | 1.09 | 10.9 | 4.13 | -0.08 | -4.46 |
| 66 | 17 | 182.4 | 1.32 | 1.00 | 10.0 | 3.84 | -0.08 | -4.30 |
| 62 | 18 | 178.1 | 1.25 | 0.92 | 9.2 | 3.57 | -0.07 | -4.15 |
| 59 | 19 | 173.9 | 1.17 | 0.85 | 8.5 | 3.33 | -0.07 | -4.00 |
| 55 | 20 | 169.9 | 1.11 | 0.78 | 7.8 | 3.10 | -0.06 | -3.87 |
| 52 | 21 | 166.1 | 1.05 | 0.72 | 7.2 | 2.90 | -0.06 | -3.73 |
| 49 | 22 | 162.3 | 0.99 | 0.67 | 6.7 | 2.70 | -0.05 | -3.61 |
| 47 | 23 | 158.7 | 0.93 | 0.62 | 6.2 | 2.53 | -0.05 | -3.49 |
| 44 | 24 | 155.2 | 0.88 | 0.57 | 5.7 | 2.36 | -0.05 | -3.38 |
| 42 | 25 | 151.9 | 0.84 | 0.53 | 5.3 | 2.21 | -0.04 | -3.27 |
| 40 | 26 | 148.6 | 0.79 | 0.49 | 4.9 | 2.07 | -0.04 | -3.16 |
| 37 | 27 | 145.4 | 0.75 | 0.45 | 4.5 | 1.94 | -0.04 | -3.06 |
| 36 | 28 | 142.4 | 0.71 | 0.42 | 4.2 | 1.82 | -0.04 | -2.96 |
| 34 | 29 | 139.4 | 0.67 | 0.39 | 3.9 | 1.71 | -0.03 | -2.87 |
| 32 | 30 | 136.5 | 0.64 | 0.36 | 3.6 | 1.61 | -0.03 | -2.78 |
|  |  |  |  |  |  |  |  |  |

## b) Outflow through Hole in Pipe Wall Connected to Vessel

In this section we refer to the specific outflow from a hole in a pipe connected to a vessel (see Figure B2.3). The outflow mass rate, $\dot{m}(\mathrm{~kg} / \mathrm{s})$ of the gas will directly depend upon the total difference between the vessel's pressure and the atmospheric pressure. More analytically, if $P_{\mathrm{o}}(\mathrm{Pa})$ denotes the pressure in the vessel and in the entrance of the pipe, $P_{\mathrm{e}}(\mathrm{Pa})$ the pressure before the hole and $P_{\mathrm{a}}(\mathrm{Pa})$ the ambient pressure, then the total pressure drop $\Delta P(\mathrm{~Pa})$ will be equal to

$$
\begin{align*}
\Delta P & =\left(P_{\mathrm{o}}-P_{\mathrm{e}}\right)+\left(P_{\mathrm{e}}-P_{\mathrm{a}}\right) \\
& =\Delta P_{\text {pipe }}+\Delta P_{\text {hole }} \tag{B2.17}
\end{align*}
$$

It should be noted that the pressure $P_{\mathrm{e}}(\mathrm{Pa})$ just before the hole, is not known.

The mass flow rate in the pipe, $\dot{m}_{\text {pipe }}(\mathrm{kg} / \mathrm{s})$ directly depends on the pressure drop in the pipe, while the outflow mass flow rate, $\dot{m}(\mathrm{~kg} / \mathrm{s})$, depends on the pressure drop in the hole. Assuming that the mass through the pipe is equal to the mass that is released, we obtain that

$$
\begin{equation*}
\dot{m}_{\text {pipe }}\left(\Delta P_{\text {pipe }}\right)=\dot{m}\left(\Delta P_{\text {hole }}\right) . \tag{B2.18}
\end{equation*}
$$

It is assumed that due to the lower pressure drop in the hole, the gas will be completely released. The above equation, in connection with Eq. (B2.13) - where, as the pressure before the hole, the pressure $P_{\mathrm{e}}$, will be assumed - will be employed for the calculation of the unknown pressure, $P_{\mathrm{e}}(\mathrm{Pa})$, and consequently of the outflow mass flow rate, $\dot{m}(\mathrm{~kg} / \mathrm{s})$, from the hole.

Outflow of Gases from Pipe

calculation procedure



Figure B2.3. Outflow of compressed gas from pipe connected to vessel.

