

RETHINKING THE PHYSICS OF A LARGE-SCALE VENTED EXPLOSION AND ITS MITIGATION

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The issue of large-scale vented deflagration modelling and mitigation is overviewed briefly. The physics of the phenomenon of coherent deflagrations, i.e. coupled internal and external explosions, in a system vented enclosure-atmosphere is studied further. Results of large eddy simulations of coherent deflagrations for an empty 547-m^3 SOLVEX enclosure are presented. Numerical simulations of initial stages of wrinkled flame front propagation inside the enclosure and pressure generation up to the well-known first pressure peak demonstrate an excellent agreement with experimental observations without introduction of any adjustable parameter. The anisotropic component of turbulent combustion in an external vortical structure after the flame touches the vent edge is thought to be responsible for the significant increase of the flame surface density during deflagration outside the enclosure. The University of Ulster's LES model, based on the renormalization group analysis of subgrid-scale modelling of isotropic turbulence and premixed combustion, is developed further to account for the anisotropic component in turbulent combustion in external vortex. The simple modification of the existent LES model allowed reproducing the experimental pressure dynamics inside and outside the enclosure at distances up to 54 m as well as the shape of the external deflagration. The numerical simulations confirmed results of former analysis that there is no extra intensification of combustion inside the enclosure. The increased second pressure peak inside the enclosure is mainly due to the pressure rise during highly turbulent external combustion and the decrease of outflow from the enclosure resulting from the pressure rise. It is concluded that in many practical cases physically sound simulations of coherent deflagrations are impossible without proper modelling of external combustion. It is suggested that in such cases the mitigation strategy should aim primarily at the suppression of combustion outside the enclosure.

INTRODUCTION

Assessments of explosion hazard and risk are crucial in obtaining an acceptable level of safety, for which validated predictive tools are required[1]. According to HSE report[2] "it appears that only those models falling into CFD class could in principle be capable of being truly predictive tools outside of their immediate range of validation". It is necessary to demonstrate that the methods used for risk assessment are valid at large scales, which are characteristic for production, distribution and storage[2]. This is supported by a recent critical review[3], where a conclusion is made that "large scale research has shown that explosions may be more severe than was previously recognised".

Significant investments have been made and valuable data on experimental large-scale explosion research are already published. However, the need to understand the physics of explosions and their effects as to permit accurate scaling and prediction has not yet conclusively been met[3]. In particular, improvements are sought in the representation of initial stages of explosions[3].

It seems that, for the first time, the importance of an external explosion on reduced pressure generated during vented deflagration was emphasised in 1957 by Swedish scientists[4]. Implicitly the critical role of external explosions was confirmed by experiments with different levels of partial filling of the confined area[5]: at high level of partial filling the pressure was similar to that attained by totally filling, and at low levels the overpressure was considerably reduced. Recently modelling studies of interaction between internal and external combustion were provided[6,7,8]. Yet there is a need for further understanding of the underlying physics, development and validation of appropriate sub-models.

The lack of understanding of the "fine" effects of vented deflagrations such as an interaction between internal and external combustion and effects of parameters of congestion of explosion overpressure is apparent. In such circumstances a million of runs by any tool either phenomenological or CFD to assess risk does not make much sense. If a tool cannot reproduce important physical effects then in such exercises the drawbacks will be reproduced millions of times. It does not mean that those drawbacks will disappear. Being supportive to probabilistic risk assessment, the authors' thrust in this paper is on the basics of this approach, i.e. the development of a deterministic physical model of the phenomenon and its validation.

It has been pointed out[3] that "it proved necessary to re-examine the relative roles of two factors which cause flame wrinkling viz flame induced turbulence in the unburnt gas and obstacle induced flame folding". It will be demonstrated in this paper that the application of RNG isotropic turbulence and premixed combustion SGS models was sufficient to reproduce wrinkled flame front propagation inside empty SOLVEX enclosure. The relative role of anisotropic "flame folding" in a vortical structure beyond the enclosure vent, which can be treated as an "obstacle", is proved here to be more significant in the generation of flame surface density than the RNG isotropic component. It is envisaged that the use of an unstructured solution adaptive mesh system with all its benefits at large-scale LES will not solve the problem and an emphasis should be placed on SGS modelling of coupled isotropic/anisotropic turbulent combustion in areas with apparent vortical structure.

