A numerical simulation of hydrogen-oxygen mixture combustion in a water-cooled combustion chamber

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Abstract. The efficiency of hydrogen combustion in an oxygen environment under various conditions is considered as a fundamental part of the nuclear power plant combination with hydrogen technology. The paper analyses two computational models: The Chemical Equilibrium and Steady Diffusion Flamelet models. A numerical simulation of the hydrogen-oxygen mixture combustion at stoichiometric conditions and heat transfer process in a water-cooled combustion chamber has been performed. It is shown that the most efficient hydrogen combustion is at a pressure of 6 MPa for both models. Additionally, the peak temperature of the cooling water is observed at a pressure of around 1.75 MPa. It is established that the Steady Diffusion Flamelet model has an advantage over the Chemical Equilibrium model while the use of the latter can fail to predict a correct combustion profile.

1. Introduction
The development strategy of the Russia’s nuclear industry provides for a significant increase in the fraction of nuclear power in the European region's power grid of the country. This rises especially relevant issues such as safety and efficiency of NPPs operation to meet the base load and off-peak electricity accumulation that allows to maintain the grid frequency. Pumped-storage plants are usually used for this purpose however their construction requires special conditions that limit it. This usually implies the impossibility of the construction near NPPs.

A solution to this may be the use of a hydrogen-powered installation in the flow diagram of an NPP that allows performing the water electrolysis for the compensation of peak demands. It should also be noted that the installation can perform an important part within the scope for safety as a redundant source of power.

The efficiency of hydrogen combustion in an oxygen environment under various flow diagrams and parameters is considered as a fundamental part of the combination of nuclear power plants and hydrogen technology. Thus, the study of the hydrogen combustion efficiency in an oxygen environment for generating steam is relevant for optimizing the parameters and flow diagrams for the hydrogen installation use in NPP cycles.

However, obtaining correct values of the parameters and combustion profile of reversible multi-stage reactions requires a significant amount of computational time, and this is a limiting factor. Therefore, it is required to select the most efficient computational method in terms of accuracy and run time. The least spent time methods are Non-premixed Combustion (NPC) Chemical Equilibrium (CE) and Steady Diffusion Flamelet (SDF), the results of those have been analyzed.
2. Computational Models

2.1. Fluid Flow Model

The hydrogen combustion in an oxygen environment has been simulated at stoichiometric conditions. The calculation has been performed via the ANSYS Fluent software. The main equations to be solved include:

The steady-state continuity equation [1, 2]:

$$\nabla \cdot (\rho \cdot \mathbf{v}) = 0,$$

where $\nabla$ — the nabla operator; $\mathbf{v}$ and $\rho$ — the velocity (m/s) and the density (kg/m$^3$) respectively.

The steady-state momentum conservation equation in an inertial reference frame excluding gravity [1, 2]:

$$\nabla \cdot (\rho \cdot \mathbf{v} \cdot \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{\tau} + \mathbf{F},$$

where $p$ — the static pressure (Pa); $\mathbf{\tau}$ — the second-order stress tensor (Pa); $\mathbf{F}$ — the external volumetric forces (Pa/m).

The stress tensor is defined as:

$$\mathbf{\tau} = \eta \left[ (\nabla \cdot \mathbf{v} + (\nabla \cdot \mathbf{v})^T) - \frac{2}{3} \nabla \cdot \mathbf{v} \cdot \delta_{ij} \right],$$

where $\eta$ — the dynamic viscosity (Pa·s); $\delta_{ij}$ — the Kronecker delta.

Turbulence is computed based on the $k$-$\varepsilon$ Realizable model comprising two additional transport equations described in [1, 3].

2.2. Chemistry Model

Two models have been used to describe the chemical interaction of hydrogen and oxygen throughout combustion. The first is the NPC Chemical Equilibrium model [1, 4]. A feature of it is that it does not solve a kinetic equation for each element, and the state and profile are determined instead via a single scalar quantity $f$ called the mixture fraction:

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i, fuel} - Z_{i, ox}},$$

where $Z_i$ — the mass concentration of the $i$-th element; $Z_{i,ox}$ — the mass concentration of the $i$-th element at the oxidizer inlet; $Z_{i, fuel}$ — the mass concentration of the $i$-th element at the fuel inlet.

In this case, the mixture fraction defines the mass concentration of the hydrogen atoms in the vapor-gas mixture.