## Outflow of Gases from Pipe

calculation procedure

Initial Conditions

Selection of Time Step


Reduction of density and temperature

New Conditions

Next Time Step

The mass flow rate, $\dot{m}_{\text {pipe }}(\mathrm{kg} / \mathrm{s})$ inside the pipe can be obtained from the Fanning relation that expresses the pressure drop in a unit length pipe, $\delta P / \delta l_{\mathrm{p}}$ $(\mathrm{Pa} / \mathrm{m})$, as a function of the Fanning friction factor, $f_{\mathrm{F}}(-)$, the gas density, $\rho$ $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$, its velocity $u(\mathrm{~m} / \mathrm{s})$, and the pipe's diameter $d_{\mathrm{p}}(\mathrm{m})$, as

$$
\begin{equation*}
\frac{\delta P}{\delta l_{\mathrm{p}}}=4 f_{\mathrm{F}} \frac{\rho u^{2}}{2 d_{\mathrm{p}}} . \tag{B2.19}
\end{equation*}
$$

The velocity of the gas can also be expressed as

$$
\begin{equation*}
u=\frac{\dot{m}_{\text {pipe }}}{\rho A_{\mathrm{p}}}, \tag{B2.20}
\end{equation*}
$$

where $A_{\mathrm{p}}\left(\mathrm{m}^{2}\right)$ is the pipe's cross-sectional area.
Integrating over the pipe's length, from Eqs. (B2.19) and (B2.20) one obtains

$$
\begin{equation*}
\dot{m}_{\mathrm{pipe}}=A_{\mathrm{h}} \sqrt{\frac{2 \int_{P_{\mathrm{e}}}^{P_{\mathrm{o}}} \rho(P) d P}{4 f_{\mathrm{F}}\left(l_{\mathrm{p}} / d_{\mathrm{p}}\right)}} . \tag{B2.21}
\end{equation*}
$$

In the case of ideal gases ( $P=C \rho^{\gamma}, C=$ constant $)$, there is an analytic solution of the above integral, and thus Eq. (B2.21) becomes

$$
\begin{equation*}
\dot{m}_{\sigma \omega \lambda}=A_{\mathrm{h}} \sqrt{\frac{\rho P_{\mathrm{o}}}{2 f_{\mathrm{F}}\left(l_{\mathrm{p}} / d_{\mathrm{p}}\right)} \frac{\gamma}{1+\gamma}\left(\left(\frac{P_{\mathrm{o}}}{P_{\mathrm{e}}}\right)^{(1+\gamma) / \gamma}-1\right)} . \tag{B2.22}
\end{equation*}
$$

The solution of the above equation together with Eq. (B2.13) and Eq. (B2.18) will produce the value for the unknown pressure, $P_{\mathrm{e}}(\mathrm{Pa})$, and consequently the outflow mass flow rate, $\dot{m}(\mathrm{~kg} / \mathrm{s})$, from the hole.

The Fanning friction factor, $f_{\mathrm{F}}(-)$, can be calculated [Fanning 1877, Pope 2000] as a function of the Reynolds number, $\operatorname{Re}=\rho u d_{\mathrm{p}} / \eta$, where $\eta$ (Pas) is the fluid kinematic viscosity, as

$$
\begin{array}{ll}
\text { for } R e<2,000 & f_{\mathrm{F}}=16 / R e, \\
\text { for } 4,000<R e<10^{5} & f_{\mathrm{F}}=0.0791 R e^{-0.25} . \tag{B2.24}
\end{array}
$$

It is worth reminding that the Fanning friction factor is a fourth of the DarcyWeisbach friction factor.

## EXAMPLE B2.2.

## Hole in Pipe Connected to Vessel

Calculate the outflow mass flow rate of compressed carbon monoxide, from a hole in a pipe connected to a vessel. The following data are available:

- Vessel's Volume, $V$

| 50 | $\mathrm{~m}^{3}$ |
| :---: | :--- |
| 1.5 | MPa |
| 288.15 | K |
| 0.15 | m |
| 100 | m |
| 0.1 | m |
| 0.62 | - |
| 0.028 | $\mathrm{~kg} / \mathrm{mol}$ |
| 745 | $\mathrm{Jkg}^{-1} \mathrm{~K}^{-1}$ |
| 1.4 | - |
| 17.3 | $\mu \mathrm{~Pa} \mathrm{~s}$ |

Initial vessel's pressure, $P_{\mathrm{o}}$
Initial vessel's temperature, $T_{\mathrm{o}}$