Another aim of this paper is to "mitigate" the criticism of CFD explosion modelling, i.e. "a number of papers seem to fulfil an advertising role rather than add to the sum of knowledge"[3]. In a topic as complex as explosion science there will be gaps in the total knowledge base of how the whole process works for the foreseeable future[3]. Particularly, one area of uncertainty in the physics of vented gaseous deflagrations will be addressed here by means of LES — what are the intrinsic processes of coherent deflagrations in a system vented enclosure–atmosphere. Filling this gap in the understanding of underlying physical phenomena will be beneficial in the development of explosion mitigation measures such as water curtains and water deluge systems.

The paper presents results and an analysis of modelling and large eddy simulations (LES) of coherent gaseous deflagrations in empty SOLVEX enclosure ($10.0 \times 6.25 \times 8.75$ m) with an initially open vent (5.86×4.66 m)[9]. The 10.5% vol. quiescent methane-air mixture was ignited at the rear wall of the enclosure by a point source. An explosion in the large-scale empty SOLVEX enclosure was chosen for simulation because it is a demanding task to model the range of combustion regimes from wrinkled to highly turbulent. The ultimate purpose was to understand the underlying phenomena the vented enclosure can encounter: a complex and not well understood interaction of physical processes inside and outside the enclosure[9].

LARGE EDDY SIMULATIONS

CALCULATION DOMAIN

The calculation domain for large eddy simulations included the 547-m^3 enclosure and hemisphere of ambient space around it with the diameter 120 m. The domain was meshed using an unstructured tetrahedral grid. Two computational grids were used for simulations: with relatively small total number of control volumes (CV) 34,302 and 87,145. The first mesh had the characteristic CV edge size 0.7–0.8 m inside the vessel. In the area of external combustion, estimated as a sphere of 10-m radius with the centre at 5 m in front of the vent centre, the CV edge size was about 2.0–2.5 m. The second grid had the same characteristic CV edge size 0.7–0.8 m inside the enclosure, but a finer grid in the area of external explosion — about 1.0–1.2 m. Outside of external combustion area the CV size gradually increased up to 23 m towards the calculation domain boundaries.

GOVERNING EQUATIONS

The LES model, used here, was previously validated against experimental data on premixed combustion of stoichiometric hydrogen-air mixture in a closed vessel[10,11] and wrinkled methane-air flame propagation in empty SOLVEX enclosure[12]. More details about the model are given elsewhere[11]. In the mentioned simulations the governing equation set comprised filtered three-dimensional mass, momentum and energy conservation equations for compressible Newtonian fluid, filtered progress variable equation to model the premixed flame front propagation, and additional species conservation equation to describe formation of non-uniform flammable mixture outside the enclosure when fuel-air mixture flowing out of enclosure is diluted by atmospheric air on its boundaries:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j) = 0, \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{u}_i) = -\frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_j}\left(\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right) + \bar{\rho}g_i, \tag{2}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{E}) + \frac{\partial}{\partial x_j}(\tilde{u}_j(\bar{\rho}\tilde{E} + \bar{p}))$$

$$= \frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}c_p}{Pr_{eff}}\frac{\partial \tilde{T}}{\partial x_j} - \sum_m \tilde{h}_m\left(-\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \tilde{Y}_m}{\partial x_j}\right) + \tilde{u}_i\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right) + \bar{S}_E, \quad (3)$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{c}) = \frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \tilde{c}}{\partial x_j}\right) + \bar{S}_c, \quad (4)$$

$$\frac{\partial}{\partial t}(\rho Y_a) + \frac{\partial}{\partial x_j}(\rho u_j Y_a) = \frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial Y_a}{\partial x_j}\right) + \bar{S}_a \quad (5)$$

