THE NATURE OF COHERENT DEFLAGRATIONS

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ABSTRACT

The nature of coherent deflagrations in an enclosure, vented into the atmosphere, is analysed. Experimental observations in an empty 547-m^3 vented enclosure of the SOLVEX programme are analysed by means of large eddy simulations (LES). The LES model is based on the renormalization group theory and the dilution of the methane-air mixture, as it flows out of the vent, is taken into account. A comparison between simulated and experimental pressure transients and, the dynamics of the propagating flame front has given an insight into the nature of the complex simultaneous interactions between flow, turbulence and combustion inside the enclosure and in expelled gases. LES processing of experimental data unveiled that the substantial intensification of premixed combustion occurs only outside the enclosure , leading to a steep coherent pressure rise in both the internal and the external deflagrations. The external explosion does not affect burning rate inside the enclosure. The LES model shows excellent agreement with experimental pressures measured at different locations within and outside the enclosure, up to the point where the flame reaches the shear layers at the edge of the external jet. The modelling of the subsequent combustion required the use of one additional ad hoc parameter. It is suggested that this quantity is necessary to account for the unresolved subgrid scale increase of flame surface density in these highly turbulent layers. The mechanism of combustion intensification in this region is discussed.

KEYWORDS: Internal and external explosion, coherent deflagrations, large eddy simulations, explosion safety engineering

INTRODUCTION

The release of a combustible gas in a petrochemical plant may result in a gas explosion with severe impact [1]. Hence, it is crucial that explosion hazards are taken into account in the safety assessment of such a plant, and reliable predictive tools have become a necessity [2]. Since the Piper Alpha disaster in 1988, gas explosion simulators have been increasingly used, particularly to design offshore structures [1], and various reviews have been published on this matter [1-3]. Computational fluid dynamics (CFD) simulation of explosions is a demanding task due to the non-linearities and disparate time scales involved in turbulent combustin compressible flows [4]. One of the unresolved questions concerns the interaction between the internal combustion during vented deflagration and the external explosion of a flammable mixture being pushed out of the enclosure after ignition, and subsequently undergoing partial dilution by atmospheric air. A similar scenario could be expected when an accidentally released fuel creates a cloud of flammable mixture that spreads throughout the site, followed by ignition in a semi-confined space.

Apparently, Swedish scientists were the first to undertake an experimental investigation that emphasised the importance of the external explosion during a vented deflagration [5]. They found that in some cases the maximum explosion overpressure outside a 203-m^3 enclosure exceeded the maximum overpressure inside of the enclosure.

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In 1980 Solberg *et al* further highlighted the danger of external explosions [6]. They found that during vented deflagrations in a 35-m^3 vessel, the flame front propagation velocity could reach 100 m/s in a lateral direction outside the vent. In their experiments the flame propagated up to 30 m outside the enclosure though the vessel was only 4 m long. In 1986 Cooper et al [7] discussed the role and onset conditions for the pressure peak inside a vented enclosure due to external explosion. Harrison and Eyre [8] came to conclusion that for "large vents, where the internally generated pressures are low, the external explosion can be the dominating influence on the internal pressure" and that this influence "could be very important for large volume, low strength structures such as buildings or off-shore modules".

In 1987 Harrison and Eyre [8], and Swift and Epstein [9], independently suggested that the mechanism of external explosion influence on the internal pressure dynamics is contained in the decrease of the mass flow rate through the vent. Theoretical analysis performed by Molkov in 1997 [10], based on the processing of experimental data by Harrison and Eyre [8] confirmed that the turbulence factor inside the enclosure was practically unaffected by the occurrence of the external explosion. Instead, a substantial decrease of the generalised discharge coefficient, i.e. mass outflow, was found for tests with pronounced external combustion. It was concluded that the decrease of the pressure drop on the vent due to combustion outside the enclosure was the main reason for reduced venting of gas outside the enclosure.