- Diameter of pipe, $d_{\mathrm{p}}$ Length of pipe (until the hole), $l_{\mathrm{p}}$
- Diameter of hole, $d_{\mathrm{h}}$ Discharge coefficient, $C_{\mathrm{d}}$
0.62 -
- Molecular weight of carbon monoxide, $W_{g}$ Specific heat at constant volume, $C_{\mathrm{v}}$ Poisson ratio, $\gamma$ $17.3 \mu \mathrm{~Pa}$ s

The steps described in Section B2.2.1, (b), are followed

1) Data: volume of vessel+pipe $V\left(\mathrm{~m}^{3}\right)=50+(\pi / 4) \times 0.15^{2} \times 100=51.77 \mathrm{~m}^{3}$, initial vessel's pressure $P_{\mathrm{o}}(\mathrm{Pa})$, and initial temperature $T_{\mathrm{o}}(\mathrm{K})$.

- From the ideal-gas equation, the density is calculated,

$$
\rho_{\mathrm{o}}=P W_{\mathrm{g}} /(R T)=1.5 \times 10^{6} \times 0.028 /(8.314 \times 288.15)=17.53 \mathrm{~kg} / \mathrm{m}^{3} .
$$

a) A value for the intermediate pressure $P_{\mathrm{e}}=1.4 \mathrm{MPa}$, is assumed.
b) The outflow mass flow rate, $\dot{m}(\mathrm{~kg} / \mathrm{s})$ is calculated from Eq. (B2.13). The flow is supersonic $\left(P_{\mathrm{e}} / P_{\mathrm{a}}=14>1.9=((\gamma+1) / 2)^{\gamma /(\gamma-1)}\right)$ and $K=0.81$, independent of pressure. From Eq. (B2.13), $\dot{m}=15.96 \mathrm{~kg} / \mathrm{s}$.
c) The mass flow rate, $\dot{m}_{\text {pipe }}(\mathrm{kg} / \mathrm{s})$ in the pipe is calculated from Eq. (B2.22). The Fanning friction factor is obtained from Eq. (B2.24) equal to 0.0015 . To calculate the velocity that is employed in the Reynolds number Re, the outflow mass flow rate obtained in step (b) is used. From Eq. (B2.22), $\dot{m}_{\sigma \omega \lambda}=17.37 \mathrm{~kg} / \mathrm{s}$.
d) If the intermediate pressure assumed in step (a) is correct, then the outflow mass flow rate in step (b) should be equal to the mass flow rate obtained in step (c).

The steps are repeated with the new assumption for the intermediate pressure. Final results, $P_{\mathrm{e}}=1.413 \mathrm{MPa}$ and $\dot{m}=16.10 \mathrm{~kg} / \mathrm{s}$.

## Outflow of Gases from Pipe

example



## Outflow of Gases from Pipe

example


| $M$ <br> $(\mathrm{~kg})$ | $t$ <br> $(\mathrm{~s})$ | $T$ <br> $(\mathrm{~K})$ | $\rho$ <br> $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ | $P$ <br> $(\mathrm{MPa})$ | $P_{\mathrm{e}}$ <br> $(\mathrm{MPa})$ | $f_{\mathrm{F}}$ <br> x 1000 | $\dot{m}$ <br> $(\mathrm{~kg} / \mathrm{s})$ | $\delta \rho$ <br> $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ | $\delta T$ <br> $(\mathrm{~K})$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 908 | 0 | 288.15 | 17.53 | 1.50 | 1.4131 | 1.49 | 16.10 | -0.62 | -4.08 |
| 875 | 2 | 284.07 | 16.91 | 1.43 | 1.3464 | 1.51 | 15.45 | -0.60 | -4.00 |
| 844 | 4 | 280.08 | 16.31 | 1.36 | 1.2761 | 1.50 | 15.68 | -0.61 | -4.15 |
| 813 | 6 | 275.93 | 15.71 | 1.29 | 1.2134 | 1.52 | 14.99 | -0.58 | -4.05 |
| 783 | 8 | 271.88 | 15.13 | 1.22 | 1.1541 | 1.54 | 14.33 | -0.55 | -3.97 |
| 754 | 10 | 267.91 | 14.57 | 1.16 | 1.0980 | 1.55 | 13.70 | -1.32 | -9.70 |
| 686 | 15 | 258.21 | 13.25 | 1.02 | 0.9671 | 1.60 | 12.23 | -1.18 | -9.18 |
|  | 20 |  |  |  |  |  |  |  |  |

## B2.2.2. Total Vessel Rupture

The total rupture of a vessel with compressed gas, irrespective of the cause, usually has the following three consequences:

- release of the contained gas,
- rupture of the vessel with possible ejection of fragments,
- creation of a shock wave due to expansion of the compressed gas.

