Numerical Simulations of Oxy-fuel Premixed Combustion in Supercritical \( \text{CO}_2 \)-diluted Environment

Abdulafeez Adebiyi\(^1\), V’yacheslav Akkerman\(^1,\ast\), and Konstantin Kemenov\(^2\)

\(^1\)Computational Fluid Dynamics and Applied Multi-Physics Center
Center for Innovation in Gas Research and Utilization (CIGRU)
Center for Alternative Fuels, Engines and Emissions (CAFEE)
Department of Mechanical and Aerospace Engineering
West Virginia University, Morgantown, WV 26506, USA
\(^2\)Symplectic Research, Inc., Atlanta, GA 30366, USA
\ast Corresponding author: vyacheslav.akkerman@mail.wvu.edu

Abstract: The design and development of advanced supercritical carbon dioxide (s\( \text{CO}_2 \)) combustors for the next-generation gas turbines require deeper understanding of the flame dynamics and morphology at highly \( \text{CO}_2 \)-diluted supercritical conditions. For this purpose, in the present work, we scrutinize the key parameters of supercritical oxy-methane premixed combustion, such as the velocity, thickness, and internal structure of the flame front. The analysis is performed by means of numerical simulations of the reacting flow equations with fully-compressible hydrodynamics, transport properties (heat conduction, diffusion and viscosity), and one-step Arrhenius chemical kinetics. The real-gas thermodynamics and molecular properties are incorporated into a reacting-flow Navier-Stokes solver along with the Peng-Robinson (PR) equation of state (EoS). It is shown that an increase in the \( \text{CO}_2 \)-dilution rate makes the flame front thicker and reduces the unstretched laminar flame speed, as compared to non-diluted oxy-combustion. Starting with planar flames (attained by means of the slip boundary conditions at the computational domain), the analysis is then extended to corrugated ones (attained by non-slip walls of the computational domain). While the corrugated flame generally spreads faster than the planar one of similar thermal-chemical characteristics, the corrugated flame velocity not only reduces with a dilution rate, but also depends on a channel width.

Keywords: supercritical \( \text{CO}_2 \) combustion, laminar premixed flames, Peng-Robinson EoS.

1. Introduction

The future generation of the fossil-fuel power systems is expected to be highly efficient to operate and exhibit extremely low (or zero) emission levels to address environmental concerns and comply with stricter government regulations. A promising technology to achieve such goals is to utilize supercritical \( \text{CO}_2 \) (s\( \text{CO}_2 \)) as the working fluid in thermal power cycles. For example, the thermal cycle efficiency in the s\( \text{CO}_2 \)-based Brayton power cycle can attain a value of 50\%, and above [1], while the higher density of the working s\( \text{CO}_2 \) fluid can potentially decrease the overall size of turbomachinery in comparison with a conventional steam (Rankine) power cycle. Moreover, the s\( \text{CO}_2 \)-based power cycles are suitable for implementation in zero-emission, fossil-fuel plants based on the oxy-combustion process which can use either pulverized coal or natural and synthesis (syngas) gases. In addition, the direct-fired s\( \text{CO}_2 \) cycle, where s\( \text{CO}_2 \) fluid resides in direct contact
with combustion sources, offers some additional benefits including the facilitation of CO₂ capture and sequestration, higher cycle thermal efficiency, and potentially simpler designs. The design and development of the future sCO₂ combustors for direct-fired cycles requires deeper understanding of flame propagation under highly CO₂-diluted conditions in supercritical environment, where typical pressure and temperature are around 300 atm and 1100 K, respectively. Such a combination of conditions is unique, poses challenges for researchers, and remains largely unexplored.

While studies of the CO₂-dilution impacts on premixed flames at supercritical conditions are virtually non-existent, the topic has been extensively studied at the atmospheric conditions (or at the typical gas turbine pressure levels) experimentally for various fuel mixtures based on CH₄ [2-5], or H₂/CO (syngas) [6-9]. The main driving force behind this research is the attractiveness of oxy-combustion technology to revamp the existing air-powered industrial burners. In oxy-combustion, air is substituted with pure oxygen diluted with recycled flue gas consisting primarily of CO₂ and H₂O to reduce the flame temperature.

