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Prediction of the Reduced Explosion Pressure During Vented Gas Explosions Using a One-Dimensional Combustion Model in Combination with the Efflux Function

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Pressure venting is a common method in process industry to limit the overpressure during a gas phase explosion to the design pressure of a vessel. The ability to predict the reduced explosion pressure for a given vent area is crucial in the design of venting devices. In preceding publications by BASF, a model to predict the reduced explosion pressure was introduced. The model describes the pressure development inside the vessel using a zero-dimensional approach for the explosion. The mass reduction due to the vented gases is calculated from the Efflux function. To improve the accordance of the predicted explosion pressures with experimental data, the existing model is refined in the present work by applying a one-dimensional model to represent the flame propagation along the vessel's centreline. This increases the accuracy of the predicted reduced explosion pressures compared to the previous version, especially for large vent areas. The explosion is described by an iterative routine for the combustion process and the induced flow velocities and turbulence. The integration of the effect of increased turbulence due to the flow of vented gases on the burning velocity was found to be crucial.

1. Introduction

Whenever explosive mixtures inside a containment cannot be avoided and the equipment cannot withstand the pressures resulting from accidental ignition, explosion pressure vents can be employed to ensure safe operation. These devices open at a certain overpressure to discharge gas from the containment. This limits the possible pressure inside the vessel to the so called "reduced explosion pressure" (p_{red}). p_{red} is defined by the vent size, the opening pressure of the venting device and the explosion characteristics of the mixture inside the vessel. For safe operation, p_{red} should not exceed the vessel's pressure resistance.
The design guidelines for pressure vents are defined in EN 14994 based on an empirical equation known as Bartknecht formula (Bartknecht 1993). The shortcomings of this formula have been pointed out in Blanchard 2013: Negative venting areas can be obtained for gases with very low K_G-value, large changes in K_G-value only result in unrealistically small changes in vent area and required vent areas for gases with low K_G-value can be predicted significantly too large. Due to these shortcomings of the present standard, BASF's safety engineering group started to develop an improved design procedure based on the physical processes involved in explosion pressure venting. In this procedure, the amount of expelled gases through the vent is calculated using the Efflux function. The first version of the model (Blanchard 2013, 2016) describes the pressure development inside the vessel using a zero-dimensional approach for the explosion. The change in the thermodynamic state of the vented gases during the explosion was determined from the pressure-time trace of a closed vessel explosion. This assumption delivers good results if the reduced explosion pressure is close to the explosion pressure in a closed vessel, i.e. if the vent area is small compared to the vessel volume. If the thermodynamic state of the vented gas is significantly different from the thermodynamic state during a closed vessel explosion, the previous approach overpredicts the reduced explosion pressure. In the present work, the existing model is refined by applying a one-dimensional model along the vessel's centreline to represent the explosion. In this way, the thermodynamic state of the vented gases is determined based on the actual pressure inside the vessel. This increases the accuracy of the predicted reduced explosion pressures

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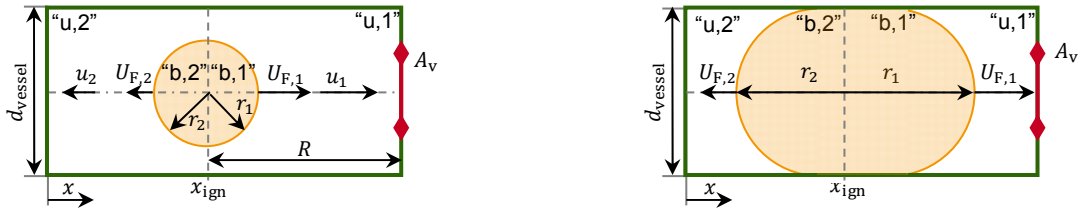
compared to the previous method, especially for large vent areas. Moreover, the effect of a variation in length-to-diameter ratio of the vessel on the reduced explosion pressure is accounted for. The explosion inside the vessel is represented by an iterative routine describing the combustion of a certain volume element of unburned mixture. To reproduce the rate of pressure increase observed in experiments, a burning velocity of the propagating flame front is required. This burning velocity is coupled to the turbulent velocity fluctuations induced by the flame propagation itself and by the flow of vented gases using a common Damköhler approach.
In the first part of this paper, the new version of the design procedure is introduced. Afterwards, the calculated pressures are compared to experimental data and results from the previous version.