In 1991 Catlin [11] studied the scaling of external explosions. He found that the external overpressure grows proportionally to the velocity of the flow and flame emerging from the vent. This emerging flame ignites the fuel-air mixture in a starting vortex outside the enclosure. Later, in 1993, Catlin *et al* [12] developed the engineering model to assess the hazard from external explosion; this was based on a previous study [11] and validated against large-scale experiments in enclosures with volumes of up to 91 m^3 , including those by British Gas.

In 1996 Puttock *et al* [13] studied the external explosions during experiments in the SOLVEX facility with and without internal obstacles. It was reported that "The effect of the external explosion, giving the final peak the curves, is particularly marked in the case of an enclosure without internal obstacles, increasing the internal pressure by about a factor of four above the previous peak". In these experiments, with typical a dimension of eight metres and a vent size of half the cross-sectional area, the effective epicentre of the external explosion, i.e. the centre of the flame-ball at the moment when the maximum pressure is measured in front of the vent, was only five metres in front of the vent. This is similar to observations in [6] and [8], where the centre of the external explosion was found to be very close to the vent too. It was concluded in [13] that the interaction between external explosion and internal pressure dynamics is still poorly understood.

To the best of our knowledge, detailed CFD modelling of external explosion dynamics has not been successfully achieved. Porosity/distributed resistance (PDR) CFD models such as EXSIM [2] manage reasonable simulations of such vented explosions, having such cases in their validation/calibration set. But they do not attempt simulation of the *details* of the external explosion dynamics. A phenomenological model such as SCOPE (Puttock *et al*. [14]) includes a representation of the external explosion, but this aspect of the formulation is essentially a correlation of experimental observations of gross parameters such as peak overpressure.

A detailed CFD simulation of a SOLVEX test with internal obstacles was reported in 1998 [15] but this over-predicted the maximum pressure by two orders of magnitude. In 1999 Fairweather *et al* stressed that "improvements in the accuracy with which the combustion process external to the vessel is modelled" are required [16].

The purpose of this study is to use experimental and theoretical analysis to clarify the nature of complex simultaneous interactions between internal and external deflagrations in a vented explosion. The theoretical analysis of the experimental data obtained during the SOLVEX programme [13] will be performed through the application of the original LES model developed at the University of Ulster and validated previously against large-scale experiments in closed and vented enclosures [17-22].

ANALYSIS OF EXPERIMENTAL DATA

The SOLVEX facility is a large-scale enclosure with size HxWxL=6.25x8.75x10.0 m and a vent HxW=4.66x5.86 m located in the centre of the wall HxW=6.25x8.75 m. The methane experiments were performed with 10.5% methane-air mixture inside the enclosure ignited by a point source located at the centre of the wall opposite the vent. Care was taken to ensure that motion in the gas-air mixture had decayed before ignition. The vent cover was allowed to drop away just before ignition. For this study, a SOLVEX test without obstacles inside the enclosure was chosen to exclude complications related to the modelling of turbulent combustion in a congested space. The SOLVEX experiments are well documented and the repeatability of the experiments was excellent, making them a reliable source of data for validation of the LES model.

The experimental snap-shots of the external explosion are shown in Fig.1, frames A to H. White lines give contours of the enclosure and the vent. Pressure transients inside and outside the enclosure are shown in Fig.2. Frames A-H in Fig.1 correspond to times after ignition A to G in Fig.2 (label H is not shown in Fig.2 as it is outside the abscissa’s upper limit). The internal pressure was recorded by a hydrophone located 2.2 meters from the rear wall on the bottom of the enclosure. The external pressure was recorded by a hydrophone located 6.1 m in front of the vent.