2. Governing Equations

The present direct numerical simulation (DNS) studies were conducted with an in-house research code, which solves a 2D system of the governing equations for a compressible reactive mixture. The code was proven to be robust and effective in numerous applications associated with aero-acoustics and combustion and was modified to include the real-gas thermodynamics, molecular properties, as well as the Peng-Robinson (PR) equation of state (EoS). In the general two-dimensional (2D) form, with respect to \((r,z)\) coordinates, the governing equations include the continuity, momentum, and total energy equations. In addition, the reactive progress variable equation was employed and written as:

\[
\frac{∂(ρY_F)}{∂t} + \frac{1}{r} \frac{∂}{∂r} \left[ r \left( ρu_r Y_F - \frac{µ_r}{Sc} \frac{∂Y_F}{∂r} \right) \right] + \frac{∂}{∂z} \left[ ρu_z Y_F - \frac{µ_z}{Sc} \frac{∂Y_F}{∂z} \right] = - \frac{ρY_F}{τ_R} \exp \left( -\frac{E_a}{R_uT} \right), \tag{1}
\]

where \(γ = 0\) for the 2D-planar Cartesian geometry and \(γ = 1\) for the cylindrical-axisymmetric geometry, respectively. A global one-step reaction mechanism representing methane CH₄ oxidation is assumed,

\[
CH_4 + 2O_2 + nCO_2 \rightarrow 2H_2O + (1+n)CO_2, \tag{2}
\]

with an Arrhenius-like reaction rate as shown in Eq. (1). Dilution is defined based on the molar fraction of CO₂ in the oxidizer stream as \(β = n/(n+n_{O_2}) = n/(n+2)\), where \(n\) and \(n_{O_2}\) denote the number of moles of diluted CO₂ and O₂, respectively. The reactive progress variable can be defined based on the mass fractions of the reactants and diluent as \(Y = Y_F + Y_{CO_2,d}\), where \(Y_F = Y_{CH_4} + Y_{O_2}\), and \(Y_{CO_2,d}\) is the mass fraction of the diluted CO₂ in the reactants. Consequently, the reactive progress variable \(Y\) monotonically changes between the unity value in the fresh reactants and some value \(Y^* = Y_{CO_2,d} >= 0\) in the fully burnt mixture, respectively, where \(Y^* = 0\) corresponds to the pure undiluted case with \(β = 0\). It is further remarked that in the progress variable transport equation, Eq. (1), the reaction rate explicitly depends on \(Y_F\) only. In this manner, the diluted portion of CO₂ in the unburnt mixture, \(Y_{CO_2,d}\), will play the role of inert gas such that it does not participate in the chemical reaction but affects all other thermal and physical processes. In this work, the PR EoS [10] is adopted to characterize the real gas effects at the supercritical conditions:

\[
P(T,v_m) = \frac{R_uT}{v_m-b} - \frac{a(T)}{v_m(v_m+b)+b(v_m-b)}, \tag{3}
\]
where \( v_m \) is the molar volume, \( R_d \) is the universal gas constant, and the cumulative quantities \( a \) and \( b \) for a mixture are given by the quadratic and linear mixing rules:

\[
    a(T) = \sum_{i=1}^{N} \sum_{j=1}^{N} X_i X_j (a_i a_j (1 - k_{ij}))^{1/2}, \quad b = \sum_{i=1}^{N} X_i b_i.
\]  

(4)

Here, \( X_i \) is the mole fraction of species \( i \), \( N \) is the total number of species, and \( k_{ij} \) characterize the binary interactions between species \( i \) and \( j \):

\[
    a_i = 0.45724 \frac{R_d^2 T_{c,i}^2}{P_{c,i}} \left[ 1 + (0.37464 + 1.5422 \omega_i - 0.26992 \omega_i^2) \left( 1 - T_{r,i}^{1/2} \right) \right]^2, \quad b_i = 0.0778 \frac{R_d T_{c,i}}{P_{c,i}},
\]  

