INITIAL EVALUATION OF FLAME QUENCHING MODELING IN FLAMEFOAM

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ABSTRACT
During a severe accident, containment integrity is threatened by a possible hydrogen explosion. Hydrogen flame can be accelerated or quenched depending on the mixture, turbulence, and geometry. At present, turbulence and steam effects on flame acceleration, deceleration, and quenching are not well reproduced by the combustion models usually implemented in the tools relevant to nuclear safety.

flameFoam is our custom open-source turbulent premixed combustion solver for OpenFOAM framework. It was developed to perform fast and adequately accurate technical simulations using RANS and TFC modeling approaches. However, in such a framework, there is no accepted flame quenching model. The most common model is based on the flame stretch effect and estimates the probability that the stretching will not quench the flame. This model is parametrized by the critical rate of strain.

This model has been recently implemented in flameFoam. This paper presents the initial validation of the implemented model based on ENACCEF facility experiments available from the SARNET2 project. Results obtained with and without quenching modeling are presented and compared. The sensitivity of the obtained results to the critical rate of strain is examined in the simulations with flame quenching. Initial validation shows that the implemented model shows high sensitivity to the critical rate of strain parameter; however, this parameter is not well defined and can be used to fit the simulation results. Implemented model tends to quench the flame in the high turbulence areas, mainly the acceleration tube of the ENACCEF facility, but underestimates the quenching intensity at the exit to the dome. This results in unsatisfactory simulations outcome, showing that quenching modeling under severe accident-relevant conditions in the given framework requires further development.

Keywords: Place any keywords here

NOMENCLATURE
\( c \) combustion progress variable
\( d \) inner diameter of the obstacle
\( D \) inner diameter of the acceleration tube
\( D_{T,t} \) time-dependent turbulent diffusivity
\( G \) stretch factor
\( g \) gravitational acceleration
\( g_{cr} \) critical velocity gradient
\( h \) enthalpy
\( k \) turbulent kinetic energy
\( K \) kinetic energy
\( L \) turbulent integral length scale
\( Le \) Lewis number
\( p \) pressure
\( R_B \) obstacle blockage ratio
\( S_c \) combustion progress variable source
\( S_i \) combustion energy source
\( S_L \) laminar flame velocity
\( S_T \) turbulent flame velocity
\( S_{T,t} \) time-dependent turbulent flame velocity
\( Sc_T \) turbulent Schmidt number
\( t \) time
\( t_{fd} \) flame development time
\( t_L \) Lagrangian time scale
\( U \) velocity
\( Y_0^{H_2} \) initial hydrogen mass fraction
\( Y^{H_2} \) hydrogen mass fraction
\( Y_{\infty}^{H_2} \) final hydrogen mass fraction
\( \alpha \) molecular thermal diffusivity
\( \alpha_{eff} \) effective thermal diffusivity
\( \varepsilon \) turbulent dissipation rate
\( \eta \) Kolmogorov length scale
\( \mu_{eff} \) effective viscosity
\( \nu \) kinematic viscosity
\( \rho \) density
\( \sigma \) standard deviation of the \( \varepsilon \) distribution
\( \rho_a \) density of a fresh mixture
\( \tau_{eff} \) effective shear stress
\( \omega \) specific turbulent dissipation rate
1. INTRODUCTION

Nuclear power plants generate electricity using nuclear reactions, but accidents at these facilities can release dangerous substances into the environment. In the event of a severe accident, hydrogen may be generated in the reactor and released into the containment building. Inside the containment, the presence of hydrogen, air, and steam can create a potentially explosive mixture, threatening the integrity of the building. The severity of the explosion would depend on the combustion regime, which can vary greatly in the case of hydrogen. Developing hydrogen flame can be accelerated or quenched depending on factors such as the mixture composition, turbulence, and geometry.

The study of hydrogen flame quenching is important for nuclear safety, as steam in the containment atmosphere can promote the quenching of flame accelerating in an otherwise dangerous combustible mixture.