To facilitate a comparison between experimental and simulated snap-shots and pressure dynamics we assume that the appearance of the flame front in the vent (snap-shot A in Fig.1) corresponds to the first pressure peak on the internal pressure-time curve (t=923 ms). It is well known that the first explosion pressure peak inside the enclosure (moment A in Fig.2) is caused by the start of venting of hot combustion products. The time of the first flame front appearance in the vent (frame A in Fig.1) was identified approximately. This is because the piece of a plastic sheet, used to cover the vent and removed shortly before ignition, screened the flame. This is why the flame appears in Fig.1 A at some distance from the vent. The movement of the plastic can be easily seen in Fig.1.

The combustion in the atmosphere outside the enclosure commences in moderate regime between frames A and B in Fig.1. The rapid intensification of combustion starts after the moment when the flame emerging from the enclosure reaches the vent edges (between frames B and C). External pressure reaches its maximum about 70 ms after intensification started (frame D). The maximum pressure inside the enclosure appears shortly after that at 1103 ms (frame E). The moment 1137 ms (frame F) relates to the pressure decay phase. At 1203 ms (frame G), the explosion pressure is close to its minimum at the negative pressure phase of the deflagration. The experimental video records show that there is still intense turbulent combustion proceeding at the top part of the vent. Frame H shows that at the final stage of the process the combustion inside the enclosure continues only at the lower part of the enclosure; this was confirmed by the numerical simulations.

At the same moment, as the pressure inside the enclosure starts to decrease due to more effective venting of hot combustion products compared to venting of a denser fuel-air mixture (moment close to A in Fig.1 and 2), the pressure outside the enclosure starts to grow more rapidly due to the initiation of combustion of flammable mixture outside the enclosure (Fig.2 A to B).

A steep rise of pressure inside the enclosure and in the atmosphere practically coincides with the visible rapid intensification of combustion in the shear layers behind the vent edges outside the enclosure (moment C in Fig.2). There are no video records of what is happening with combustion inside the enclosure at this time. The nature of observed coherent deflagrations inside the vented enclosure and in the atmosphere is not obvious from the analysis of experimental data only. Harrison and Eyre [8] pointed out “there is a widely held belief that any increase in internal pressure that is not predicted by simple venting theory should be attributed to increase in the combustion rate inside the chamber” yet “it is wrong to attempt to represent the peaks caused by external explosions in this way”. That means that Harrison and Eyre [8] as well as Swift and Epstein [9] and Molkov [10] dealt with experiments when decrease of pressure drop on the vent was a significant phenomenon. However, Catlin *et al* [12] stated “the combustion external to the enclosure can provide a source of overpressure and velocity which upon arrival at the vent can interact with the flame inside the enclosure to cause a marked increase in burning rate”.