where t = time, $x_{i,j,k}$ = spatial coordinates, ρ = density, $u_{i,j,k}$ = velocity components, p = pressure, μ_{eff} = effective dynamic viscosity, g_i = component of vector of gravity acceleration, E = total energy, T = temperature, c_p = specific heat capacity at constant pressure, h_m = enthalpy of mth specie ($h = \int_{298.15}^{T} c_p dT$), Y_m = mass fraction of mth specie, c = progress variable (normalised product mass fraction), Pr_{eff} = effective Prandtl number, Sc_{eff} = effective Schmidt number, S_c, S_a = source terms for progress variable and additional species conservation equation, S_E = source term in energy conservation equation ($S_E = S_c \cdot H_c$), H_c = heat of reaction. Here and below overbar ¯ stands for filtered quantities and tilda ˜ stands for mass-weighted filtered quantities[13].

The gradient combustion method[14], which is simple to realise and inexpensive in sense of computational resources, was used to model the mass burning rate:

$$\bar{S}_c = \rho_u S_u |grad\ \tilde{c}| \Xi_{SGS}, \quad (6)$$

$$\bar{S}_a = -\frac{Y_a}{Y_f + Y_a}\rho_u S_u |grad\ \tilde{c}| \Xi_{SGS}, \quad (7)$$

where ρ_u = unburned mixture density, S_u = laminar burning velocity, Ξ_{SGS} = SGS flame front wrinkling factor, Y_a, Y_f = mass fractions of air and fuel.

The laminar burning velocity of non-uniform fuel-air mixture was modelled according to data from[15]. The heat of reaction as a function of composition was obtained from a thermodynamic equilibrium model[16]. For 10.5% vol. methane-air mixture $S_u = 0.44$ m/s and $H_c = 2.58$ MJ/kg.

The simplest LES filter — top hat filter — was found to be the most successful in conjunction with unstructured grids in[17] and was utilised in present simulations. Here the filtering was implicitly introduced by finite-difference discretization with the filter size equal to the size of CV. The LES employed the SGS turbulence[18] and SGS premixed combustion[19] models, which are based on the renormalization group (RNG) analysis. The following SGS effective viscosity, effective Prandtl number and turbulent burning velocity were used in LES:

$$\mu_{eff} = \mu\left[1 + H\left(\frac{\mu_s^2 \mu_{eff}}{\mu^3} - 100\right)\right]^{1/3}, \tag{8}$$

$$\left|\frac{1/Pr_{eff} - 1.3929}{1/Pr - 1.3929}\right|^{0.6321}\left|\frac{1/Pr_{eff} + 2.3929}{1/Pr + 2.3929}\right|^{0.3679} = \frac{\mu}{\mu_{eff}}, \tag{9}$$

$$S_t = S_u\ \Xi_{SGS} = S_u \exp(u'^2/S_t^2), \tag{10}$$

where $\mu =$ dynamic viscosity, $\mu_s = \bar{\rho}(0.157V_{CV}^{1/3})^2\sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$, $\tilde{S}_{ij} =$ strain rate tensor, V_{CV} – volume of a control volume, used for meshing, $H(x)$ is the Heaviside function, $S_t =$ turbulent burning velocity, $S_u =$ laminar burning velocity, $u' =$ SGS (residual) velocity. The effective Schmidt number was equal to the effective Prandtl number. The choice of RNG SGS models was based on their ability to describe both laminar and turbulent flows. This feature might be particularly important in the considered experiment, where a relatively long initial phase of wrinkled flame front propagation was anticipated.

INITIAL AND BOUNDARY CONDITIONS

At the initial moment the mixture was quiescent, pressure equal to $p = 101{,}325$ Pa, temperature was equal $T = 285$ K. The initial concentrations of fuel, air and products (progress variable) inside the vessel were equal $Y_f = 0.061$, $Y_a = 0.939$, $c = 0$ and $Y_f = 0$, $Y_a = 1$, $c = 0$ in the ambient atmosphere. The no-slip impermeable adiabatic boundary condition was used in simulations at vessel walls and at the surfaces, representing the ground. Non-reflecting flow conditions were used at the domain boundary in the atmosphere. Combustion was initiated by slow increase of progress variable in one control volume in the centre of the enclosure's rear wall during 50 ms.