The release of the contained gas can result in secondary effects such as the creation of a fire ball (Section C2.2), flash fire (Section C2.4), vapor cloud explosion (Section C3) or dispersion of toxic cloud (Section C5). The appearance (or not) of these secondary effects depends entirely upon the flammability limits and the toxicity of the contained gas. All the above mentioned effects will be discussed in the corresponding sections.

Part of the internal energy of the compressed gas contained in the vessel transforms into kinetic energy of fragments, which can become high velocity projectiles that travel great distances and hit whatever they find in their way.

Another part of this internal energy is transformed into dynamic energy (expansion of the vessel's content). This type of mechanical energy is carried in the surrounding atmosphere as a shock wave. The shock wave is detected as a sudden change in the pressure, density and velocity of the gas. The resulting overpressure can destroy or eject objects and facilities (Section C3).

Usually there are two reasons for total rupture of a vessel either the internal pressure exceeds the vessel's design pressure, or the strength of the vessel is reduced due to its length of operation. Increase of the internal pressure of a vessel can be a consequence of overfilling, overheating from internal or external sources, failure of a pressure regulator, an inside run-away reaction, internal explosion, etc. Reduction of the strength of the vessel's wall can be the consequence of oxidation, rusting, overheating, metal fatigue, the impact of another object on it, etc.

Total Vessel Rupture
calculation procedure

## Characteristic

Time
ransient
Outflow Mass Flow Rate nal Time


## B2.3. Outflow Due to Total Pipe Rupture

The instantaneous rupture of a pipe with compressed gas is another case which can lead to the outflow of a large volume of gas from a pipe. The instantaneous rupture of one side of the pipe produces an instantaneous shock wave that moves with the speed of sound from the rupture point to the other end of the pipe (that is, in direction opposite to the flow of gas).

There are many models in literature that describe this situation [Bell 1978, Wilson 1979, Picard \& Bishnoi 1989, Chen, Richardson \& Saville 1992]. Here, the empirical model of Bell, as modified by Hanna \& Drivas [Hanna \& Drivas 1987, Lees 2003], is described. This model agrees well with the rest, but additionally is easy in its use. Its validity is restricted to the time taken for the shock wave to travel from the rupture point to the other side of the pipe. It also estimates the outflow mass flow rate based on the initial conditions.

According to the model of Bell [Hanna \& Drivas 1987], the transient mass flow rate $\dot{m}(t)(\mathrm{kg} / \mathrm{s})$ from the pipe is calculated as a function of the time $t(\mathrm{~s})$, from the expression

$$
\begin{equation*}
\dot{m}(t)=\frac{\dot{m}}{1+S}\left\{S \exp \left(-\frac{t}{t_{\mathrm{B}}}\right)+\exp \left(-\frac{t}{t_{\mathrm{B}} S^{2}}\right)\right\}, \tag{B2.25}
\end{equation*}
$$

where

$$
\begin{equation*}
S=\frac{M}{\dot{m} t_{\mathrm{B}}} . \tag{B2.26}
\end{equation*}
$$

In relation to Eqs. (B2.25) and (B2.26) we note the following:

- The outflow mass flow rate $\dot{m}(\mathrm{~kg} / \mathrm{s})$, in the above two equations, refers to the outflow mass flow rate from a hole, obtained from Eq. (B2.13). In the case of the total pipe rupture examined here, the discharge coefficient, $C_{d}(-)$, has a value equal to 1 .
- $\quad$ The initial mass, $M(\mathrm{~kg})$, of the gas in the pipe is calculated from the pipe's dimensions (length, $l_{\mathrm{p}}(\mathrm{m})$, and diameter, $d_{\mathrm{p}}(\mathrm{m})$ ), the density, $\rho\left(\mathrm{kg} / \mathrm{m}^{3}\right)$, of the gas, and the pipe cross-sectional area $A_{\mathrm{p}}\left(\mathrm{m}^{2}\right)$, as

$$
\begin{equation*}
M=\rho l_{\mathrm{p}} A_{\mathrm{p}}=\rho l_{\mathrm{p}}(\pi / 4) d_{\mathrm{p}}^{2} . \tag{B2.27}
\end{equation*}
$$