However, current combustion models implemented in the computational tools relevant to nuclear safety do not accurately reproduce the effects of turbulence and steam on flame acceleration, deceleration, and quenching, as was demonstrated in recent international benchmarks.

flameFoam [1–3] is a custom for OpenFOAM [4] framework-based open-source turbulent premixed combustion solver developed at Lithuanian Energy Institute. While it supports both RANS and LES modes, it is mostly intended for fast and accurate technical simulations using progress variable, RANS, and TFC [5,6] modeling approaches. In the context of nuclear safety, such simulations require capabilities to estimate both turbulent flame acceleration and quenching.

However, there is no accepted flame quenching model in the discussed framework. The most common model is based on the flame stretch effect and estimates the probability that the stretching will not quench the flame. This model is parametrized by the critical rate of strain [5]. However, even though this model has been proposed some time ago, it is still not extensively used and validated. In the frame of international benchmarks, experiments with quenched flame have been simulated in OECD NEA ISP49 [7] and EU FP7 SARNET2 [8] projects. In the SARNET2 project, it was shown that quenching can be promoted by higher contents of steam in the mixture. In both blind and open cases of these projects, no participant presented satisfactory simulation results of the quenching phase. Since then, there has been no significant improvement in application-relevant turbulent hydrogen flame quenching simulation.

This paper aims to implement a RANS/TFC-suitable quenching model into the flameFoam solver and evaluate its performance. The model is tuned by the critical velocity gradient, and the influence of this parameter on the obtained results will also be studied. The results of the performed study are useful for further development of quenching modeling capabilities for RANS/TFC combustion simulations.

The flameFoam solver and newly implemented quenching model will be presented in the second section of the paper. The third section will describe the facility and experiment selected for simulation, the fourth section will discuss the performed simulations and obtained results.

2. COMBUSTION AND QUENCHING MODELING IN FLAMEFOAM

2.1 flameFoam solver

The presented simulations were performed using the internal development version of flameFoam, a solver built on top of OpenFOAM v7. flameFoam is not a direct copy of any existing solvers, but rather a combination of standard OpenFOAM solvers rhoPimpleFoam, buoyantPimpleFoam, and chtMultiRegionFoam, enhanced with custom progress variable equation and combustion models. The current stable version of the solver has been developed and tested for the simulation of turbulent combustion in homogeneous hydrogen-air mixtures.

Base elements of flameFoam are standard buoyant compressible Navier-Stokes equations (continuity (1), momentum (2), and energy (3)) with progress variable equation (4) and combustion source terms $S_c$ and $S_t$:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{U}) = 0 \quad (1)$$

$$\frac{\partial \rho \vec{U}}{\partial t} + \nabla \cdot (\rho \vec{U} \times \vec{U}) = \nabla \cdot \vec{t}_{\text{eff}} - \nabla p + \rho \vec{g} \quad (2)$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \vec{U} h) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \vec{U} K) = \frac{\partial p}{\partial t} + \nabla \cdot (\rho \vec{U} \vec{g}) \quad (3)$$

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho \vec{U} c) = \nabla \cdot \left( \frac{\mu_{\text{eff}}}{S_T} \nabla c \right) + S_c \quad (4)$$

Progress variable $c$ is equal to the fraction of the expected burnt mixture:

$$c = \frac{\gamma S_{0}^{H_2} - \gamma H_2}{\gamma S_{0}^{H_2} - \gamma H_2} \quad (5)$$

The thermophysical properties of the mixture depending on its composition (molar mass, specific enthalpy, and others) are linearly interpolated from the properties of burnt and unburnt mixtures and the value of $c$.

The progress variable transport equation can be closed using several approaches. For RANS simulations, flameFoam supports TFC (6) and extended TFC (ETFC) (7) [9], currently in validation, models (for details and LES case, see [1,2]):

$$S_c = \rho_u S_T |\nabla c| \quad (6)$$

$$S_c = \frac{s_Q}{4(\alpha/Le + D_{T,T})} \rho_u c(1-c) + \rho_u S_{T,I} |\nabla c| \quad (7)$$

Closing progress variable equation requires estimation of turbulent flame velocity $S_T$. This can be done in several ways in flameFoam. In RANS simulations $S_T$ can be estimated using one...
of three universally accepted correlations – Zimont [6], Bradley [10], or Bray [11].