The molecular mass of 10.5% vol. methane-air mixture and its combustion products were calculated as $M_u = 27.47$ kg/kmole and $M_b = 26.78$ kg/kmole respectively. The temperature of combustion products of 10.5% vol. methane-air mixture was $T_b = 2156$ K. The densities of initial fuel-air mixture and its combustion products were $\rho_u = 1.175$ kg/m^3 and $\rho_b = 0.151$ kg/m^3, that gives the expansion coefficient of combustion products at initial conditions $E_i = 7.8$.

NUMERICAL DETAILS

The coupled solver was used for simulations with explicit time-stepping scheme and fourth order Runge-Kutta method to solve linear equation set. A second order upwind scheme was used for discretization of convective terms. The Courant-Friedrichs-Lewy number was equal $CFL = 0.8$ to ensure numerical stability. Simulations required about 18 hours CPU time using 6 Power-4 processors' IBM p650 server for an 87,145 CV grid.

RESULTS AND DISCUSSION

INITIAL STAGES OF COHERENT DEFLAGRATIONS AND VORTEX FORMATION

Simulation results for the flame arrival time along enclosure centreline axis are shown in Figure 1 in comparison with the experimental data reported in[20]. The flame front position in Figure 1 is associated with iso-value of progress variable $c = 0.5$. During the initial stage of simulations the flame front profile, which requires at least 3–4 CV, is forming and it is not shown for the radius below 1 m. The simulated propagation of the wrinkled flame front beyond the "ignition zone" of about 1 m is in a good agreement with both experimental records and theoretical predictions[20]. Such an agreement is achieved due to the application of SGS RNG models for turbulence and turbulent combustion, featuring the ability to resolve transitional flows.

The experimental pressure transient inside the enclosure and simulated pressure dynamics for described above LES model are given in Figure 2. There first pressure peak in experimental pressure dynamics at $t = 920$ ms corresponds to the start of venting of combustion products. The simulated pressure dynamics are in excellent agreement with experimental data for both grids until the first pressure peak. This assumes that the key physical phenomena inside the enclosure are properly modelled by RNG approach and mesh resolution inside the enclosure is adequate for simulations of wrinkled flame propagation in conditions of low-intensity turbulent flow in empty SOLVEX enclosure.

However, the LES model based on RNG subgrid modelling of isotropic turbulence and turbulent premixed combustion was unable to reproduce experimental pressure dynamics after the first pressure peak. It is clear that the model should be developed further. The comparison between two simulations on two different grids demonstrates

