THE ACOUSTIC RESPONSE OF REACTING SPRAYS IN CROSS FLOW MODELS TO FORCED EXCITATIONS

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Thermo-acoustic instabilities can occur in combustion systems due to unsteady heat release. The derivation of transfer functions is a method to describe the systems dynamics, which is applied to analyse and to control these instabilities. In this work, validated models for spray atomization, evaporation and combustion in OpenFOAM are used to investigate their response to acoustic forcing. Mono-frequency excitations are employed, with a frequency range from 100Hz to 1000Hz in 100 Hz intervals. The fuel considered in this study is hexadecane, for which a reduced kinetic mechanism is available. A primary atomization model, together with a secondary atomization model, is employed to simulate a spray in cross flow. The evaporation model is a zero-dimensional model developed for multicomponent droplets at high ambient pressures and temperatures. The combustion model comprehends a blend of the FGM (Flamelet Generated Manifold) and the SCRS (Simple Chemical Reaction System) models. The acoustic response of each model, in terms of its transfer function, is determined by applying forcing at the inlet boundary. The penetration and global SMD are monitored at 80 mm downstream from the injection point and forcing frequencies are clearly found in the response of both quantities. The rate at which the droplet diameter shrinks is tracked in the droplet vaporization, and a non-linear response is encountered due to its dependence on the relative velocity. Similarly, the heat release is used for 1-D premixed flames, showing forcing frequencies in the model response too.

1. Introduction

Lean premixed combustion systems are predominant in modern heavy duty gas turbines due to increasing restrictions of combustion emissions [1]. Lean operation leads to low flame temperatures and therefore to low NOx production. Drawbacks of this technology are flame quenching, auto-ignition and flashback. Furthermore, lean premixed combustion systems are prone to unsteady heat release that can trigger thermo-acoustic instabilities [2, 3]. The interaction between pressure waves and unsteady heat release drive the oscillations, resulting in noise and vibration that can induce severe damage to the engine. For this reason, analyses of flame dynamics, i.e. thermo-acoustics, are essential for advanced gas turbine engine development. A sophisticated method to analyse the thermo-acoustic stability is found by the forced response approach. The flame is excited artificially and the response on velocity perturbations is used to determine the Flame Transfer Function (FTF) [4, 5]. This gives a relationship between the heat release and the velocity fluctuations. Transfer functions of reacting flows can be obtained by means of Computational Fluid Dynamics (CFD). To predict combustion instabilities correctly, Large Eddy Simulations (LES) are found to be a convenient
method [6]. The determination of transfer functions helps to describe the systems dynamics and to control instabilities.

This work aims to investigate the thermo-acoustic behaviour of models to simulate a spray flame for gas turbine fuel oil operation. The examined processes are the breakup and secondary atomization of a liquid jet in cross flow, the evaporation and mixing of the formed droplets and the combustion of the fuel-air mixture. For this, the acoustic response of previously validated models for spray atomization, evaporation and combustion to forced excitation are analysed using the CFD tool OpenFOAM.

The atomization model, reviewed in [7] and by Guildenbecher et al [8], considers jet breakup, primary and secondary atomization. The impact of forced excitation has been experimentally examined by Anderson et al. [9] for the process of fuel oil disintegration, providing information on the acoustic response for the investigated fuel injector. The introduction of acoustic perturbations to the liquid fuel jet in cross flow was investigated by Anderson et al. [10]. Song et al. [11] stated that the liquid jet atomization is enhanced by an oscillating crossflow, resulting in a greater number of smaller droplets (i.e. SMD). For the droplet breakup and evaporation, investigated in [7] and by Cossali et al. [12] and Moon et. al [13], the droplet surface shape is strongly influenced by acoustic waves and consequently the evaporation is enhanced.

An introduction to spray combustion is given by Tanner in [7], where different schemes and approaches for combustion modelling are discussed. The droplet evaporation and combustion processes are introduced by Law [14]. Ha [15] investigated the evaporation and combustion of a single droplet under oscillating flow. The magnitude of the relative velocity between air and droplet, due to the acoustic excitations, was found to increase the heat and mass transfer in the evaporation process. Furthermore, droplet combustion time is found to be smaller for increasing amplitudes.

The impact of acoustic oscillations on spray combustion has been numerically examined by Zhu et al. [16]. For the influence of air perturbations, it was found that smaller droplets are formed in the process of atomization. Therefore, the evaporation time is reduced and the fuel supply and hence consumption increases, which has a stronger influence on the combustion stability.