- The characteristic time, $t_{\mathrm{B}}$ (s), in Eq. (B2.26), is given by the empirical expression

$$
\begin{equation*}
t_{\mathrm{B}}=\frac{4}{3} \frac{l_{\mathrm{P}}}{u_{\text {sound }}} \sqrt{\frac{\gamma f_{\mathrm{F}} l_{\mathrm{P}}}{d_{\mathrm{p}}}}, \tag{B2.28}
\end{equation*}
$$

where $f_{\mathrm{F}}(-)$ is the Fanning friction factor, Eqs. (B2.23)-(B2.24) and $u_{\text {sound }}$ $(\mathrm{m} / \mathrm{s})$ is the speed of sound, equal to

$$
\begin{equation*}
u_{\text {sound }}=\sqrt{\frac{\gamma R T}{W_{\mathrm{g}}}} \tag{B2.29}
\end{equation*}
$$

In the above expression, $\gamma(-)$ is the Poisson ratio, $R$ the universal gas constant $\left(=8.314 \mathrm{Jmol}^{-1} \mathrm{~K}^{-1}\right), T(\mathrm{~K})$ the gas temperature and $W_{\mathrm{g}}(\mathrm{kg} / \mathrm{mol})$ its molecular weight.

As mentioned before, the model of Bell [Hanna \& Drivas 1987] is valid for the time period until the shock wave that moves with the speed of sound, $u_{\text {sound }}(\mathrm{m} / \mathrm{s})$, travels the pipe's length, $l_{\mathrm{p}}(\mathrm{m})$. Hence it is valid for time $t_{\mathrm{E}}(\mathrm{s})$, equal to

$$
\begin{equation*}
t_{\mathrm{E}}=\frac{l_{\mathrm{p}}}{u_{\text {sound }}} \tag{B2.30}
\end{equation*}
$$



Fire and explosion on February 18, 2008, in Big Spring Refinery, TX, U.S.A. (Reproduced by kind permission of Texas Forest Service U.S.A.)

Total Vessel Rupture
calculation procedure



Calculate the transient outflow mass flow rate of propane from a pipe that suddenly ruptures. The following data are available:

| - | Initial pressure of pipe, $P_{\mathrm{o}}$ | $:$ | 0.5 |
| :--- | :--- | :---: | :--- |
| MPa |  |  |  |
| Initial temperature of pipe, $T_{\mathrm{o}}$ | $:$ | 288.15 | K |
| - | Pipe diameter, $d_{\mathrm{p}}$ | $:$ | 1 |
| m |  |  |  |
| Pipe length (until rupture point), $l_{\mathrm{p}}$ | $: 10,000$ | m |  |
| - $\quad$ Discharge coefficient, $C_{\mathrm{d}}$ | $:$ | 1 | - |
| - $\quad$ Molecular weight of propane, $W_{\mathrm{g}}$ | $:$ | 0.0441 | $\mathrm{~kg} / \mathrm{mol}$ |
| Poisson ratio, $\gamma$ | $:$ | 1.19 | - |
| Viscosity of propane, $\eta$ | $:$ | 82 | $\mu \mathrm{~Pa} \mathrm{~s}$ |

The transient outflow mass flow rate will be calculated from Eq. (B2.25)

$$
\dot{m}(t)=\frac{\dot{m}}{1+S}\left\{S \exp \left(-\frac{t}{t_{\mathrm{B}}}\right)+\exp \left(-\frac{t}{t_{\mathrm{B}} S^{2}}\right)\right\} \quad \text { where } \quad S=\frac{M}{\dot{m} t_{\mathrm{B}}} .
$$

Subsequently, we will calculate in turn
a) the outflow mass flow rate $\dot{m}(\mathrm{~kg} / \mathrm{s})$,
b) the characteristic time $t_{\mathrm{B}}(\mathrm{s})$ and
c) the parameter $S(-)$.
a) Initially we need to calculate the outflow mass flow rate $\dot{m}(\mathrm{~kg} / \mathrm{s})$, from the hole, calculated from Eq. (B2.13).

$$
\dot{m}=C_{\mathrm{d}} A_{\mathrm{h}} P_{\mathrm{o}} K \sqrt{\frac{W_{\mathrm{g}}}{\gamma R T}} .
$$

The flow is supersonic as

$$
50=\frac{P_{\mathrm{o}}}{P_{\mathrm{a}}} \geq\left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}}=1.7,
$$

where $P_{\mathrm{a}}(\mathrm{Pa})$ is the ambient pressure.