All three \( S_f \) correlations require a value of laminar flame velocity \( S_L \). flameFoam offers several methods to set \( S_L \). In the simplest case, it can be set as a user-selected constant value. In the case of lean mixtures, Malet correlation [12] can be used to estimate \( S_L \) values. And, recently, the third method has been implemented – a deep neural network based on the experimental data and valid for dry hydrogen-air mixtures [3].

### 2.2 Quenching model

In this work, the flamelet quenching through stretching model presented by Zimont et al. in [5] was implemented in flameFoam. In this model, the progress variable source term \( S_c \) is multiplied by the stretch factor \( G \) (8), which corresponds to the probability of not-quenching the flame:

\[
G = 0.5 \text{erfc} \left( - \frac{1}{2\sigma} \left( \ln \frac{15\nu g_{cr}^2}{\varepsilon} + \frac{\sigma}{2} \right) \right) \quad (8)
\]

\[
\sigma = 0.26 \ln \frac{L}{\eta} \quad (9)
\]

The model is parametrized by the critical velocity gradient \( g_{cr} \). There is no established model for the estimation of \( g_{cr} \) value for turbulent flows and, presently, this value needs to be tuned for the specific conditions [5].

### 3. ENACCEF FACILITY AND SELECTED EXPERIMENT

To evaluate the implemented model, the experiment from the ENACCEF facility in Orleans, France, operated by ICARE-CNRS was selected for the simulation. It was originally presented and published in the frame of the European Union Framework Programme 7 SARNET2 project [8].

The ENACCEF facility, schematically shown in Figure 1, consists of a vertical acceleration tube and a wider dome at the upper exit of the tube. The heights of these elements are 3.3 m and 1.9 m, respectively, and their inner diameters are 154 mm and 726 mm. In the simulated experiment [8], nine annular obstacles of 2 mm thickness were inserted at the lower part of the tube to accelerate the flame. These obstacles are characterized by the blockage ratio:

\[
R_B = 1 - \left( \frac{d}{D} \right)^2 \quad (10)
\]

The first (lowest) obstacle is located at 0.638 m from the ignition point, and the subsequent obstacles are spaced 0.154 m apart. The mixture is ignited using two thin tungsten electrodes connected to a high voltage source, 0.138 m from the bottom of the facility. The flame propagation was detected using 16 photomultipliers tubes, and the maximum pressure load was measured using 9 pressure sensors.

The experiment studied the upward flame propagation and obstacle-induced acceleration in a homogenous 13% hydrogen-30% steam-air mixture at normal conditions.
However, the intense mixing with a colder unburnt mixture causes the flame to be quenched at the exit of the acceleration tube into the dome. In the base calculations, no quenching is modeled, and the increased turbulence at the pipe exit accelerates the flame instead of quenching it.

To investigate the possibility of simulating flame quenching in this experiment, the model described in section 2.2 was implemented into flameFoam. The model is tuned by the $g_{cr}$ parameter, which needs to be set by the user. To assess the influence of the $g_{cr}$ parameter on the quenching process simulation, calculations were performed with various $g_{cr}$ values. Based on the results of the modeled flame propagation, several groups of $g_{cr}$ parameter values were identified as high, intermediate, and low. Simulation results obtained with very high values of $g_{cr}$ showed no discernible or significant differences compared to the simulations without the quenching model, and are not discussed in this paper.

Figure 3 shows the vertical flame propagation velocity profile obtained from the calculations with the quenching model and high $g_{cr}$ values (in the range of $50000 – 100000 \text{ s}^{-1}$). With these $g_{cr}$ values, the influence of the quenching model is visible but not significant. The main effect of the quenching model seems to be a decrease in the maximum flame propagation velocity values. The results in this range do not appear to be very sensitive to the value of $g_{cr}$, with a lot of overlap between the results of calculations with different $g_{cr}$ values.