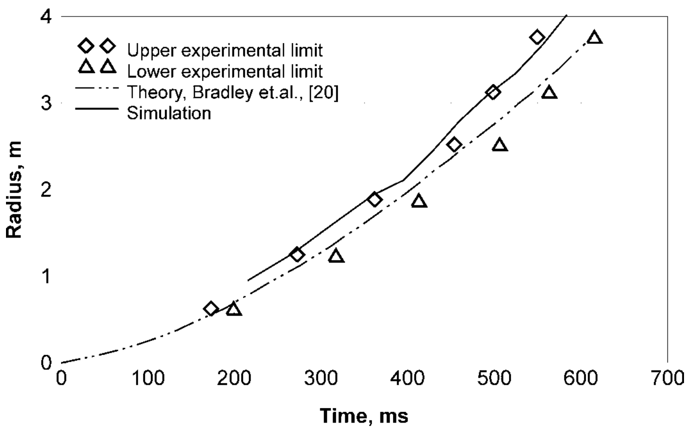

Figure 1. Flame front position along a centreline of the SOLVEX enclosure

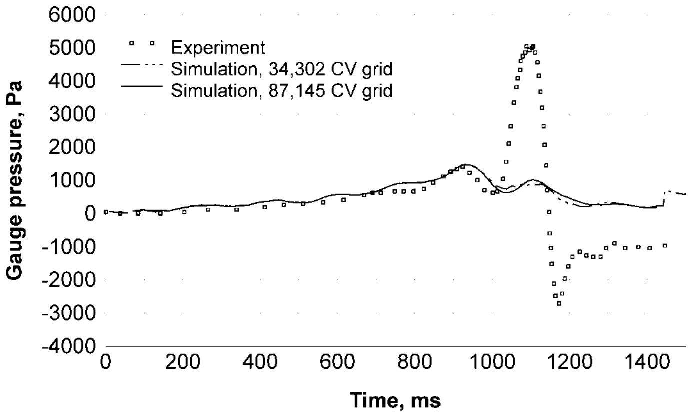

Figure 2. Experimental and simulated pressure dynamics inside the SOLVEX enclosure with SGS RNG turbulence and combustion models

that it is hard to expect that any further improvement of LES predictions of the second peak is possible with further refinement of the computational grid.

It was unclear until now what is a nature of the "unexpectedly" high second pressure peak. The reason for the high explosion overpressure could be the acceleration of turbulent combustion inside the enclosure, the effect of external explosion, when the flow through vent is choked by external pressure rise, or both these phenomena.

The simulations clearly demonstrate the formation of external vortical cloud and flame front propagation throughout it. Figure 3 shows successive snap-shots of methane mass fraction distribution in the forming vortex of combustible mixture pushed out of the enclosure. This predetermines the origin of an anisotropic component of highly turbulent combustion occurring outside the enclosure. An analysis of experimental video records established that transition to highly turbulent combustion commences when flame front touches the edges of the vent and enters highly turbulent mixing layer[7,8]. The vent structure plays the role similar to a "bluff body" or a "baffle". The mechanism of turbulent combustion outside the enclosure is different compare to initial stages of wrinkled flame propagation inside the enclosure. Apparently, the RNG SGS models, based on assumption of isotropic turbulence, cannot reproduce an "additional" increase of flame surface density due to the effect of turbulence anisotropy in the vortex and the development of subsequent SGS model is necessary.

SIMPLE MODEL OF TURBULENT COMBUSTION IN AN EXTERNAL VORTEX

As has been shown above the application of SGS RNG turbulent premixed combustion model based on the assumption of isotropic turbulence does not allow reproduction of experimental