The paper is structured in the following way: first the models employed are introduced, followed by the exemplification of the approach and by the selection of the boundary conditions for the simulations. Subsequently, CFD results are presented and discussed.

2. Method

2.1 Models

2.1.1 Atomization

The primary atomization of the liquid jet is modelled according to Rachner [17]. The liquid jet is discretized by an individual set of Lagrangian particles, each being treated as a cylindrical part of the liquid column. The disintegration of the jet is governed by two breakup mechanisms, shear breakup and column breakup. The shear breakup determines the mass rate of droplets being shed from the jet surface due to the shearing action of the air. The size of these droplets is correlated with the boundary layer displacement thickness within the jet. The column breakup results from the development of surface waves along the jet axis, which finally disintegrate the column into ligaments.

The instant of column breakup is determined by a characteristic time governed by the liquid/gas density ratio and the relative velocity. The ligaments undergo further breakup according to the shear breakup mechanism until the aerodynamic Weber number falls below a stable value.

The secondary breakup is modelled following the Kelvin-Helmholtz-Rayleigh-Taylor (K-H/R-T) approach and is applied for droplets which have been formed due to mass stripping [18]. The R-T model predicts instabilities on the droplet surface in terms of the growth of waves. Rayleigh-Taylor breakup is initiated as the droplet diameter is larger than the wave length of the fastest growing wave and the time of the disturbance growth is larger than the characteristic breakup time. Similar-
ly, the Kelvin-Helmholtz mechanism assumes the droplet to behave like liquid jet with perturbation waves growing on its surface inducing the stripping of mass. The K-H breakup is then characterized by the breakup time using the fastest growing wavelength and an aerodynamic Weber number reaching a stable value.

2.1.2 Evaporation

A zero-dimensional multicomponent evaporation model by Le Clercq [19] is employed which has been validated for pure heptane and has been extended for emulsions. The model solves the governing equations for evaporated droplet mass, species mass fraction and droplet temperature. A uniform temperature distribution within the droplet is assumed. Natural and convective heat transfer to the droplet is accounted by means of the Sherwood and Nusselt numbers [19].

Droplet properties are obtained by mass averaging calculated liquid and gas properties. Furthermore, the surface mixture fraction is calculated from the component’s vapour pressure using the droplet temperature and the ambient pressure. For this, Raoult’s law is applied at low pressures whereas a correction for real gas effects are comprised at elevated pressures.

Further information on the evaporation model can be deduced in the work done by Le Clercq [19].

2.1.3 Combustion

The combustion model is implemented following Dederichs et al. [20] and comprises a blend of the Flamelet Generated Manifold (FGM) and Simple Chemical Reaction System (SCRS) models.

The SCRS model assumes an infinitely fast chemistry and it is based on a single-step stoichiometric reaction. The FGM model consists in the tabulation of the internal flame structure (i.e. transport properties, temperatures, mass fractions and progress variable, source terms) from detailed laminar flame solutions. Prior to CFD simulations one-dimensional laminar premixed flames are calculated using Cantera a kinetic mechanism provided by Biet el al. [22]. From these calculations, chemistry tables are extracted for being used by the CFD solver.

The first variable of the tables denominates the regress variable. This variable determines the flame location. In this model, the progress variable is based on the CO2 product species and it is zero for burned mixtures and unity for unburned regions. The fuel mixture fraction corresponds to the second variable. In order to account for the effect of pressure waves (due to acoustic excitations) and the temperature decrease (due to droplet evaporation) on the chemistry, the enthalpy is used as a third variable in the tables. Based on these values, the progress variable source term (i.e. \( \omega_{\text{CO2}} \)) is read from the tables. The mixture composition is calculated from the mixture fraction and the CO2 mass fraction, which is solved in a transport equation, assuming a one-step global reaction.

Flame thickening is modelled using the artificial flame thickening (AFT) approach, which combines inherent and explicit flame thickening [20], to have an accurate prediction and resolution of the flame. Turbulence chemistry interaction, due to flame wrinkling, is considered following Bradley [21].

2.2 Boundary conditions and approach

The fuel considered in this study is hexadecane, as a reduced kinetic mechanism for the combustion model is available [22]. The acoustic response of the provided models for spray atomization, evaporation and combustion to forced excitation, in terms of its transfer function, is determined by monitoring model characteristics. For this, each of the applied models is investigated individually. For spray atomization simulations, a 3-D rectangular channel is set up with flow entering the domain from one end. Liquid fuel is injected into the cross flow at the centre of a channel wall. For this case, the spray penetration and the downstream droplet distribution (i.e. SMD) are tracked. For the evaporation case, a single droplet is injected into a 1-D domain with the mean velocity of air...
and the surface regression rate \( SRR = -\frac{d(d^2)}{dt} \) is computed for the entire droplet lifetime. For combustion simulations, a 1-D domain is set up, where the air velocity is equal to the laminar flame speed to have a flame which is spatially fixed. The flame heat release is tracked.