(5)

where for species \( i \) the respective critical pressure and temperature are \( P_{c,i} \) and \( T_{c,i} \), with the reduced temperature \( T_{r,i} = T/T_{c,i} \), and the Pitzer’s acentric factor \( \omega_i \). In particular, the following acentric factors are employed in this work: \( \omega_{CH_4} = 0.01142 \), \( \omega_{O_2} = 0.0222 \), \( \omega_{CO_2} = 0.344 \), \( \omega_{H_2O} = 0.22394 \). As for the binary interaction parameters, they are taken to be \( k_{ij} = 0 \) for \( i = j \), while otherwise, \( k_{CH_4,O_2} = 0.03 \), \( k_{CH_4,CO_2} = 0.0919 \), \( k_{CH_4,H_2O} = 0.5 \), \( k_{CO_2,O_2} = 0.0015 \), \( k_{H_2O,CO_2} = 0.0046 \), and \( k_{H_2O,CO_2} = 0.1896 \). The mole fractions for each species are calculated from the progress variable \( Y_F \) as \( X_{CH_4} = Y_F/3 \), \( X_{O_2} = 2Y_F/3 \), \( X_{H_2O} = 2(1 - Y_F)/3 \), and \( X_{CO_2} = (1 + n - Y_F)/3 \), with \( Y_F \) changing in the range \( 0 \leq Y_F \leq 3/(3+n) \). Obviously, in the case of no dilution \(( n = \beta = 0 \) we have \( 0 \leq Y_F \leq 1 \) and \( X_{CO_2} = (1 - Y_F)/3 \).

Molecular viscosity of the mixture is calculated employing the dense-gas Lucas model [11], which has often been used in the supercritical combustion DNS studies. The other transport properties such as thermal conduction and molecular diffusivity are computed based on the Prandtl, Pr, and Schmidt, Sc, numbers which are taken to be \( Pr = Sc = 1 \) such that the Lewis number is \( Le = Sc/Pr = 1 \) to avoid the diffusional-thermal instability. The specific heats are implemented as:

\[
    C_V = C_{V, id}(T) + C_{V, real}(T, v_m), \quad C_p = C_{P, id}(T) + C_{P, real}(T, v_m),
\]  

(7)

where the ideal gas components are computed using the NASA polynomial approximations [10], while the real gas correction is given by:

\[
    C_{V, real}(T, v_m) = \frac{T d''}{b \sqrt{8}} \ln \left( \frac{v_m + b(1 + \sqrt{2})}{v_m + b(1 - \sqrt{2})} \right),
\]  

(8)

and \( C_{P, real} \) is computed from the PR EoS as:

\[
    C_{P, real}(T, v_m) = C_{V, real}(T, v_m) - T \left( \frac{\partial P}{\partial T} \right)_{v_m}^2 \left( \frac{\partial P}{\partial v_m} \right)_T.
\]  

(9)

3. Computational Configuration

The governing equations are integrated employing a cell-centered, finite-volume computational scheme in the plane Cartesian geometry \(( \gamma = 0 \) ). The scheme is of the 2nd-order accuracy in time,
and it features the 4th-order accurate discretization for the convective terms and the 2nd-order accurate discretization for the diffusive terms, respectively. Specifically, we deal with a semi-open 2D channel such that one (left) end of the channel is closed, and an initially planar flame front propagate from the closed end to the open (right) one. The non-reflecting boundary conditions are implemented at the open end. As for the upper and lower boundaries ("walls"), they are adiabatic ($n \cdot \nabla T = 0$), and either slip ($n \cdot u = 0$), to keep the flame shape planar, or non-slip ($u = 0$), which distorts the flame front. Here $n$ is the unit normal vector at the walls. The channels of widths $D = 5 \mu m$ and $10 \mu m$ are considered.