Figure 4 shows the velocity profiles obtained using intermediate values of $g_{cr}$. The expected tendency of lower flame acceleration and maximal flame propagation velocity values (higher average quenching) with decreasing $g_{cr}$ values is clearly observed. However, the influence of the implemented quenching model seems to differ in the tube and dome parts of the facility. In the acceleration tube, quenching is clearly simulated, with lower $g_{cr}$ values corresponding to lower flame propagation velocities. However, in this part of the facility, the simulation of flame acceleration was already sufficiently accurate without the quenching model, and the occurrence of quenching was expected to be modeled with low probability in this region to maintain obtained results.

On the other hand, without quenching modeling, the flame propagation velocity was overestimated in the dome region, and the modeled quenching was expected to have the greatest impact there. However, even with the intermediate values of $g_{cr}$, the average simulated quenching rate in the dome seems to be very low and has little influence on the obtained results. Furthermore, this influence appears to be very stochastic, as while there is a small tendency for the peak flame propagation velocity to decrease with $g_{cr}$, the peak velocity obtained with the lowest presented $g_{cr}$ value ($15000 \text{ s}^{-1}$) is almost the same as without the quenching model.
Figure 4: Vertical Flame Propagation Velocity Profiles, Intermediate \( g_{cr} \) Values

Figure 5: Vertical Flame Propagation Velocity Profiles, Low \( g_{cr} \) Values

To further examine simulated quenching and flame propagation dynamics, a fragment of the acceleration tube (from the 5th to 8th obstacles) and the simulated turbulent kinetic energy \( (k) \) and stretch factor \( (G) \) field distributions when flame (red curve) goes past the 7th obstacle are shown in Figure 6 with \( g_{cr} \) values of a) 100000 s\(^{-1}\) and b) 15000 s\(^{-1}\). These \( g_{cr} \) values correspond to the characteristic cases of a) insignificant influence of quenching and b) significant influence in the acceleration tube only.

The flame is significantly faster in the acceleration tube in case a) compared to b) (Figures 3 and 4), resulting in more intense turbulence as well. However, the turbulent kinetic energy distributions are qualitatively similar in both cases. The relationship between \( G \) and \( k \) distributions, on the other hand, is significantly different. In case a), quenching occurs only partially \((0 < G < 1)\) and only in the regions with the highest \( k \). The majority of the flame brush is located in the \( G = 1 \) region and experiences little quenching. In b) case, quenching is strong enough to occur everywhere, at least partially. In the unburnt zone, even in regions with low turbulence, \( G \) has values below 0.5. In the burnt zone, \( G \) values are higher, likely due to higher viscosity. These results show the expected sensitivity of the quenching model to the tuning parameter \( g_{cr} \). However, surprisingly, the predicted flame propagation velocities in the dome were similar in both cases (Figures 3 and 4).
This discrepancy is explained by the examination of the corresponding vertical gas velocity component distribution, presented in Figure 8.

The vertical velocity of the gas entering the dome is above 400 m/s, which corresponds to the flame propagation velocity at this height (Figure 4). This means that the flame’s propagation velocity against the gas is already quite low and the flame is simply carried by the gas flow into the dome.

With the implemented combustion and quenching models, the following flame propagation dynamics are simulated in the presented cases: the flame is accelerated in the obstacle region of the tube, then decelerates, but is pushed together with the fast gas flow into the dome. In the experiment, the flame is quenched when entering the dome, but in the simulations, only partial quenching occurs in this region, and flame propagation is registered at the velocity of the flowing gas. This velocity depends on the previously obtained flame acceleration and partial quenching in the tube. With high \( g_{cr} \) values, flame acceleration is only slightly affected by quenching, gas velocities and flame behavior in the dome are similar to the unquenched case. With intermediate \( g_{cr} \) values, quenching starts to visibly decrease the maximum flame velocities achieved in the acceleration tube, but they are still high enough to have a fast gas flow and flame behavior in the dome is only slightly different from the unquenched case. Only with low \( g_{cr} \) values is flame acceleration in the tube suppressed enough to diminish gas flow velocities and, correspondingly, observed flame propagation speed in the dome.