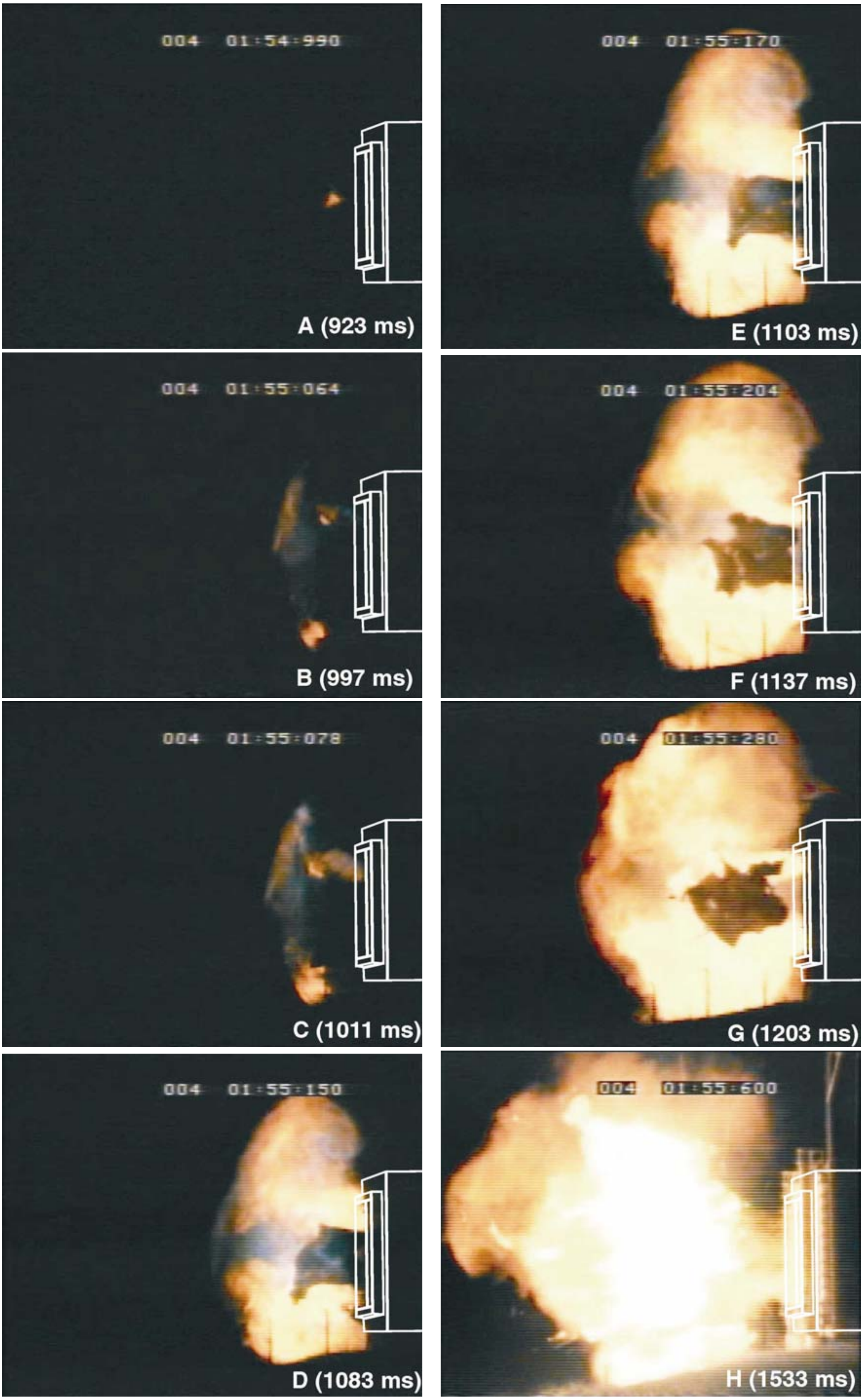

FIGURE 1. Dynamics of external deflagration in experiment.