A fully developed flow state for the gas phase is achieved before the droplet injection or the flame initialization processes. Forced excitation is introduced to the flow as quasi-stationary state is reached. Following Poinset [6], non-reflecting boundary conditions (NRBC) are applied within the LES to guarantee that pressure waves do not reflect, leading to unphysical behaviour, but rather leave the domain. Forced excitation is applied to the flow field using oscillating inlet boundary conditions for the velocity. Thus, travelling sinusoidal waves are introduced to the flow resulting in pressure waves. Investigated forcing frequencies are from 100 to 1000 Hz with 100 Hz intervals.

Structured meshes are employed for the simulations. The number of cells and the cell size for each mesh is included in Table 1. The mesh for the 3-D Atomization case contains a refinement level around the fuel injector, where the cell size is about 0.5 mm.

<table>
<thead>
<tr>
<th>Case name</th>
<th>Number of cells / 1000</th>
<th>Cell size / mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-D Atomization</td>
<td>470</td>
<td>1</td>
</tr>
<tr>
<td>1-D Evaporation</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1-D Combustion</td>
<td>2.4</td>
<td>0.04</td>
</tr>
</tbody>
</table>

The kinetic mechanism, introduced by Biet et al. [22], provides the chemical reactions for the combustion of a hexadecane-air mixture. The fuel-air-ratio is unity for the 1-D combustion case. Initial conditions for droplet diameter and temperature are 0.45 mm and 293 K for 3-D simulations comprising the liquid jet disintegration, whereas 0.1 mm and 300 K are applied for the 1-D evaporation.

<table>
<thead>
<tr>
<th>Case name</th>
<th>T / K</th>
<th>p / bar</th>
<th>U / m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-D Atomization</td>
<td>280</td>
<td>5.8</td>
<td>100</td>
</tr>
<tr>
<td>1-D Evaporation</td>
<td>700</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>1-D Combustion</td>
<td>600</td>
<td>8</td>
<td>0.82</td>
</tr>
</tbody>
</table>

The thermodynamic inlet conditions of the simulations are presented in Table 2. For all the simulations, the applied forcing amplitude, defined as \( U' / \overline{U} \), is 20%. The conditions for the atomization case are selected from the stationary experimental data available in [21]. For the evaporation and combustion cases, conditions have been selected to be the similar to those of a 3-D case that will be computed in a future work, from which stationary data is also available. The temperature for the combustion is taken assuming 100 K decay due to the fuel evaporation

3. Results

For the primary atomization of a liquid jet in cross flow, the characteristic time for column breakup and mass stripping due to shear stresses is determined by the relative velocity between fuel jet and air. The latter is also ascertaining the process of secondary atomization [17, 18]. Simulation results, in terms of the Bode diagram for the liquid jet penetration and global SMD at the measurement plane (i.e. both 80 cm downstream of the point of injection), are depicted in Figure 1. The response amplitude of the penetration reveals a similar level of the introduced inlet forcing amplitude for low frequencies, particularly at 100 Hz and 200 Hz frequencies where the amplitude is slightly amplified. This entails that the spray trajectory is very sensitive to the upstream flow velocity. At higher frequencies the amplitude of the response is significantly reduced, showing low-pass
filter behaviour. The global SMD, however, reveals a lower response to the forcing frequencies. Furthermore, it is found that amplitudes are slightly decreasing as frequencies are increasing, which is in agreement with the droplet inertia to large gradients in the cross flow. From this, rough low-pass filter behaviour can be estimated. Additionally, the computed SMD mean values indicate a greater number of smaller droplets due to acoustic oscillations, which is in agreement with the findings obtained in [11]. Regarding the phase difference between each variable and the inlet excitation, it has been plotted so that it decreases with frequency by subtracting multiple of 360 degrees. For lower frequencies the phase is similar for both the SMD and spray penetration. As the frequency increases a higher phase lag is obtained for the SMD, which can be interpreted as a slower response to the inlet excitation.