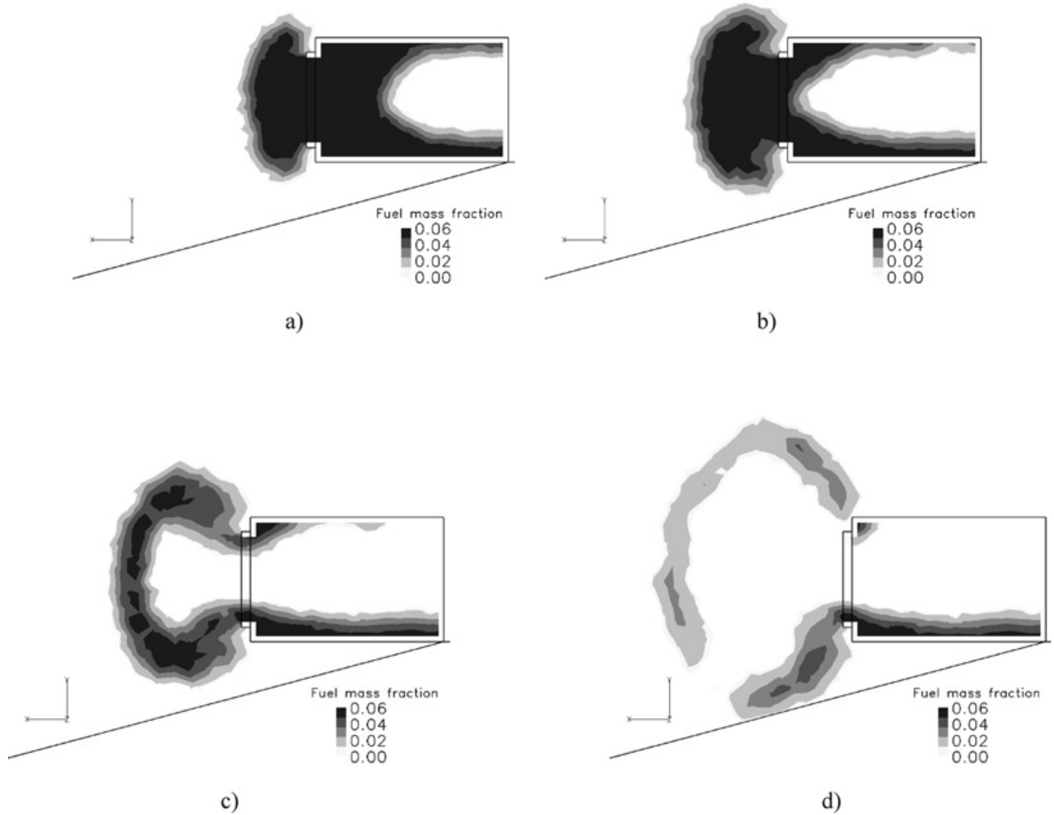

Figure 3. Formation and combustion of the external vortex (fuel mass fraction for methane; 87,145 CV grid): a) $t = 755$ ms, b) $t = 882$ ms, c) $t = 1001$ ms, d) $t = 1203$ ms

pressure transients. It was found that with such model a flame front shape outside the enclosure does not match the shape observed in experiment too[8]. Simulations confirmed the formation of a vortical structure outside the enclosure. Experimental results demonstrated that the flame surface area for methane-air mixture in a vortex in test conditions[21] is growing proportionally to the vorticity. Based on this knowledge an additional SGS factor Ξ^a_{SGS} taking into account the increase of the flame surface density due to anisotropic component of the turbulence was introduced into the combustion model in the area where the pronounced vortical structure was observed (outside the enclosure). The Ξ^a_{SGS} factor begins to grow linearly from its initial value 1, when the flame front touches the vent edge, and reaches value $\Xi^a_{SGS} = 2$ in 100 ms. It remains constant afterwards. The pressure dynamics simulations for the model with additionally introduced Ξ^a_{SGS} factor are presented in Figure 4 for both employed grids (for the coarser grid the value 1.8 was used for Ξ^a_{SGS} factor instead of 2). The introduction of this physically justified adjustment into the LES model provides nearly perfect match for the pressure dynamics inside the enclosure. After this model modification all stages of pressure development inside the vessel are reproduced with high accuracy: the initial stages of pressure growth, the first pressure peak, the second pressure peak and finally the negative pressure peak. The simulation with the modified combustion model reproduced the experimentally observed shape of developing deflagration outside the enclosure too[8]. The final stage of outside combustion can be seen in Figure 3d, when the flame front engulfs sides of the enclosure. This is in agreement with experimental observations[9] and can not be achieved with only the RNG premixed combustion model.

INTERACTION BETWEEN EXTERNAL AND INTERNAL DEFLAGRATIONS

Some reasoning on physics of coherent deflagrations is given in papers[7,8]. The LES model was used here as a "knowledge vehicle" to study the phenomenon. Figure 5 shows pressure

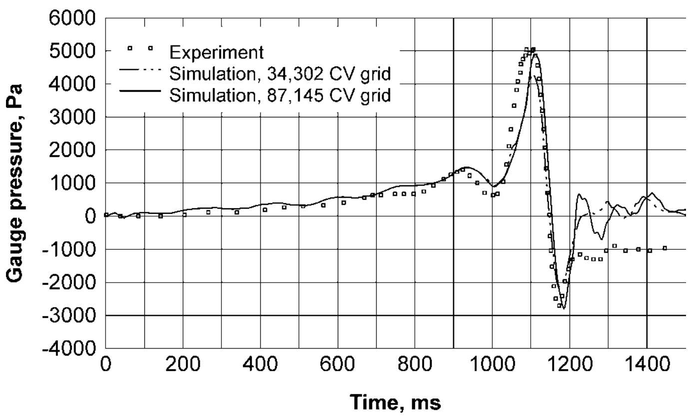

Figure 4. Experimental and simulated pressure dynamics inside the enclosure with additional flame surface density factor Ξ^a_{SGS} applied outside the enclosure for two different grids