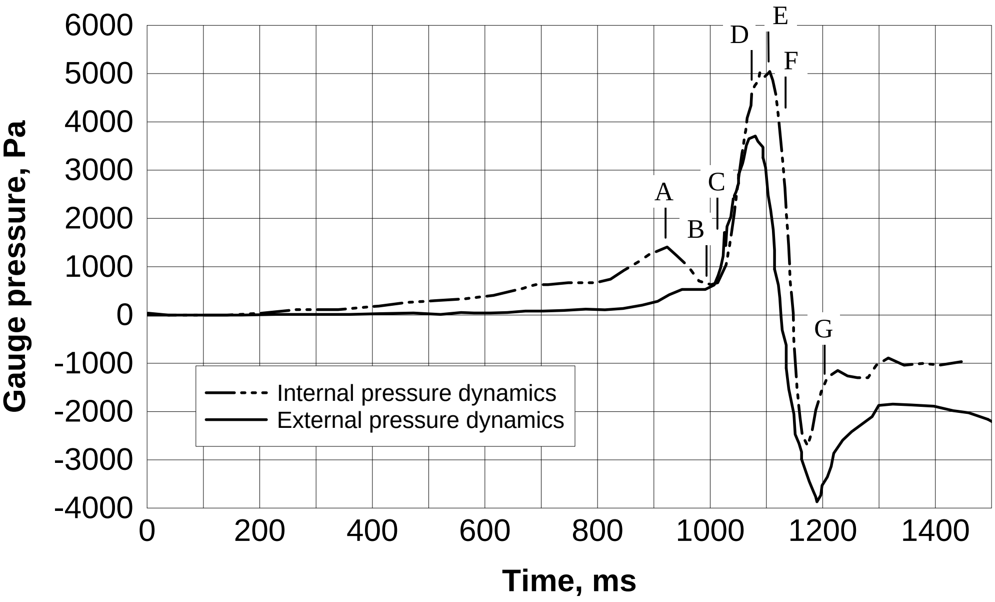

FIGURE 2. Experimental pressure transients inside and outside the enclosure.

MODELLING

The LES model for simulation of gaseous deflagration is described in detail in [17]. It is validated against experimental data on pressure dynamics of stoichiometric hydrogen-air deflagration in a closed 2.3-m diameter spherical vessel [18-21], on the development of a cellular structure and its fractal dimension in a large-scale hydrogen-air confined deflagration and the cellular structure of methane-air premixed flames in the SOLVEX enclosure [18, 22]. The model formulation solves compressible, Favre-filtered (top-hat filter) Navier-Stokes equations and energy equation. The subgrid-scale (SGS) model of turbulence and SGS model for turbulent burning velocity are based on the renormalization (RNG) group analysis [23, 24]. The deflagration flame front propagation was modelled using the progress variable equation and the gradient method was used for the modelling of mass burning rate

$$\frac{\partial}{\partial t}(\rho c)+\frac{\partial}{\partial x_j}(\rho u_j c)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial c}{\partial x_j}\right)+\rho_u S_u |grad\, c|, \tag{1}$$

where c - progress variable (normalised product mass fraction, c=0 in unburned mixture and c=1.0 in combustion products), ρ - density, ρ_u - unburned fuel-air mixture density, u_j - velocity component along x_j coordinate, μ_{eff} and Sc_{eff} - effective viscosity and effective Schmidt number, S_u - turbulent burning velocity as a function of dependent of pressure and temperature laminar burning velocity and the SGS velocity residual.

To account for the combustion of non-uniform fuel-air mixture outside the enclosure the LES model was extended by an additional conservation equation for air concentration

$$\frac{\partial}{\partial t}(\rho Y_a)+\frac{\partial}{\partial x_j}(\rho u_j Y_a)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial Y_a}{\partial x_j}\right)-\frac{Y_a}{Y_f+Y_a}\rho_u S_u |grad\, c|, \tag{2}$$

where Y_a - air concentration, Y_f - initial flammable mixture concentration.

The laminar burning velocity and the heat of reaction were dependent on the methane concentration in the flammable mixture. The combustion products composition did not vary with the fuel concentration and were equal to those of the initial 10.5% methane-air mixture; this led to a negligible error in the molecular mass and the specific heat capacity.

The governing equations were solved by means of the second-order accurate upwind scheme for convective terms and the central-difference scheme for diffusion terms. The explicit scheme was used for time stepping, with the CFL number being equal to 0.8, yielding a time step in the order $2.5\ 10^{-5}$ s.

The calculation domain comprised of the enclosure itself, surrounded by comparatively large hemispherical area (R=60 m) to exclude the effects of boundary conditions on the external combustion and to capture the diverging pressure wave generated by coherent deflagrations. The calculation domain was discretised using an unstructured tetrahedral grid, which allows the meshing of arbitrary complex calculation domains and local refinement in the area of interest, thereby reducing the total number of control volumes to a minimum. There are no preferential directions as is the case with structured grids. The performance of LES on tetrahedral unstructured grids was studied in [25], where the most simple filter - a top-hat filter - was found to be the most successful. The average edge length of the CV was 0.8 m inside and outside the enclosure where combustion took place. The characteristic CV size increased gradually to 23 m in the rest of the domain. The total number of CVs was 87,156 which is a moderate number in view of the complex geometry and size of the problem.