The NPC model consists of two equations for $\langle f \rangle$ — the mean mixture fraction and its standard deviation $\sqrt{\langle (f - \langle f \rangle)^2 \rangle}$:

$$\nabla \cdot (\rho \cdot \mathbf{v} \cdot \langle f \rangle) = \nabla \cdot \left( \frac{\eta_t + \eta_r}{\sigma_t} \cdot \nabla \langle f \rangle \right),$$

$$\nabla \cdot (\rho \cdot \mathbf{v} \cdot \langle f^2 \rangle) = \nabla \cdot \left( \frac{\eta_t + \eta_r}{\sigma_t} \cdot \nabla \langle f^2 \rangle \right) + C_s \cdot \eta_t \langle \nabla \langle f^2 \rangle \rangle^2 - C_d \cdot \rho \frac{\varepsilon}{k} \langle f^2 \rangle,$$

where $\sigma_t$, $C_s$, $C_d$ — the dimensionless constants equal to 0.85, 2.86, and 2.0 respectively; $\eta_t$ and $\eta_r$ — the dynamic viscosities of the laminar and turbulent flows respectively (Pa·s); $k$ and $\varepsilon$ — the turbulent kinetic energy (J/kg) and its dissipation rate (J/(kg·s)) respectively.

The second applied model is the NPC Steady Diffusion Flamelet described in [1, 5]. It, in contrast to the first, includes an equation of elements conservation and does not imply that the system is
equilibrium. This may enable to avoid incorrect results, whereas the first model fails. Nevertheless, the SDF model cannot completely characterize the process occurring in the reaction volume since pre-tabulated values of the dissipation rate are used, which are necessary to solve the equation for this model. The table of dissipation rate values has been generated via the chemical reactions shown in table 2 [6].

The steady-state energy conservation law for the combustion process of the NPC-based models, expressed as a sum of enthalpies, is represented by the following equation [1, 7]:

\[
\vec{v} \left( \rho \cdot \vec{v} \cdot \sum_{i=1}^{n} h_i \cdot Y_i \right) = \vec{v} \left[ \frac{\lambda}{c_p} \cdot \vec{v} \cdot \sum_{i=1}^{n} h_i \cdot Y_i \right] + S,
\]

where \( h_i \) – the enthalpy of the \( i \)-th element (J/kg); \( Y_i \) – the mass concentration of the \( i \)-th element; \( \lambda \) – the thermal conductivity (W/(m\(^2\)·K)); \( c_p \) – the heat capacity at constant pressure (J/(kg·K)); \( S \) – the value that accounts for the heat exchange and the radiation in the system (W/m\(^3\)).

2.3. Radiation Model
Accounting for the radiation is done by applying the \( P_1 \) – approximation used as a special case of the \( P_n \) – method based upon the angular intensity expansion in the spherical harmonics of the 1st moment. As a result, the heat flux for radiation is obtained [1, 2]:

\[
\vec{q}_\gamma = -\frac{1}{3 \cdot (\Sigma_a + \Sigma_s - \langle \theta \rangle \cdot \Sigma_s)} \vec{v} \cdot \vec{G},
\]

where \( \Sigma_a \) – the absorption coefficient (m\(^-1\)); \( \Sigma_s \) – the scattering coefficient (m\(^-1\)); \( \langle \theta \rangle \) – the mean cosine of the scattering angle in the L-frame between the wave and the medium; \( G \) – the incident radiation (W/m\(^2\)).

This function for the radiation flux \( \vec{q}_\gamma \) yields the following transfer equation:

\[
4 \cdot \alpha \cdot n^2 \cdot \sigma \cdot T^4 = -\vec{v} \cdot \vec{q}_\gamma - \Sigma_a \cdot \vec{G},
\]

where \( n \) – the refractive index of the medium the radiation interacts with; \( \sigma \) – the Stefan-Boltzmann constant, (J/(K\(^4\)·m\(^2\))).

Finally, \(-\vec{v} \vec{q}_\gamma\) is directly substituted into the energy conservation law to implement the radiation. This model makes it possible to comprise not only the Stefan-Boltzmann radiation but also the computationally inexpensive anisotropy of a scattering event in the L-frame.