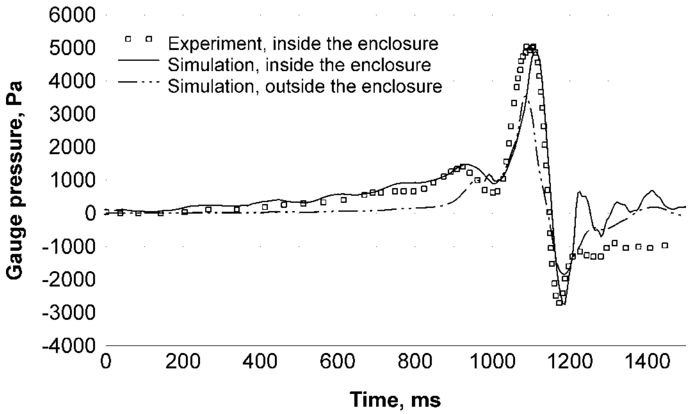

Figure 5. Experimental and simulated pressure dynamics (inside and 6.1 m outside of the enclosure) with additional flame surface density factor Ξ^a_{SGS} applied **outside** the enclosure only (87,145 CV grid)

dynamics of coherent deflagrations inside and 6.1 m outside the enclosure. Later we will see that it is the intensification of combustion in external vortex what is leading the pressure build up both inside and outside the enclosure. The mechanism is not the extra intensification of combustion inside the enclosure yet the decrease of mass outflow from the enclosure due to pressure rise outside of it as was suggested in 1987 independently by Harrison and Eyre[22] and Swift and Epstein[23] and proved later by theoretical analysis in study[24].

It was found[8] that the experimental pressure dynamics both inside and outside the enclosure could be reproduced only with additional anisotropic intensification of combustion applied to external deflagration (Figure 5). Figure 6 shows simulated pressure dynamics obtained with the same factor Ξ^a_{SGS} but applied both inside and outside the enclosure. The simulation for the case with application of Ξ^a_{SGS} factor only inside the enclosure is presented in Figure 7. It is obvious that two last cases are unsatisfactory as the positive second pressure peak is much higher than experimental one whereas the negative pressure peak is much less. Contrary, in the case of combustion intensification only beyond the enclosure both positive and negative phases of experimental pressure development are perfectly reproduced (Figure 5). This CFD based study explains that exactly the external deflagration is responsible for observed pressure growth inside and outside the enclosure.

These results give more information to designers of mitigation techniques. Particularly, the water deluge systems were demonstrated to be effective in situations, where the water spray decreased flame acceleration in confined areas[25]. In situations with external explosions the most of combustion acceleration occurs outside of area of water spray application and the effectiveness of such systems may be reduced.

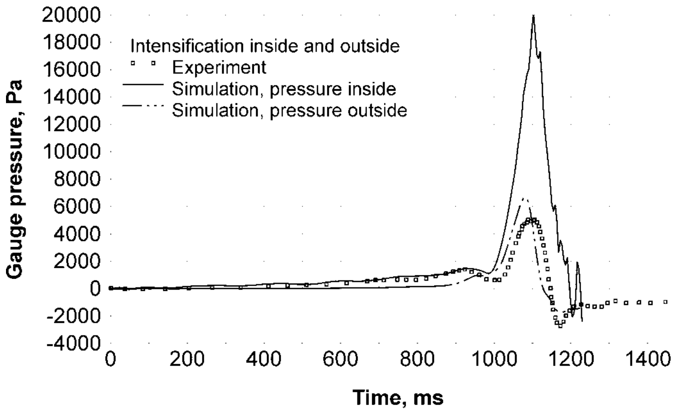

Figure 6. Experimental and simulated pressure dynamics (inside and 6.1 m outside of the enclosure) with additional flame surface density factor Ξ^{a}_{SGS} applied both **inside and outside** the enclosure (87,145 CV grid)

MODELLING OF BLAST OUTSIDE THE ENCLOSURE

The development of coherent deflagrations inside and outside the enclosure is the source of formation and outward propagation of explosion pressure wave able to affect nearby structures. The blast outside the enclosure was measured by pressure gauges at distances