A structured rectangular mesh was employed with the cell sides being parallel to the radial and axial directions. The mesh is adaptive, to ensure that the flame is always kept within a fine grid zone, such that the axial size of the computational domain changes dynamically and follows the leading pressure wave. The 3rd-order splines are employed to re-interpolate the variables during a periodic grid reconstruction to preserve the 2nd-order accuracy of the numerical scheme. The grid size is chosen to ensure that the internal flame structure is resolved, with several grid points embedded in the flame front. In the majority of the present high-pressure simulations, the finest grid size was as small as $0.1 \mu m$. The appropriateness of such a resolution is justified by the resolution test discussed below.

4. Results and Discussion

4.1 Planar Flames

In this subsection, we employ the slip boundary conditions at the walls to ensure planar flame propagation. To validate the computational platform, we first considered the conventional conditions (the initial temperature of the fuel mixture is $T_f = 300$ K and pressure is $P = 1$ atm), with the ideal-gas (ID) EoS, in order to reproduce the experimental measurements of the unstretched laminar flame speed for the stoichiometric oxy-methane mixture [12], which was found to be about $S_L = 2.9$ m/s. This experimental result was reproduced by the lowest curve in Fig. 1a. The computational thermal-chemical parameters chosen to obtain this particular value of $S_L$ were chosen as follows: the activation energy $E_a = 126.885 kJ/kg$, and the energy release from the reaction $Q = 4896.577 kJ/kg$.

We next extended our analysis to the elevated initial temperature of $T_f = 800$ K, but keeping the atmospheric pressure, and compare the ID and PR EoS models. The results are shown by the two upper curves in Fig. 1a. We observe a substantial increase of the laminar flame speed as compared to the room temperature conditions with values of $S_L$ being about 10 m/s, approximately. It is also seen that in both PR and ID cases, the laminar flame speed values are well correlated with the $S_L$ for the PR case being little smaller in magnitude. Obviously, such a correlation is expected as long as the pressure is strongly subcritical.

However, the situation conceptually changes when we extend the investigation to the supercritical conditions. This consideration starts by Fig. 1b, which provides the resolution test for stoichiometric oxy-methane combustion (with no dilution) at $P = 300$ atm and $T_f = 800$ K (this is considered to be the "master-case" for the present work). Specifically, the time evolution of $S_L$ is shown in Fig. 1b, for three various mesh sizes, namely: $\Delta x = 0.05 \mu m$, $0.1 \mu m$ and $0.2 \mu m$. It is seen that all three meshes yield essentially the same value of $S_L$, about 1.11 m/s, approximately, thereby justifying that the resolution of $0.1 \mu m$ was be reasonable to be employed in the
rest of simulations, for given $P = 300$ atm and $T_f = 800$ K. In fact, this grid resolution is in good agreement with that provided by the characteristic flame thickness $\delta_f$. Indeed, the latter quantity is traditionally defined as

$$\delta_f = \mu_f / \text{Pr} \rho_f S_L,$$

(10)

where $\mu_f$ and $\rho_f$ are the dynamic viscosity and density in the unburnt matter. In our case, this formula yields $\delta_f \approx 0.3 \mu m$ such that we have about three grid cells per $\delta_f$ with the grid size $\Delta x = 0.1 \mu m$, which is reasonable. It should be also noted, in this respect, that the quantity (10) is only a parameter of the length dimension (a characteristic transport length scale), while the real size of the burning zone may substantially exceed $\delta_f$. For this reason, in the present study we used an alternative estimation for the flame thickness defined as:

$$L_F = (T_b - T_f) / |\nabla T|_{max},$$

(11)