3. Boundary Conditions
The applied boundary conditions are specified in table 1:

| Table 1. Simulation boundary conditions (per 1/8). |
|-----------------------------------------------|
| Parameter                          | Inlet   | Outlet |
|-------------------------------------|---------|--------|
| Mass flow rate of \( H_2 \) (kg/s)  | 3.125·10\(^{-5}\) | –       |
| Mass flow rate of \( O_2 \) (kg/s)  | 25.0·10\(^{-5}\)  | –       |
| Cooling water mass flow rate (kg/s) | 0.015   | –      |
| Gauge pressure (Pa)                | 0.0     | 0.0    |
| Temperature of \( H_2O \) (K)      | 300     | –      |

The hydrogen-oxygen mixture combustion has been simulated using a 515 mm length combustion cylindrical chamber. There are channels on the periphery for the cooling water supply. Through the cylinder axis, an oxygen nozzle is set while the hydrogen nozzles are radially set around the oxygen nozzle. The chamber interior is 500 mm long. Figure 1 shows a part of the chamber design. In order to
accelerate the computation, an 1/8 part of the chamber has been used, the periodic condition has been applied by making the pressure gradient equal to zero at the boundaries of the cut.

The chamber radius has been considered as a variable to provide the time of the mixture being inside close to a constant to obtain similar conditions for different pressures. Additionally, the sizes of the inlet nozzles have been assumed as variables too otherwise it unavoidably leads to underburning due to high velocities in the case of low pressures.

List of reactions used in simulation is specified in Table 2 [8, 9]:

| Reaction                                                                 | Reaction                                                                 | Reaction                                                                 | Reaction                                                                 |
|--------------------------------------------------------------------------|--------------------------------------------------------------------------|--------------------------------------------------------------------------|--------------------------------------------------------------------------|
| \( H + O_2 \rightleftharpoons O + OH \)                                | \( H + O_2 (+M) \rightleftharpoons HO_2 (+M) \)                          | \( H_2O_4 (+M) \rightleftharpoons 2OH (+M) \)                          | \( OH + H_2O_2 \rightleftharpoons HO_2 + H_2O \)                        |
| \( OH + HO_2 \rightleftharpoons H_2O + O_2 \)                          | \( 2HO_2 \rightleftharpoons O_2 + H_2O_2 \)                             | \( H_2O + H_2O \rightleftharpoons OH + H + H_2O \)                      | \( OH + OH \rightleftharpoons H_2O + O \)                               |
| \( O + H_2 \rightleftharpoons H + OH \)                                 | \( O + H_2 \rightleftharpoons H + OH \)                                  | \( H + HO_2 \rightleftharpoons OH + OH \)                              | \( H + HO_2 \rightleftharpoons H_2O + O \)                              |
| \( H + HO_2 \rightleftharpoons H_2 + O_2 \)                            | \( O + HO_2 \rightleftharpoons OH + O_2 \)                              | \( H_2O_2 + H \rightleftharpoons HO_2 + H_2 \)                         | \( H_2O_2 + H \rightleftharpoons H_2O + OH \)                           |
| \( H_2O_2 + O \rightleftharpoons OH + HO_2 \)                          | \( H_2 + M \rightleftharpoons H + H + M \)                              | \( O + O + M \rightleftharpoons O_2 + M \)                            | \( O + H + M \rightleftharpoons OH + M \)                              |

4. Results of Numerical Modelling

The main computation results according to the set boundary conditions are shown in table 3 and table 4.
In the concentration of CH₂CH₂CH₂CO₂H₂OCH₃CH₂CO₂, it falls. This is inconsistent with the free path of molecules at the chamber outlet.

The total concentrations of hydrogen and oxygen atoms remain close to the stoichiometric ratio of 1:8 in all the cases, this confirms the correctness of the obtained results from the point of preserving atoms.