Boundary conditions used for simulations were: no-slip, non-permeable, adiabatic conditions on all walls and ground surfaces and non-reflecting flow conditions at the domain boundary in the atmosphere. Initially, the flammable mixture inside the enclosure and air in the atmosphere were quiescent, pressure was equal to atmospheric, p=101325 Pa, and temperature was equal to T=285K. The initial values c=0, Y_f =0.061, Y_a=0.939 were used inside the enclosure and c=0, Y_f =0, Y_a=1 in the atmosphere. Combustion was initiated by a slow increase of the progress variable in one CV at the centre of the rear wall over 50 ms.

RESULTS OF LARGE EDDY SIMULATIONS

The LES model previously developed at the University of Ulster, based on SGS RNG modelling of turbulence [23] and turbulent premixed combustion [24], was applied directly. It failed to reproduce experimental pressure dynamics in different locations inside and outside the empty SOLVEX enclosure. This numerical experiment showed that an additional ad-hoc parameter is needed to account for the unresolved increase of flame surface density in the starting vortex region outside the enclosure. Results of LES presented in this paper have therefore been obtained with the SGS flame surface density in the area outside the enclosure multiplied by a factor that increases linearly from 1 to 2 during the 100 ms after the emerging flame front first reaches the edge of the vent. It is believed that, with the use of control volumes of typical dimension of 0.8 m, the shear layers at the boundary of the external jet were not sufficiently resolved for the flame surface area generation in this region to be modelled correctly. The use of a much finer mesh was not feasible for these runs.