2. Modified Design Procedure

A one-dimensional model is used to describe the process of an explosion inside a cylindrical vessel. The considered system is depicted in Fig. 1. At the beginning of the simulation, the complete vessel is filled with a homogeneous combustible/oxidant/inert gas mixture (labelled “u,1” and “u,2”). Then, the mixture is ignited at the position x_{ign}. The position of ignition can be varied along the vessel’s centreline. Depending on the location of ignition one or two flame fronts are initiated and propagate into the unburned mixture. At the beginning of the explosion, spherical flame propagation is assumed until the flame front reaches the vessel wall ($r = d_{\mathrm{vessel}}/2$). It is assumed that from that point on, the flame fronts propagate as hemispheres with a constant flame front area of $A_F = \pi\, d_{\mathrm{vessel}}^2/2$. The thermodynamic state of the gas expelled through the vent (burned “b,1” or “b,2” or unburned “u,1” or “u,2”) is determined depending on the position of the flame fronts.



a) Initially spherical flame propagation *b) Flame propagation for $r_i > d_{\mathrm{vessel}}/2$, $i \in \{1;2\}$*

Figure 1: One-dimensional model of an explosion inside a vessel with venting device (red) and two propagating flame fronts (orange). The orange region marks the already burned mixture.

2.1 Basic Model Structure

The structure of the modified design procedure is presented in Fig. 2.

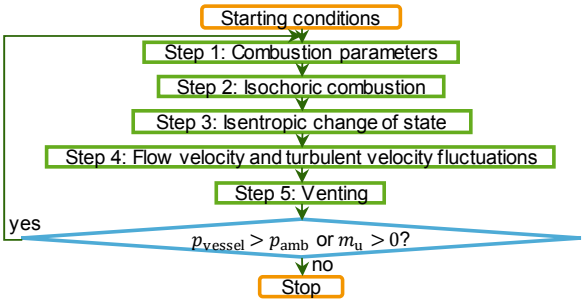


Figure 2: Iterative calculation routine of modified design procedure for explosion pressure vents.

The calculation routine basically consists of five steps: In the first step, the chosen time step Δt is translated into mass and volume elements of unburned mixture which are combusted in the current iteration. For this purpose, the mixture’s laminar burning velocity is transformed into a turbulent burning velocity using the turbulence parameters generated in the fourth step of the previous iteration. The second step describes the combustion of the unburned mixture elements defined in the first step under constant volume conditions. This step results in different pressures in the unburned and burned mixture regions which are equalized in the third step in an isentropic change of state. After the third step, the thermodynamic state of the burned and unburned mixture is constant for the remaining steps of the iteration. In the fourth step, the flow velocities and velocity fluctuations in the unburned mixture are calculated. The parameters calculated in this step are used in the first step of the subsequent iteration to calculate the turbulent burning velocity. In the fifth step, the mass flow expelled through the venting device is calculated depending on the thermodynamic state of the gases

inside the vessel close to the vent. For this purpose, the Efflux function is used which has already been applied in Blanchard 2013, 2016.

2.2 Model Details

First, the thermodynamic state in the different mixture regions after the mass reduction due to venting is determined: The temperature in the mixture regions is obtained from the change in internal energy caused by the enthalpy flux attributed to the vented gas. The corresponding pressure is calculated from the ideal gas law. Afterwards, the influence of velocity fluctuations and corresponding flame front instabilities on the burning velocity is defined using a common Damköhler approach (Peters 2004):

$$S_\mathrm{t} = S_\mathrm{l}\left(1 + C_\mathrm{St}\left(\frac{u'}{S_\mathrm{l}}\right)^{0.5}\right). \tag{1}$$

In this approach, the turbulent burning velocity S_t is computed from the laminar burning velocity S_l and the turbulent velocity fluctuations u'. The pre-exponential parameter C_St depends on the sensitivity of each combustible-oxidizer mixture to flame front instabilities and can be adapted to reproduce the rate of pressure increase in a closed vessel explosion. From the turbulent burning velocity, the flame surface area A_F (cf. Fig. 1) and the time step Δt, the volume elements of unburned mixture consumed by the two flame fronts are obtained:

$$\Delta V_\mathrm{comb} = S_\mathrm{t} A_\mathrm{F} \Delta t. \tag{2}$$

They can be transformed to mass elements Δm_comb. These mass/volume elements are converted to burned mixture in the second step of the iteration. The pressure in the burned mixture is obtained from volumetric averaging of the explosion pressure from isochoric combustion of ΔV_comb and the pressure in the burned mixture from the previous iteration. The resulting pressure differences in the different mixture regions are equalized in the third step assuming an isentropic change of state to the same pressure in all mixture regions:

$$p_\mathrm{i} = {p'}_\mathrm{i}\left(\frac{{V'}_\mathrm{i}}{V_\mathrm{i}}\right)^{\kappa},\ i \in \{\mathrm{u},1;\ \mathrm{u},2;\mathrm{b},1;\mathrm{b},2\},\ p_{\mathrm{u},1} = p_{\mathrm{u},2} = p_{\mathrm{b},1} = p_{\mathrm{b},2},\ \sum V_\mathrm{i} = V_\mathrm{vessel}. \tag{3}$$

After this step, the thermodynamic state of the gas and the position of the flame fronts are constant for the remaining steps of the iteration. Therefore, the flame positions can be calculated from the volume of the burned mixture assuming the flame shapes shown in Fig. 1. The flame speeds with respect to the vessel walls are derived from the change of volume of the unburned mixture regions.
In the fourth step, the flow velocity in the unburned mixture is computed from the flame speed, the turbulent burning velocity and the mass flow rate of the vented gases. In the vented case, it is assumed that the flame propagating towards the vent dominates the explosion process. For that reason, the acceleration of the flow in the product gas of this flame is accounted for in the calculation of the flow velocity for the second flame propagating in the opposite direction. From the flow velocity u and a turbulence intensity Tu, the turbulent velocity fluctuations are obtained:

$$u' = \mathrm{Tu}\,|u|. \tag{4}$$

The turbulence intensity is defined as shown in Fig. 3. In the closed vessel, it is assumed that the turbulence intensity first increases linearly while the flame propagates from the location of ignition $r = 0$ towards the wall at $r = R$. Close to the wall a quadratic increase of turbulence intensity due to the sudden deceleration of the flow ahead of the flame is implemented. In the vented case, it is assumed that the turbulence intensity for the flame approaching the vent increases quadratically from the point on when the venting device is opened due to the acceleration of the flow by the vented gases. It is furthermore assumed that the wall effect is reduced because the flow approaching the wall is less decelerated by the wall but accelerated while passing the vent. Hence, it is assumed that the maximum turbulence intensity at $r = R$ is reduced from 0.25 to 0.16. For the second flame propagating in the direction opposite to the vent, the turbulence intensity distribution of the closed vessel is applied. The dependence of Tu on r/R is held constant for all calculations presented here.
If the pressure inside the vessel increases above the opening pressure of the vent (p_stat), the status of the vent is set to “open”. For an open vent, the vented mass

$$\Delta m_\mathrm{vent} = \alpha\, A_\mathrm{vent} \psi\, p_\mathrm{vent}\sqrt{\frac{2\,M}{T_\mathrm{vent}\,R}}\Delta t \text{ with } \psi = \left(\frac{p_\mathrm{amb}}{p_\mathrm{vent}}\right)^{1/\kappa}\sqrt{\frac{\kappa}{\kappa-1}\left[1-\left(\frac{p_\mathrm{amb}}{p_\mathrm{vent}}\right)^{(\kappa-1)/\kappa}\right]} \text{ for } \frac{p_\mathrm{vent}}{p_\mathrm{amb}} < \Pi_\mathrm{crit} \text{ and}$$
$$\psi = \left(\frac{2}{\kappa+1}\right)^{1/(\kappa-1)}\sqrt{\frac{\kappa}{\kappa+1}} \text{ for } \frac{p_\mathrm{vent}}{p_\mathrm{amb}} \geq \Pi_\mathrm{crit}, \text{ critical pressure ratio: } \Pi_\mathrm{crit} = \left(\frac{\kappa+1}{2}\right)^{\kappa/(\kappa-1)} \tag{5}$$

is calculated from a vent efficiency factor α (set to unity throughout this work), the vent area A_{vent}, the Efflux function ψ and the thermodynamic state (p_{vent}, T_{vent}) of the vented gases (R, M and κ denote the universal gas constant, the mixture's molar mass and isentropic exponent). The thermodynamic state of the vented gases is determined depending on the position of the flame front and the resulting mixture region present at the vent. Furthermore, the mass flow rate $\Delta m_{\mathrm{vent}}/\Delta t$ is converted to a flow velocity inside the vessel.