### Table 3. Main results of SDF model calculation.

| №  | Pressure (MPa) | Mixture temperature (K) | Cooling water temperature (K) | $C_m(H_2)$ | $C_m(H_2O)$ | $C_m(O)$ | $C_m(O_2)$ | $C_m(OH)$ | $C_m(H)$ |
|----|----------------|-------------------------|--------------------------------|-------------|-------------|-----------|------------|------------|-----------|
| 1  | 6.0            | 1,903                   | 326                            | 0.0156      | 0.7726      | 0.0180    | 0.0791     | 0.1118     | 0.0023    |
| 2  | 4.0            | 1,872                   | 338                            | 0.0159      | 0.7634      | 0.0197    | 0.0837     | 0.1142     | 0.0025    |
| 3  | 3.0            | 1,820                   | 357                            | 0.0165      | 0.7589      | 0.0207    | 0.0854     | 0.1153     | 0.0027    |
| 4  | 2.0            | 1,739                   | 380                            | 0.0171      | 0.7517      | 0.0223    | 0.0888     | 0.1169     | 0.0030    |
| 5  | 1.75           | 1,717                   | 382                            | 0.0171      | 0.7490      | 0.0229    | 0.0901     | 0.1174     | 0.0030    |
| 6  | 1.5            | 1,665                   | 377                            | 0.0172      | 0.7458      | 0.0236    | 0.0919     | 0.1180     | 0.0031    |
| 7  | 1.25           | 1,596                   | 366                            | 0.0175      | 0.7430      | 0.0243    | 0.0932     | 0.1185     | 0.0033    |
| 8  | 1.0            | 1,489                   | 342                            | 0.0177      | 0.7390      | 0.0252    | 0.0952     | 0.1191     | 0.0034    |
| 9  | 0.5            | 1,310                   | 332                            | 0.0185      | 0.7282      | 0.281     | 0.1007     | 0.1204     | 0.0039    |
| 10 | 0.25           | 1,262                   | 337                            | 0.0191      | 0.7176      | 0.0310    | 0.1067     | 0.1211     | 0.0043    |
| 11 | 0.101          | 1,221                   | 338                            | 0.0199      | 0.7055      | 0.0347    | 0.1139     | 0.1210     | 0.0050    |

$C_m(x)$ – the mass concentration of the element $x$ at the chamber outlet.

Table 4 evidently shows the CE model fails to preserve mass concentrations of atoms in the case of 0.1 MPa, therefore this point is omitted.

Figure 2 presents the vapor concentration dependence at the outlet on the chamber pressure. In the case of the SDF model, it is observed that the change occurs according to a function close to exponential, and the highest vapor concentration in the mixture is achieved at a pressure of 6 MPa. A different situation is observed in the case of the CE model, whereas starting from 6 MPa the vapor concentration falls and then at the point of 2 MPa increases. This is inconsistent because decreasing pressure leads to the decline in concentrations, that is, the free path of molecules rises, and consequently this shall negatively affect the combustion efficiency. The profile for the other products of the SDF model is shown in figure 3.

As shown in figure 3 the concentrations increase following approximately an exponential law while the pressure decreases. In this case, a high concentration of OH is observed, and it increases with the pressure decline. This cannot be explained from the dissociation point inasmuch as this process shall become significant to be noticed at a temperature of above 2000°C [10], and the concentrations shall fall likewise the temperatures. However, according to the multi-step chemistry shown in table 2, it can
be concluded that such OH concentrations can be considered as a consequence of the underburning resulted from the non-equilibrium state assumption, taken into account by the SDF model and intrinsically neglected by the CE model.

![Figure 2](image1.png)

**Figure 2.** The vapor concentration of the combustion profile at the outlet: 1 – Chemical Equilibrium; 2 – Steady Diffusion Flamelet.

![Figure 3](image2.png)

**Figure 3.** The combustion profile (except H\textsubscript{2}O) for the SDF model at the outlet.

The cooling water temperature dependence on the chamber pressure is depicted in figure 4, whereas with a decrease in pressure a growth in this temperature at the outlet is observed and peaks at the region of 1.75 MPa, and then a drop is experienced until 0.1 MPa. Also, additional points have been taken near this domain to exclude the possibility of wrong set conditions.
This can be explained that the heat transferred to the surface is proportional to the heat exchange area and the temperature gradient $Q \propto S \cdot \nabla T$, hence to the set chamber radius and the temperature gradient, since the chamber length is constant. Following the data in Table 3, the chamber relative radius increases faster than the relative temperature gradient declines since it is proportional to the square root of the relative pressure, therefore a rise in the cooling water temperature would be seen, which is shown by the computation at a pressure from 6 to 1.75 MPa. However, a decrease from 1.75 to 0.1 MPa then occurs, which can be explained by a significant drop in the convective heat transfer coefficient.

How the convection heat transfer coefficient changes using the example of the SDF model is considered. The heat transfer coefficient is determined using the Nusselt criterion [11]:

$$\alpha = \frac{Nu \cdot \lambda}{d},$$

$$Nu = Re^{0.33} \cdot Pr^{0.43},$$

$$Re = \frac{w \cdot d}{\eta},$$

where $\alpha$ – the convection heat transfer coefficient (W/(m²·K)); $Nu$ – the Nusselt number; $Re$ – the Reynolds number; $\lambda$ – the thermal conductivity coefficient (W/(m·K)); $d$ – the chamber inner diameter (m); $Pr$ – the Prandtl number; $w$ – the mean velocity (m/s); $\eta$ – the dynamic viscosity (Pa·s).