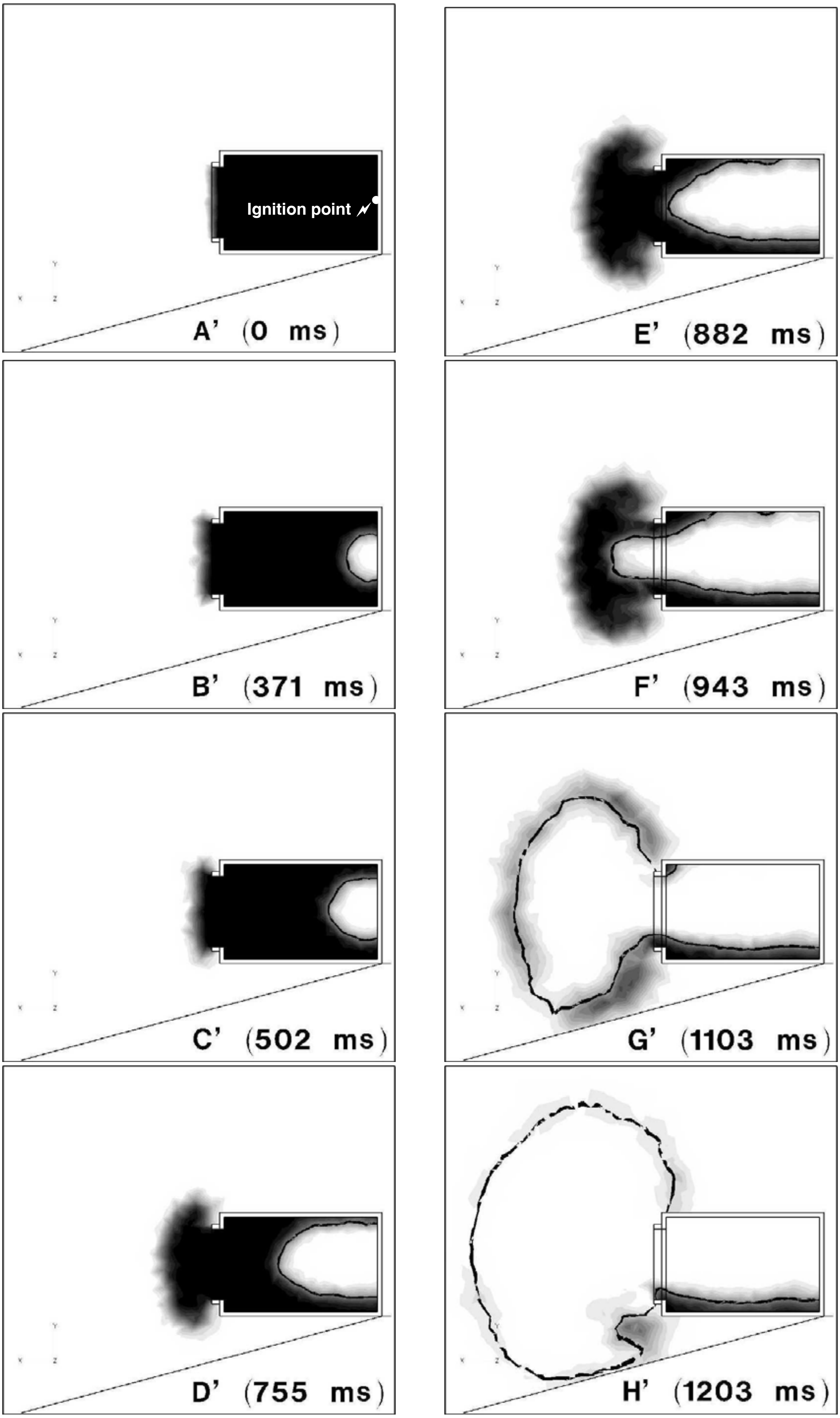

FIGURE 3. Simulated dynamics of external deflagration: flame front position (black line), location of flammable mixture and fuel concentration (black/grey scale palette) in a centre-line cross section.

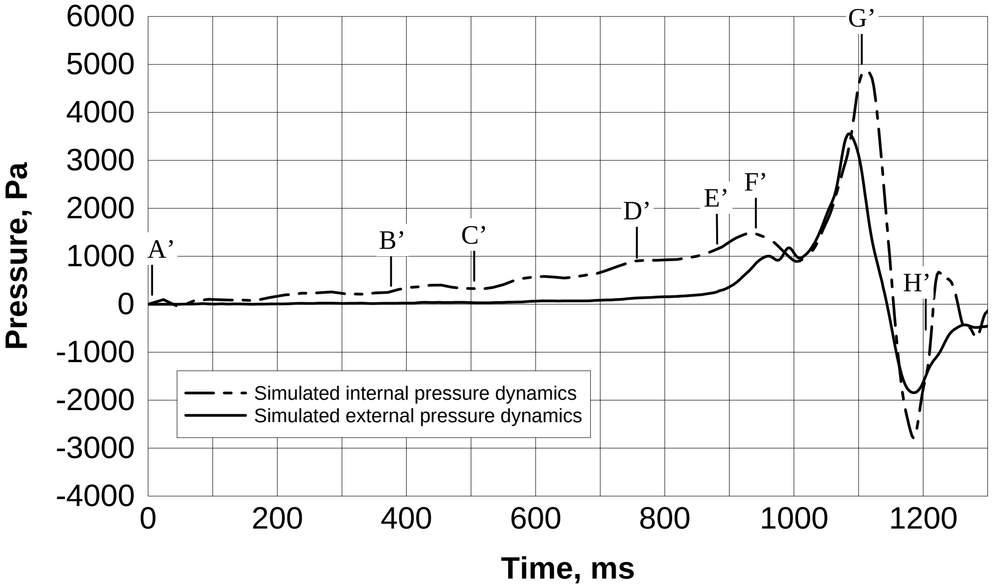

FIGURE 4. Simulated pressure transients inside and outside the enclosure.