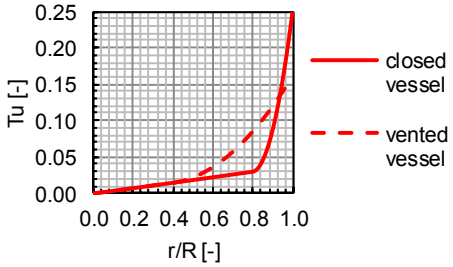
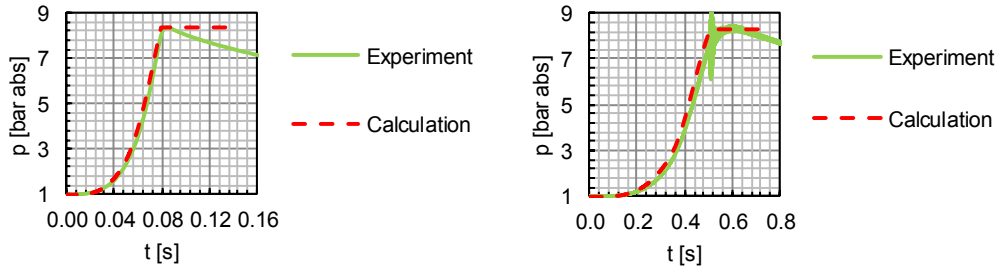


Figure 3: Turbulence intensity depending on flame radius r normalized by R (distance of location of ignition from the wall) for an explosion in a closed and a vented vessel. In a vented vessel, the dashed line is used for the flame approaching the vent. For the flame propagating in opposite direction, the solid line is applied.

3. Model Validation

3.1 Explosions in Closed Vessels

The explosion characteristics ($p_{\mathrm{ex}}/p_{\mathrm{u}}|_T, K_{\mathrm{G}}$) of a specific fuel-oxidizer mixture are typically determined in a spherical 0.02 m³ vessel with an ignitor in the center by recording the pressure development during the explosion. A pressure-time trace resulting from such an experiment is shown in Fig. 4 a) compared to the results from the calculation procedure. The combustion parameters for the near stoichiometric methane-air mixture were set as follows: $C_{\mathrm{St}} = 1.9$, $S_{\mathrm{l0}} = 0.36\ \mathrm{m/s}$, $p_{\mathrm{ex}}/p_{\mathrm{u}}|_{25\,^{\circ}\mathrm{C}} = 8.3$. Figure 4 b) depicts the measured and calculated pressure-time trace obtained for a similar mixture in a cylindrical 5 m³ vessel. The experiments were performed at "Bundesanstalt für Materialforschung und -prüfung" BAM (Rosenow 2016 and Blanchard 2016). The good agreement between experimentally obtained and calculated pressure-time traces for both vessels shows that the sub-model for the flame propagation (turbulent burning velocity and turbulence distribution) included into the vent design procedure is suitable to describe a gas explosion in a closed vessel. For that reason, the probability is high that it also reasonably well represents the flame propagation in a vented explosion.



a) 0.02 m³ spherical vessel, 9.5 vol.-% methane *b) 5 m³ cylindrical vessel ($L/D = 1.18$), 9.7 vol.-% methane*

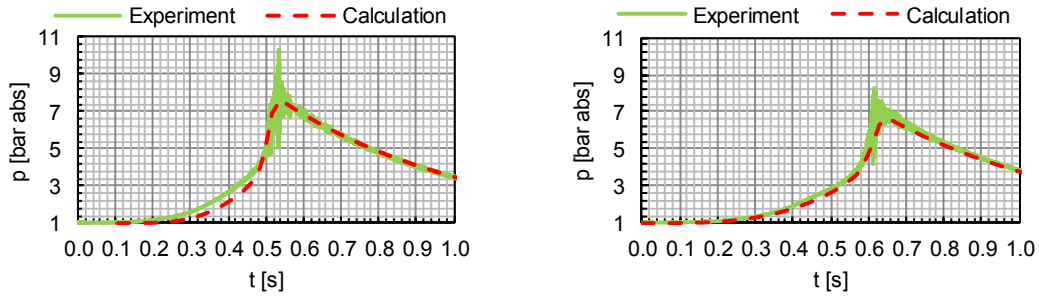
Figure 4: Pressure-time traces of closed vessel explosions of near stoichiometric methane-air mixtures at ambient initial conditions. For the spherical vessel calculation, the procedure was adjusted to a mere spherical flame propagation. The experiment in the spherical vessel was performed at BASF, the experiment in the cylin-drical vessel at BAM (Rosenow 2016, Blanchard 2016). Note: the experiment in the cylindrical vessel shows unphysical pressure oscillations in the region of the pressure maximum due to disturbances of the sensor.