which better reproduces the width of the temperature gradient field. We next investigated the impact of the CO$_2$-dilution on the supercritical laminar flame propagation. For this purpose, we performed the simulation runs for the dilution rate in the range of $0 \leq \beta \leq 0.8$. The results are presented in Figs. 2-5. In particular, Fig. 2 exhibits the effect of dilution on the laminar flame speed. Here, the time evolution of $S_L$ is shown in Fig. 2a for various dilution rates, $\beta = 0\%, 20\%, 40\%, 60\%$ and $80\%$, while Fig. 2b presents $S_L$ versus $\beta$. It is seen that the dilution diminishes the laminar flame velocity significantly, namely, $S_L$ reduces almost twice at $\beta = 40\%$, as compared to that at $\beta = 0$, and it drops to a small value, $S_L \approx 0.06$ m/s at $\beta = 80\%$. This effect is due to the fact that while an inert diluent does not participate in the combustion reaction, it nevertheless participates thermodynamically by absorbing the energy released from the reaction. It is also of interest to investigate the internal flame structure for various dilution rates. This question is addressed in Figs. 3 and 4. Specifically, Fig. 3 presents the instantaneous profiles of the progress variable $Y$, while the respective instantaneous temperature profiles are shown in Fig. 4.
Figure 2: (a), (left): Time evolution of the unstretched laminar flame speed $S_L$ for various dilution rates $\beta = 0\%, 20\%, 40\%, 60\%$ and $80\%$; and (b), (right): $S_L$ vs $\beta$. $P = 300$ atm and $T_f = 800$ K in both cases.

Figure 3: Instantaneous profiles of the progress variable $Y$ for $P = 300$ atm, $T_f = 800$ K and various dilution rates $\beta = 0\%, 20\%, 40\%, 60\%$ and $80\%$.

In addition, based on the results of Fig. 4b, presents the adiabatic flame temperature $T_{ad}$ versus the dilution rate $\beta$. The plots and outcomes of Figs. 4a and 4b, generally resemble that of Figs. 2(a,b): the presence of the inert diluent consumes the energy form the combustion reaction, and thereby diminishes the adiabatic flame temperature significantly, from $T_{ad} \approx 3000$ K at $\beta = 0$ till $T_{ad} \approx 1600$ K at $\beta = 80\%$. The dependence of $T_{ad}$ on $\beta$ is near-linear for $\beta \leq 60\%$, but it substantially drops thereafter.

One more result observed in Figs. 3 and 4 is that an increase in $\beta$ makes the $Y$- and $T$-profiles smoother by reducing the gradients of temperature and progress variable fields which leads to thickening of the flame front. To address this point in more details, Fig. 5 shows the flame thickness $L_f$, defined based on the temperature gradient, Eq. (11), versus the dilution rate $\beta$. It is seen that the flame front gets thicker as $\beta$ increases. Again, the dependence is practically linear up to $\beta \leq 60\%$, but it drastically rises thereafter. To be specific, being $L_f \approx 0.85 \mu m$ in the case of no dilution, the
Figure 4: (a), (left): Instantaneous temperature profiles inside a flame front for various dilution rates $\beta = 0\%, 20\%, 40\%, 60\%$ and $80\%$; and (b), (right): the adiabatic flame temperature $T_{ad}$ vs $\beta$. $P = 300$ atm and $T_f = 800$ K in both cases.

flame thickness attains the value of $L_f \approx 1.2 \mu m$ at $\beta = 60\%$ and even $L_f \approx 2.2 \mu m$ at $\beta = 80\%$. It is noted that all these values of $L_f$ significantly exceed the value of $\delta_f \approx 0.3 \mu m$ given by Eq. (10). This provides another justification for the grid resolution $\Delta x = 0.1 \mu m$ employed in the present work. Indeed, we have from 8 (in the case of no dilution) till 22 (for $\beta = 80\%$) grid cells inside the burning zone, which is enough to resolve the flame front.