![Figure 1: Bode diagram of droplet distribution and spray penetration.](image)

The droplet evaporation process is governed by the heat transferred from the gas to the droplet and the amount of mass evaporated. The former depends on the gaseous properties, the intensity of the convective field and the gas-liquid temperature difference. The latter depends on the droplet temperature (which is determined from the time-evolution of the heat balance), pressure level and the gaseous fuel concentration at the droplet surface. In general, the introduction of forced excitation to the mean velocity of the air flow results in a faster heating period and therefore in a shorter evaporation time [15]. Correlations for the convective mass and heat transfer, in terms of Sherwood and Nusselt numbers respectively, are strongly impacted by the by the Reynolds number. This is calculated from the absolute value of the difference between air and droplet velocity (relative velocity). As a result, the heat transferred to the droplet oscillates with double the frequency of the inlet excitation. This is a source of non-linearity, which leads to complex results that are hard to analyse with a Bode diagram.

Simulation results for 100 Hz, shown in Figure 2, have been chosen to exemplify the effect of forced excitations on the evaporation model. Droplet velocity and diameter are obtained from the Lagrangian parcel properties, while air velocity is monitored at the domain inlet. The time series of the droplet velocity, air velocity and absolute relative velocity fluctuations (non-dimensionized with the mean air velocity) are depicted in the right graph. The temporal evolution of the droplet surface regression rate is shown on the upper left plot. The frequency content of the aforementioned quantities is shown in the lower left graph. At the initial heating stage, the SRR is negative (i.e. the droplet
expands) because the liquid density decreases. As the droplet temperature increases, the SRR raises accordingly.

![Figure 2: 100 Hz forcing of a single droplet: SRR time series (top left); Fourier transform of SRR, gas and magnitude of relative velocity (bottom left); fluctuations time series for droplet velocity, gas phase velocity and magnitude of droplet relative velocity, non-dimensionalized with the mean gas velocity (right).](image)

A maximum value is reached for both quantities, after which they decrease until the droplet is completely vaporized. This droplet temperature and SRR reduction is caused by reduction of the relative velocity, as the droplet has less inertia and is able to respond faster to the gas phase oscillations. The latter can be observed in the velocity time series: At the beginning the phase between the droplet and the air velocity fluctuations is 90°; as the droplet is vaporized, the frequency and amplitude increases to get in phase with gas phase velocity fluctuations.

The Fourier Transform of the SRR shows an initial peak, which corresponds to the frequency of the droplet lifetime, and a second peak at the frequency of the relative velocity, showing a clear dependency on it. This behaviour is also found for higher forcing frequencies.

In the case of the combustion model, the pressure is solved in the governing energy equation [6] and consequently temperature oscillations are induced. Due to the correlation between temperature and enthalpy, the latter oscillates too. Therefore, the combustion model uses the enthalpy as an entry variable for the chemistry tables, from which the progress variable source term is read.

Figure 3 presents the simulation results for the 1-D combustion case. The Bode diagram of the flame transfer function, defined as the ratio between the volume integrated heat release amplitude and the inlet velocity amplitude and the phase difference between them, is shown for single frequency forcing. The transfer function at the investigated frequencies reveals that the forcing frequency is found in the response of the heat release fluctuations, with an amplitude of about 40% the triggered amplitude. Similarly to the penetration and SMD variables in the atomization case, the phase difference between the heat release and the inlet velocity fluctuations is linearly decreasing with the forcing frequency. Particularly, they are almost in phase for all the frequencies investigated.
Future work will focus on the analysis of the response to coupled models. Simulations for an evaporating spray (atomization + evaporation), a 1-D spray flame (evaporation + combustion) and a 3-D test case (atomization + evaporation + combustion) will be performed for this study.

4. Conclusion

A thermo-acoustic study on the response of validated models for spray atomization, evaporation and combustion to forced excitation is performed. The investigated frequency range is from 100 Hz to 1000 Hz in 100 Hz interval. A 3-D spray in cross flow is simulated for the atomization model, and fluctuations of the spray penetration and global SMD at a downstream plane are monitored. The forcing frequencies are found in the FFT obtained for both variables, being the spray penetration more sensitive to acoustic waves. For the evaporation model of a single evaporating droplet in a 1-D domain, the surface regression rate is tracked during the droplet lifetime. Non-linear behaviour is found when applying forcing, since the evaporation depends strongly on the relative velocity between the air and the droplet, resulting in SRR fluctuations with double the frequency of the inlet excitation. Regarding the combustion model, the forcing frequencies are found in the response for the heat release fluctuations of a 1-D premixed flame, with an amplitude about 40% the one from the inlet. Future work aims to investigate the effect of acoustic wave on coupled simulations. The main outcome of this paper is that, for all simulations, the amplitude of the acoustic response for each investigated model characteristic is lower than the forcing amplitude.

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