3.2 Vented Explosions

Experiments of vented explosions of methane-air mixtures have been performed at BAM for varying methane concentrations in a 5 m³ vessel (Rosenow 2016, Blanchard 2016). The pressure time traces of two mixture compositions are presented in Fig. 5 compared to the results of the calculation routine presented in Sec. 2. For the near stoichiometric case with 9.7 vol.-% methane, the combustion parameters chosen for the closed vessel explosions shown in Fig. 4 are applied. For the lean case with 8.4 vol.-%, the parameters are set as follows: $C_{\mathrm{St}} = 1.5$, $S_{\mathrm{l0}} = 0.3\ \mathrm{m/s}$, $p_{\mathrm{ex}}/p_{\mathrm{u}}|_{25\,^{\circ}\mathrm{C}} = 7.4$. The laminar burning velocities for methane-air mixtures are

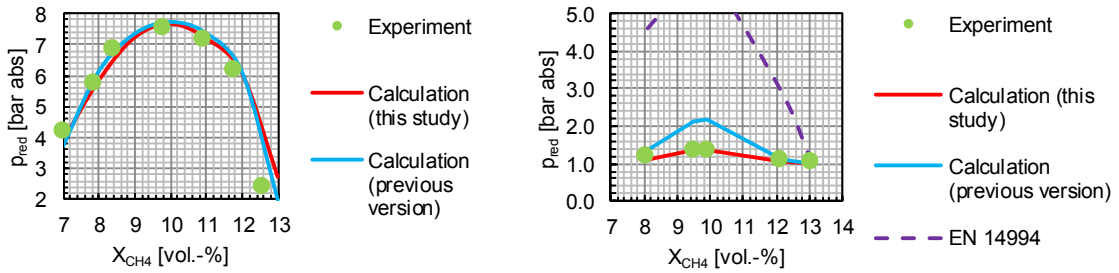
taken from Chen 2011, the explosion pressure ratio from closed vessel explosions performed at BAM. Figure 5 shows that the pressure development during the explosion is well reproduced for both mixtures. (Note: As in Fig. 5 b) unphysical pressure oscillations are observed in the experimental data around the pressure maximum. These oscillations originate from disturbances of the pressure sensor presumably due to oscillations of the vessel structure. The actual reduced explosion pressure is obtained from the average value of the oscillation.) In Fig. 6 a), the reduced explosion pressures of the experiments conducted in the 5 m³ vessel are compared to the predictions from the current and the previous version of BASF's vent design procedure. In the previous version, the turbulence parameter is set to $A_{\mathrm{T}} = 3$ (cf. Blanchard 2016). The pre-exponential factors C_{St} in the current version are adjusted to reproduce the rate of pressure increase in closed vessel explosions at similar methane concentrations. Both calculations well represent the reduced explosion pressures for a broad mixture composi-tion range. The reason for the good agreement of the previous version with the experimental data is the fact that the reduced explosion pressure is close to the explosion pressure in the closed vessel and that the K_G-value used as input parameter was measured in the same vessel geometry (same L/D). The results for a vessel with larger L/D and lower p_{red} are shown in Fig. 6 b) (Kasmani 2008). In this case, the previous version of the design procedure strongly overpredicts the reduced explosion pressures whereas the modified procedure well reproduces the experimental data. The same result is found in Fig. 7 a) for near stoichiometric methane-air explosions with varying vent size. The reason for the much better performance of the new model in case of elongated vessels is the fact that for increasing L/D, the influence of the initially spherical flame propagation shown in Fig. 1 a) attributed to a high rate of pressure increase decreases. This leads to a lower rate of pressure increase compared to spherical or cylindrical vessels with low L/D. This effect of vessel geometry on the rate of pressure increase is not included in the zero-dimensional approach of the previous model version.

The effect of different combustibles on the accuracy of the one-dimensional design procedure presented in this work is depicted in Fig. 7 b) for hydrogen-air mixtures and in Fig. 8 for a stoichiometric propane-air mixture. In both cases, C_{St} is adjusted to reproduce the rate of pressure increase of a closed vessel explosion. Combustion parameters are taken from Konnov 2008 and Huzayyin 2008. For both combustibles, the modified design procedure delivers satisfactory agreement with the experimental data, especially regarding the low reduced explosion pressures.