4.2 Corrugated Flames

In the previous subsection, we have demonstrated that the CO$_2$-dilution diminishes the velocity and temperature of a supercritical oxy-methane flame, and it makes burning zone thicker. In other words, the dilution mitigates oxy-methane combustion, with a risk of extinction. How to prevent this effect? The primary idea is to facilitate combustion and promote the flame propagation velocity by means of distortion of the flame shape. Indeed, it is well known that a corrugated flame has a larger surface area relative to a planar one involving the same mixture and under the same conditions. Thus, it is expected to consume more fuel per unit time and release more heat, thereby propagating more rapidly. In particular, flames in tubes are known to accelerate due to wall friction. However, the effect depends on a tube/channel width, the flame thickness and their ratio. On the one hand, a flame front is known to accelerate faster in a narrower channel than in a wider one. On the other hand, a finite (and noticeable) flame thickness may work against this trend because the wider the flame front is, the harder to corrugate it. The latter, however, will depend on the dilution rate which thickens the flame front. Consequently, a nontrivial interplay between the dilution rate and the channel width is expected, and this constitutes the focus of the present subsection.

The slip boundary conditions of the previous subsection are replaced now with the non-slip ones, in order to generate a corrugated flame front and scrutinize its dynamics and morphology. Two channels, of widths $D = 5 \mu m$ and $10 \mu m$ are considered, with various dilution rates, $\beta = 0\%, 20\%, 40\%, 60\%$ and $80\%$, in both cases. The initial conditions are kept to be $P = 300$ atm and $T_f = 800$ K. We start the analysis of corrugated flames with the temperature snapshots of Fig. 6 which shows the evolution of a non-diluted flame ($\beta = 0$) in a channel of width $D = 5 \mu m$.
Sub Topic: IC and GT Engines

Figure 5: The flame thickness evaluated by Eq. (11) vs the dilution ratio $\beta$ for $P = 300$ atm and $T_f = 800$ K.

Figure 6: Consecutive color temperature snapshots describing a corrugated flame evolution in a channel of width $D = 5 \mu m$ in the case of no dilution ($\beta = 0$) with $P = 300$ atm and $T_f = 800$ K.
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Figure 7: Time evolution of the instantaneous corrugated flame velocity \( S_w \) [(a), (left)] and scaled flame surface area (length) \( A_F/D \) [(b), (right)] in a channel of width \( D = 5 \mu m \) for various dilution rates \( \beta = 0\%, 20\%, 40\%, 60\% \) and 80\%, with \( P = 300 \) atm and \( T_f = 800 \) K in all cases.

Obviously, the flame surface area (and thereby propagation velocity) are promoted in the course of flame acceleration.

We next quantify this effect by means of the plots in Figs. 7-13. In particular, Fig. 7a compares the time evolution of the corrugated flame velocities \( S_w \) in a channel of width \( D = 5 \mu m \) for various dilution rates in the range \( 0 \leq \beta \leq 0.8 \). For simplicity, \( S_w \) is evaluated here by means of the flame tip velocity, which is a reasonable approximation accounting for a moderate and self-similar manner of flame propagation/acceleration. Figure 7a shows that for all dilution rates the \( S_w \) values eventually exceed the corresponding \( S_L \) values (for the same \( \beta \)) several times. On the other hand, the larger values of \( \beta \) are, the lower \( S_w \), and the slower the acceleration trends are. Figure 7b shows the time evolution of the scaled flame surface area (taken to be the length of the flame front in 2D), \( A_F/D \). It is seen that qualitatively, the flame speed evolution is well correlated with the flame length evolution, such that the corresponding plots in both figures show similar trends (at fixed \( \beta \)). Nevertheless, \( S_w \) is not exactly proportional to \( A_F/D \): (i) because of the impact of the final flame thickness, and (ii) because the flame tip velocity still slightly differs from the total burning rate. Overall, both Fig. 7(a,b) supports the observation that the corrugated flames accelerate, but the dilution diminishes the flame propagation speed and acceleration.

Figures 8(a,b) are the counterparts of 7(a,b) but for a twice wider channel, \( D = 10 \mu m \). All the trends here are qualitatively the same as in Fig. 7, the corrugated flame accelerates, but the higher values of the dilution mitigates flame propagation, and moderates its acceleration. At the same time, it follows that an increase in the channel width also weakens the flame acceleration. Indeed, all the quantities and trends of Fig. 8 are a little lower than that of Fig. 7.