The simulated deflagration front propagation, locations of flammable mixture moving outside the enclosure and fuel concentrations in the flammable mixture are shown in Fig.3. Simulated pressure transients were obtained at the same locations inside and outside the enclosure as in the experiment and are shown in Fig.4. Snap-shots A’ through H’ in Fig.3 correspond to the moments A’ through H’ in Fig.4.

The development of a simulated turbulent combustion zone outside the enclosure shown in Fig.3 is similar to that observed experimentally and presented in Fig.1. The geometrical centre of the external explosion at the final stage of combustion (Fig.3 H’) is at the distance about 5-6 m from the vent, which corresponds to experimental observations [13]. A formation of the vortex structure in flammable mixture flowing out to the atmosphere through the vent is clearly seen in Fig.3.

Simulated pressure dynamics of coherent deflagrations given in Fig.4 fit the observations (Fig.2) very well. Flame arrival time to the vent is very close to the experimental one.

The combustion inside the enclosure proceeds in a wrinkled mode. The LES model based on RNG SGS turbulence and turbulent combustion models perfectly reproduces the internal deflagration during the whole period of the development of the coherent deflagrations without an introduction of any ad hoc parameter to describe complex interactions of flow, turbulence and combustion inside the enclosure.

The internal pressure dynamics are reproduced very well in simulations for the whole period of combustion, including the first pressure peak associated with a start of outflow of combustion products from the enclosure, the second pressure peak associated with the coherent external/internal combustion, and the negative pressure peak; the negative pressure is created by the momentum of the outward flow from the external explosion after combustion ceases. The amplitude of the negative pressure peak appears to be significantly under-predicted. However, in this phase the measurement is suspect because this sensor was engulfed in a high-velocity jet of flame, which caused a displacement of the reading by up to 2000 Pa..

The combustion at the top part of the vent at 1203 ms (frame G in Fig.1 and moment H’ in Fig.3), which appears in the video records is not “seen” in Fig.3. The reason is that Fig.3 shows the snap-shots of the process in a centre-line vertical cross section whereas the combustion at the upper part of the vent seen in the video originates from the top corners of the enclosure.

Finally there is a “residual” combustion at the bottom side of the enclosure (after the time of Fig.3 H’) that gives rise to somewhat higher pressure in the enclosure compared to the outside pressure after the negative pressure peak.

CONCLUSIONS

The phenomenon of coherent deflagrations in the SOLVEX empty vented enclosure has been studied. The analysis was based on available experimental data and the results of large eddy simulations. The comparison of pressure transients inside and outside the enclosure by the LES model led to some important conclusions on the nature of coherent deflagrations.

The formation of the turbulent starting vortex in the flammable mixture pushed out of the enclosure during the internal deflagration is a prerequisite for a subsequent intense combustion outside the enclosure. The rapid acceleration of combustion outside the enclosure commences not at the moment when the flame front emerges from the vent, but after the flame front “touches” the edges of the vent. At this point the flame reaches the region of strong turbulence generated in the shear layers at the perimeter of the external jet. There is consequently a rapid increase in the rate of combustion and a coherent steep pressure rise is observed both inside and outside the enclosure. The external pressure rise in the atmosphere is a direct consequence of the highly turbulent deflagration there, but there is no increase of the burning rate inside the enclosure. The pressure rise inside the enclosure is caused by the decrease of mass flow rate from the enclosure to the atmosphere due to the high pressure just outside the vent.

It was found necessary to introduce an additional ad-hoc parameter into the LES model to account for the increase of the SGS flame surface density in the shear layers at the vent edge. These shear layers were not adequately resolved by the mesh size used in these simulations. The parameter was a factor increasing the flame surface density generation. It was steadily increased from 1 to 2 in a time equal to that needed for the completion of the external combustion. The LES model then produced an excellent simulation of experimental pressures at different locations inside and outside the enclosure and the development of the deflagration in the atmosphere.

Further research and development of theoretical SGS models are required for reliable LES of vented gaseous deflagrations in arbitrary practical conditions.

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