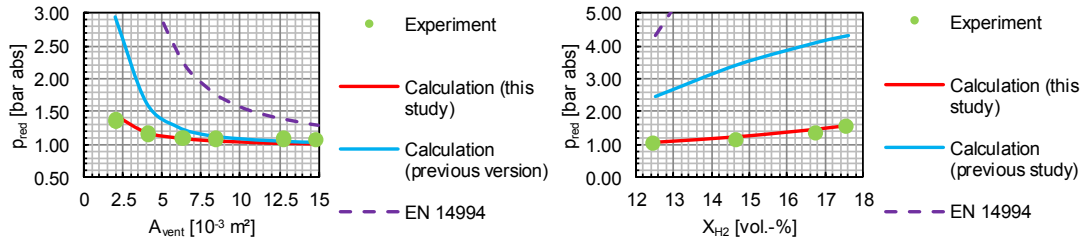
a) 9.7 vol.-% methane *b) 8.4 vol.-% methane*

Figure 5: Pressure-time traces of vented explosions of methane-air mixtures in a 5 m³ cylindrical vessel ($L/D = 1.18$, ambient initial conditions, central ignition, $A_{\mathrm{vent}} = 0.0113\ \mathrm{m}^2$, $p_{\mathrm{stat}} = 3.6\ \mathrm{bar\ abs}$, experiment is described in Rosenow 2016 and Blanchard 2016).



a) 5 m³ vessel, $L/D = 1.18$, $A_{\mathrm{vent}} = 0.0113\ \mathrm{m}^2$, central ign. *b) 0.196 m³ vessel, $L/D = 2$, $A_{\mathrm{vent}} = 0.0206\ \mathrm{m}^2$, end wall ign.*

Figure 6: Reduced explosion pressures of vented explosions of methane-air mixtures in cylindrical vessels at ambient initial conditions and varying methane concentrations (5 m³ vessel experiment: BAM, Rosenow 2016, Blanchard 2016; 0.196 m³ vessel experiment: Kasmani 2008).



a) 0.01 m³ vessel, 10 vol.-% methane, $L/D = 2.8$ *b) 0.196 m³ vessel, hydrogen, $L/D = 2$, $A_{\mathrm{vent}} = 0.0206\ \mathrm{m}^2$, $C_{\mathrm{St}} = 2.7$*

Figure 7: Reduced explosion pressures of vented explosions with end wall ignition of combustible-air mixtures in cylindrical vessels at ambient initial conditions (0.01 m³: Fakandu 2016; 0.196 m³: Kasmani 2008).

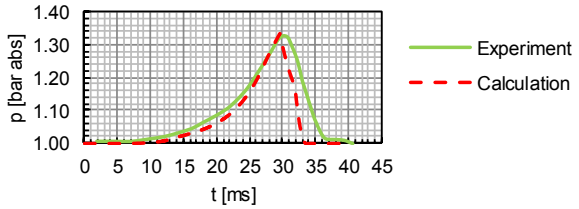


Figure 8: Pressure-time traces of a vented explosion of a stoichiometric propane-air mixture in a 0.003 m³ cylindrical vessel ($L/D = 10.7$, ambient initial conditions, end wall ignition, $A_{\mathrm{vent}} = 0.001\ \mathrm{m}^2$, $p_{\mathrm{stat}} = 1.0\ \mathrm{bar\ abs}$, $C_{\mathrm{St}} = 1.7$, $S_{\mathrm{l0}} = 0.45\ \mathrm{m/s}$, $p_{\mathrm{ex}}/p_{\mathrm{u}}|_{25\,^{\circ}\mathrm{C}} = 8.5$, experiment: Ponizy 2014).

4. Conclusions

The modified vent design procedure including a one-dimensional representation of the flame propagation inside the vessel and the effect of increased turbulence due to the outflowing gases well reproduces the pressures observed in vented explosions of methane-air, hydrogen-air and propane-air mixtures. Especially for large vent areas compared to the vessel volume, this means low reduced explosion pressures, and vessels with a large length-to-diameter ratio, the prediction accuracy of the design procedure was significantly improved compared to its previous version and compared to the present standard method.
In future work, the influence of non-explosive mixture regions inside the vessel and of discharge ducts downstream of the vent on the reduced explosion pressure will be analysed and integrated into the model.

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