To scrutinize this effect further, we also compared the corrugated flame speed \( S_w \) and scaled flame length \( A_F/D \) time evolution in two channels with \( D = 5 \mu m \) and 10 \( \mu m \), and with different dilution rate \( \beta \). This is shown in Figs. 9-13 for \( \beta = 0\%, 20\%, 40\%, 60\% \) and 80\%. In all cases, the solid lines represent the narrower channel, \( D = 5 \mu m \), while the wider channel, \( D = 10 \mu m \) is shown by the dashed lines. In line with our expectations, it is seen that an increase in the channel width moderates flame acceleration in all the cases considered. Nevertheless, the effect is minor in the case of high dilution such as \( \beta = 80\% \).
Figure 8: Time evolution of the instantaneous corrugated flame velocity $S_w$ [(a), (left)] and scaled flame surface area (length) $A_F/D$ [(b), (right)] in a channel of width $D = 10\mu m$ for various dilution rates $\beta = 0\%, 20\%, 40\%, 60\%$ and $80\%$, with $P = 300$ atm and $T_f = 800$ K in all cases.

Figure 9: Time evolution of the instantaneous corrugated flame velocity $S_w$ [(a), (left)] and scaled flame surface area (length) $A_F/D$ [(b), (right)] in the channels of width $D = 5\mu m$ (solid, blue) and $10\mu m$ (dashed, red) in the case of no dilution ($\beta = 0$) with $P = 300$ atm and $T_f = 800$ K.

Figure 10: Time evolution of the instantaneous corrugated flame velocity $S_w$ [(a), (left)] and scaled flame surface area (length) $A_F/D$ [(b), (right)] in the channels of width $D = 5\mu m$ (solid, blue) and $10\mu m$ (dashed, red) for the dilution rate $\beta = 20\%$ with $P = 300$ atm and $T_f = 800$ K.
Figure 11: Time evolution of the instantaneous corrugated flame velocity $S_w$ [(a), (left)] and scaled flame surface area (length) $A_F/D$ [(b), (right)] in the channels of width $D = 5\mu m$ (solid, blue) and $10\mu m$ (dashed, red) for the dilution rate $\beta = 40\%$ with $P = 300$ atm and $T_f = 800$ K.

Figure 12: Time evolution of the instantaneous corrugated flame velocity $S_w$ [(a), (left)] and scaled flame surface area (length) $A_F/D$ [(b), (right)] in the channels of width $D = 5\mu m$ (solid, blue) and $10\mu m$ (dashed, red) for the dilution rate $\beta = 60\%$ with $P = 300$ atm and $T_f = 800$ K.

Figure 13: Time evolution of the instantaneous corrugated flame velocity $S_w$ [(a), (left)]; and scaled flame surface area (length) $A_F/D$ [(b), (right)] in the channels of width $D = 5\mu m$ (solid, blue) and $10\mu m$ (dashed, red) for the dilution rate $\beta = 80\%$ with $P = 300$ atm and $T_f = 800$ K.
5. Conclusions

In the present work, we explored the key parameters of supercritical oxy-methane premixed combustion, such as the flame speed, flame thickness, and internal structure of the flame front. The analysis is performed by means of the 2D numerical simulations of reacting mixtures with fully-compressible hydrodynamics, transport properties (heat conduction, diffusion and viscosity), and the one-step Arrhenius chemical kinetics. The real-gas thermodynamics and molecular properties are incorporated into a reacting-flow Navier-Stokes solver along with the Peng-Robinson EoS.

It is shown that an increase in a CO₂-dilution rate makes a flame front thicker and reduces the laminar flame speed significantly, as compared to non-dilated combustion. Starting with the planar flames, the analysis is then extended to the corrugated ones. While the corrugated flame generally propagates faster than the planar one of similar thermal-chemical characteristics, the corrugated flame velocity not only reduces with the dilution rate, but also depends on the channel width.

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