These results show that the performed simulations fail to accurately capture the experimental phenomena.

One possible interpretation of the obtained results is that instead of simulating partial quenching in the tube and dome, more intense quenching should be observed in the dome, while no quenching should be observed in the acceleration tube. In this case, it is currently unclear how the quenching model itself needs to be modified to enable simulation of the presented experimental transient, or whether a dynamic definition of \( g_{cr} \) that takes into account different geometrical and mixing
conditions in the tube and its exit would help. It seems that a turbulence parameters-based model may be insufficient to predict full quenching and the influence of diluent, 30% of steam in this case, as a suppressant should be taken into account more explicitly.

Furthermore, in this case, using the stock TFC approach as it is most widely presented in the literature, it would not be possible to fully simulate quenching, even when the quenching model predicts it. When the quenching model predicts $G$ values close to zero, the combustion does not permanently terminate. Instead, the flame burning rate just drops close to zero, but as soon as the turbulence decays, the flame propagation resumes due to the still present gradient of $c$.

Therefore, in this case, further work on the problem would involve modifications to both the TFC and quenching models. The TFC model would need to be modified in a way that does not significantly increase its computational requirements but allows for the termination of combustion in the presence of a progress variable gradient. The quenching model would also need to be modified so that it can accurately predict full quenching in the dome while having little impact on flame propagation in the acceleration tube in the simulated case.

Another possible interpretation of the obtained results is that gas flow and turbulence are simulated incorrectly at the exit of the tube, leading to an incorrect prediction of flame propagation as well. Figure 9 is presented to further elaborate on this potential issue.

![Figure 9: Vertical Flame Propagation Velocity Profiles, No Quenching, 10% and 30% Steam Concentration Cases](image)

Figure 9 presents the velocity profiles from two different experiments performed with mixtures containing 10% and 30% steam. It is important to note that the simulations correctly predict the flame propagation velocity in the tube in both cases, demonstrating the effectiveness of the applied models and mesh in estimating flows and turbulence prior to flame entering the dome.

However, in the case of the 10% steam concentration, the flame reacted as a reactive turbulent jet at the exit of the tube and accelerated, unlike in the 30% steam concentration case, where it was quenched. The simulation results in the 10% case show that while the flame velocity in the upper part of the dome corresponds to the experimental results, discrepancies are observed at the exit of the tube. The flame velocity is overestimated, similarly to the 30% steam concentration case. In the experiment, flame acceleration occurs further in the dome than in the simulations. This indicates that while the applied models and mesh are generally effective in predicting flow and turbulence in these simulations, the complex conditions that arise locally when the flame enters the dome in a jet-like configuration might not be accurately simulated. Another possibility is that these conditions might exhibit partial quenching, which is not considered in the simulation.

These results highlight the need for further study to improve both the quenching modeling and the flow and turbulence modeling at the tube exit. It is important to consider multiple factors that could affect the accuracy of the simulation results, and to conduct additional tests to validate the conclusions drawn.

5. CONCLUSION

In this study, the flame propagation in a hydrogen-air mixture with 30% diluents in the ENACCEF facility was simulated using the flameFoam solver. The aim was to explore the possibility of simulating flame quenching using a well-established quenching model. The results showed that the current implementation of the quenching model did not accurately capture the experimental phenomena. Instead of low quenching probability in the tube region and complete quenching in the dome region, the model predicted partial quenching in both regions.

It is noted that the inaccuracies in the simulation could also be a result of incorrect simulation of the gas flow and turbulence at the exit of the tube. This is supported by the results of the simulations with 10% steam concentration, where the flame is carried into the dome as a reactive turbulent jet and accelerates, but the simulations overestimate the flame velocity at the exit of the tube compared to the experimental results.

Further research is needed to explore the modeling of gas flow and turbulence, as well as modifications to the flame quenching models. This includes the termination of combustion in the presence of a progress variable gradient in the TFC model, and more explicit inclusion of the diluent effect or a dynamic definition of the tuning parameter $g_{cr}$ in the quenching model.

The obtained results highlight the importance of considering multiple factors that might impact the accuracy of the simulation results.
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