Additionally, according to the condition $w \approx const$, the following can be supposed:

$$Re \propto \frac{r}{\eta}.$$

The four points at different regions of the graph are chosen to verify this behavior: 1, 1.75, 3, 6 MPa. The parameters required for the calculation at the central domain are presented in Table 5, and the calculation results – in Table 6. The thermophysical properties have been estimated according to [10]. The calculation is performed in relative units and this yields the final formulation:

$$\frac{Q}{Q_0} = \frac{(\alpha \cdot \Delta T \cdot S)}{(\alpha \cdot \Delta T_0 \cdot S_0)} = \frac{\lambda}{\lambda_0} \cdot \frac{Re}{Re_0}^{0.33} \cdot \frac{Pr}{Pr_0}^{0.43} \cdot \frac{\Delta T}{\Delta T_0}.$$
Table 5. Parameters at central part.

| Point | $P$ (MPa) | $T$ (K) | $T_{cw}$ (K) | $\eta 10^4$ (Pa·s) | $Pr$ | $\lambda$ (W/(m·K)) |
|-------|-----------|---------|--------------|-----------------|------|-------------------|
| 0     | 6.0       | 2,650   | 318          | 80              | 1.02 | 0.43              |
| 1     | 3.0       | 2,500   | 332          | 77              | 0.737| 0.47              |
| 2     | 1.75      | 2,450   | 345          | 76              | 0.728| 0.48              |
| 3     | 1.0       | 2,200   | 324          | 70              | 0.887| 0.30              |

where $T$ and $T_{cw}$ are the mixture and cooling water temperatures respectively at the central part of the chamber.

Table 6. Results of heat transfer calculation in dimensionless units.

| Point | $r$ | $\Delta T$ | $Re$ | $Pr$ | $\lambda$ | $\alpha$ | $Q$ |
|-------|-----|-------------|------|------|------------|----------|-----|
| 0     | 1.0 | 1.0         | 1.0  | 1.0  | 1.0        | 1.0      | 1.0 |
| 1     | 1.41| 0.93        | 1.46 | 0.72 | 1.09       | 0.76     | 1.005|
| 2     | 1.80| 0.90        | 1.90 | 0.71 | 1.12       | 0.66     | 1.08 |
| 3     | 2.24| 0.80        | 2.56 | 0.87 | 0.70       | 0.40     | 0.72 |

The calculation has been done using the relative units to show that the heat transfer power firstly grows and then declines, which can be seen from the last column of table 6. However, the estimation cannot completely show the heat exchange process since it has been performed for the average vapor parameters at the chamber central part.

Figure 5 reveals the temperature dependence at the chamber outlet on pressure. This graph is similar to the shape of figure 2, which is logical because the heating of the mixture is mainly determined by the amount of generated steam. At the same time, there is a slight drop on the graph in the region of 1.75 MPa in both cases, which evidently can be explained by figure 4. There is also a significantly higher temperature in the case of the CE model, which is explained by a higher concentration of the generated vapor (hence the underburning is lower) than in the SDF case.

Figure 5. The combustion products temperature at the outlet:
1 – Chemical Equilibrium; 2 – Steady Diffusion Flamelet.
5. Conclusion
As a result of the combustion modeling of the hydrogen-oxygen mixture in the water-cooled combustion chamber, it has been shown that the highest vapor concentration is achieved at the highest pressure. In this case, the combustion of hydrogen in the oxygen environment at 6 MPa is the most efficient for both computational models.

It should be also noted although the CE model results can be inaccurate at low pressures, a similar pattern of the cooling water temperature dependence has been obtained. This behavior is rather connected to the specificity of the set conditions for the modeling than to the pressure variation. Thus, using the chamber for a heating purpose at a pressure of about 1.75 MPa can be an effective but inefficient way in terms of underburning.

Besides, the SDF model includes the preservation of individual molecules, thereby this certainly has an advantage over the CE model that may lead to inaccuracies in calculation of the combustion profile, which has been shown. However, as mentioned above, the SDF model is not ideal because it does not include the chemical kinetic equations. Therefore, for more accurate results, it is necessary to perform the simulation considering chemistry based on the Arrhenius formulation. For instance, the Species Transport model, which includes the Eddy Dissipation Concept model with detailed chemistry based on the ANSYS software, may become the most suitable for this purpose. However, this model is computationally expensive to obtain reference results.

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