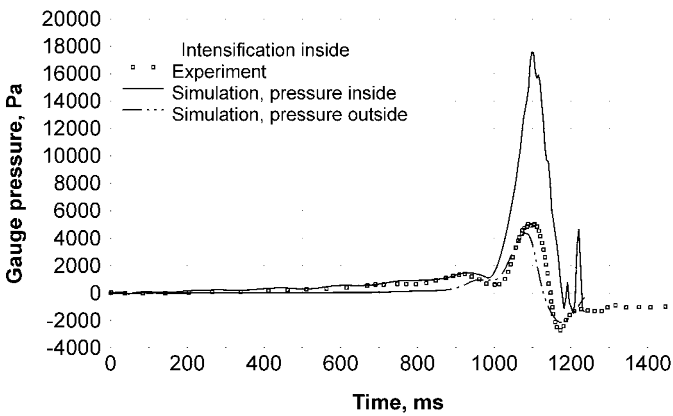

Figure 7. Experimental and simulated pressure dynamics (inside and 6.1 m outside of the enclosure) with additional flame surface density factor Ξ^{a}_{SGS} applied inside the enclosure only (87,145 CV grid)

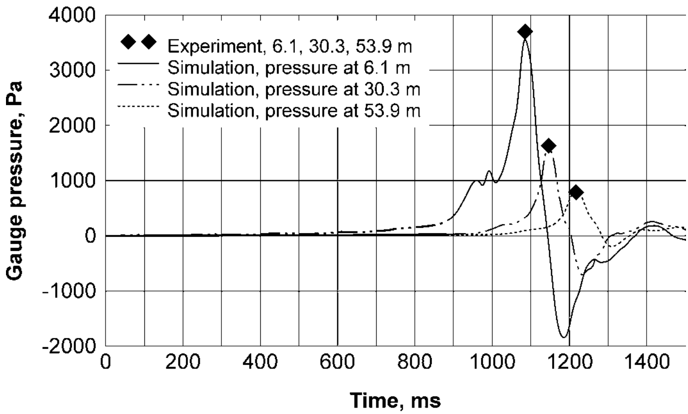

Figure 8. Experimental pressure peaks and simulated pressure dynamics outside the enclosure at locations 6.1, 30.3, and 53.9 m from the vent (87,145 CV grid)

6.1, 30.3 and 53.9 m during SOLVEX tests. Figure 8 demonstrates that the LES model perfectly reproduced pressure wave peaks at all these locations too.

CONCLUSIONS

The LES model of coherent deflagrations in a system vented enclosure–atmosphere, based on RNG SGS turbulence and premixed combustion submodels, has been developed further to account for additional intensification of turbulent combustion due to anisotropy in a vortical flow structure outside the enclosure. There was no extra mechanism required in addition to isotropic RNG SGS premixed combustion mechanism to proper model the initial stages of turbulent combustion inside the empty SOLVEX enclosure up to the moment before the second pressure peak.

The application of the LES model to processing of experimental data obtained during tests in large-scale empty SOLVEX enclosure gave a new insight into the physics of the processes involved. The intensification of combustion outside the enclosure commences in the model after the flame front touches the vent edge. It has been demonstrated that the shape of external deflagration and experimental pressure dynamics inside and outside the enclosure at different locations can be reproduced only in the case when the extra intensification of turbulent combustion is applied outside of the enclosure. It is demonstrated that without the proper modelling of the turbulent external deflagration the explosion pressure dynamics can be significantly under predicted.

The stages of coherent deflagrations from the ignition, the accelerated wrinkled flame propagation inside enclosure towards the vent, the formation of the vortex of non-uniform mixture outside the enclosure, the fully developed turbulent external combustion with simultaneous wrinkled flame propagation inside the enclosure, the development of positive and negative pressure peaks and the formation of outwardly propagating pressure wave were accurately reproduced in large eddy simulations according to modified LES model. The clarified nature of coherent deflagrations in the system vented enclosure–atmosphere pointed out directions for the development of explosion mitigation technologies by combustion suppression outside the enclosure.

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