Hence the coefficient $K(-)$ is calculated from Eq. (B2.16) as

$$
K=\gamma\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}}=0.71
$$

Thus the outflow mass flow rate $\dot{m}(\mathrm{~kg} / \mathrm{s})$ obtained is equal to $1,089.2 \mathrm{~kg} / \mathrm{s}$. In the calculations we employed $C_{\mathrm{d}}=1$ and $A_{\mathrm{h}}=(\pi / 4) \times 1^{2} \mathrm{~m}^{2}$.
b) The characteristic time, $t_{\mathrm{B}}(\mathrm{s})$, is obtained from the empirical equation, Eq. (B2.28), as

$$
t_{\mathrm{B}}=\frac{4}{3} \frac{l_{\mathrm{P}}}{u_{\text {sound }}} \sqrt{\frac{\gamma f_{\mathrm{F}} l_{\mathrm{P}}}{d_{\mathrm{p}}}} .
$$

The speed of sound, $u_{\text {sound }}(\mathrm{m} / \mathrm{s})$, is obtained from Eq. (B2.29) as

$$
u_{\text {sound }}=\sqrt{\frac{\gamma R T}{W_{\mathrm{g}}}}=254.3 \mathrm{~m} / \mathrm{s}
$$

while the Fanning friction factor, $f_{\mathrm{F}}(-)$, is calculated from Eq. (B2.24),

$$
f_{\mathrm{F}}=0.0791 R e^{-0.25}=1.23 \times 10^{-3}
$$

where $R e=\rho u d_{\mathrm{p}} / \eta$ and

$$
\begin{aligned}
& \rho=P_{\mathrm{o}} W_{\mathrm{g}} /\left(R T_{\mathrm{o}}\right)=9.2 \mathrm{~kg} / \mathrm{m}^{3}, \\
& u=\dot{m} /\left(\rho A_{\mathrm{h}}\right)=150.7 \mathrm{~m} / \mathrm{s} \text { and finally } \\
& R e=1.69 \times 10^{7} .
\end{aligned}
$$

Hence according to the above, the characteristic time $t_{\mathrm{B}}=201 \mathrm{~s}$.
c) The initial mass, $M(\mathrm{~kg})$, of the gas in the pipe is obtained from the dimensions of the pipe (length, $l_{\mathrm{p}}(\mathrm{m})$, and diameter, $d_{\mathrm{p}}(\mathrm{m})$ ) and the density, $\rho\left(\mathrm{kg} / \mathrm{m}^{3}\right)$. Thus the initial mass of the gas is equal to $72,275 \mathrm{~kg}$.

Therefore

$$
S=\frac{M}{\dot{m} t_{\mathrm{B}}}=0.33 .
$$





Table B2.4. Temporal Change of Transient Outflow Mass Flowrate of Propane.

| $t, \mathrm{~s}$ | $\dot{m}(t), \mathrm{kg} / \mathrm{s}$ |
| ---: | :---: |
| 0 | 1,089 |
| 25 | 500 |
| 50 | 294 |
| 100 | 173 |

In Table B2.4 the temporal change of the transient outflow mass flow rate of propane is shown.

As already mentioned, the model of Bell [Hanna \& Drivas 1987] is valid for the time period until the shock wave that moves with the speed of sound, $u_{\text {sound }}(\mathrm{m} / \mathrm{s})$ covers the entire length, $l_{\mathrm{p}}(\mathrm{m})$ of the pipe.

Hence the model is valid for time

$$
t_{\mathrm{E}}(\mathrm{~s})=l_{\mathrm{p}} / u_{\text {sound }}=39 \mathrm{~s}
$$

For this reason, in Table B2.4 no higher times are given.


[^0]:    * The expression was derived from the change in internal energy $\delta U(\mathrm{~J} / \mathrm{kg})$, assuming
    - reversible adiabatic outflow and thus $\quad \delta U=-P \delta V$,
    - neglecting internal pressure (ideal gas) and thus $\delta U=C_{\mathrm{V}} \delta T$,
    - from the definition of density per unit mass in the vessel $\rho=1 / V$ and $\delta V=-\delta \rho / \rho^{2}$.

