CFD modelling of gas-turbine fuel droplet heating, evaporation and combustion

Mansour Al Qubeissi

Acknowledgement to colleagues: Geng Wang, Nawar Al-Esawi, Oyuna Rybdylova, Sergei S. Sazhin

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Aim of study

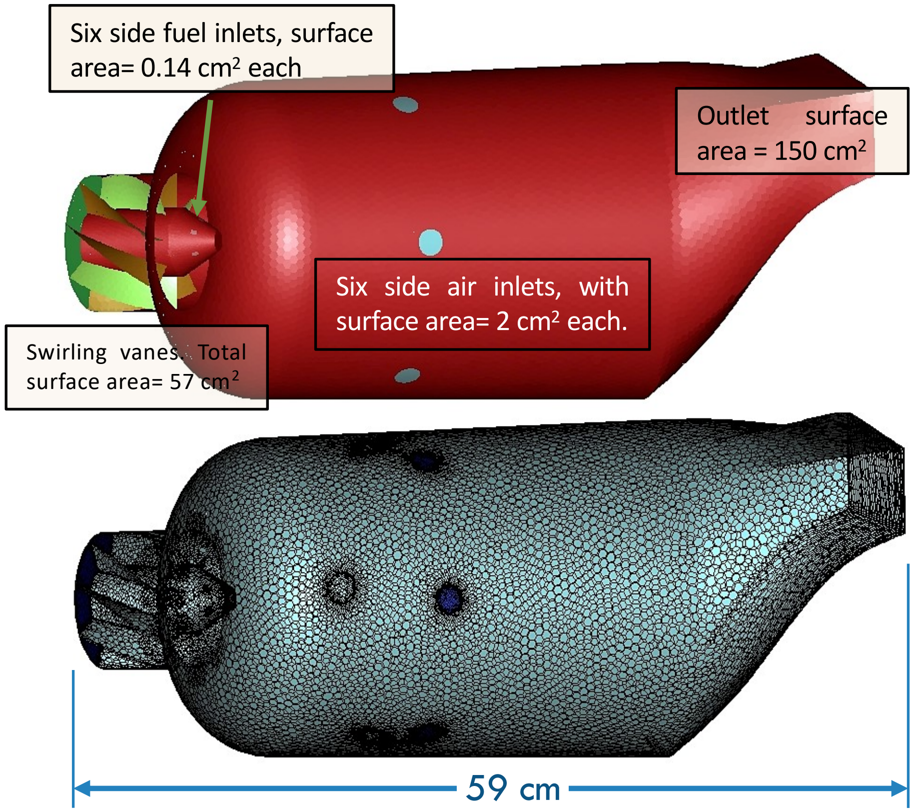
The simulation of heating, evaporation, and combustion of kerosene fuel droplet in turbine combustion chamber and conditions.

Objectives

- Reduce the kerosene fuel composition (40 species) to 2 surrogates, using the multi-dimensional quasi-discrete model.
- Simulate fuel droplet heating and evaporation, using the Discrete-Component model (DCM).
- Implement a user-defined function (UDF) of DCM into commercial CFD software (ANSYS-Fluent).
- Simulate the kerosene fuel combustion in turbine combustor conditions.

Input parameters

A full scale turbine can combustor geometry is used for a full combustion process, including liquid spray penetration, evaporation and combustion.



Primary, secondary Inj. air velocity	10, 6	m/s
Stoichiometric ratio	15.6 : 1	-
Fuel mass flowrate	0.003	Kg/s
Amb. pressure	4	Bar
Air Temp	293	K
Fuel Temp	300	K
Oxide Temp	800	K

Flamelet generated manifolds (FGM) table is used to understand the combustion processes with $\kappa - \varepsilon$ RANS – PDF model for the turbulent simulation.

Kerosene fuel compositions

The molar fraction of each component in kerosene fuel is show below (divided into 5 hydrocarbon groups according to their chemical structure).

CN	Alk	Cycloalk	Alkyb	Ind & Tet	Naph
C7	0.6666	0.2820	0.1590	0	0
C8	0.8272	0.9145	0.9356	0	0
C9	2.8071	3.0581	2.1136	0.3031	0
C10	5.4843	6.7705	3.3002	1.3056	0.1143
C11	6.3470	7.3163	2.4058	2.0156	0.2862
C12	7.1920	7.1614	3.0108	3.5362	0.3126
C13	5.2398	4.0110	2.6882	0.8410	0.0574
C14	4.9514	3.1355	1.4889	0.2076	0
C15	4.7625	1.2929	0.2789	0	0
C16	1.5539	0.5371	0	0	0
C17	0	0.3279	0	0	0
Total	39.8	34.8	16.4	8.2	0.8

Discrete Component Model (DCM)

- The solutions to **heat transfer** and **species diffusion** equations are based on the **effective thermal conductivity** and **effective diffusivity** (ETC/ED) models.
- Several physics, underlying the evolutions of droplet heating and evaporation, are accounted for (e.g. **transient** and **gradient fuel composition** inside droplet).

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Modelling of biodiesel fuel droplet heating and evaporation

CrossMark

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Multi-Dimensional Quasi-Discrete Model (MDQDM)

- MDQDM is used to **reduce the computational time** of DCM, without a sacrifice to accuracy.
- It replaces high number of fuel components with **a small number** of representative components (with averaged molecular formulae).
- These representative components have **non-integer carbon numbers** $\bar{n}$, so called quasi-components (QCs).
- Each set of QCs are **formed within a group of components** (e.g. alkanes, cyclo-alkanes), based on their thermodynamic and transport properties, and chemical structures.

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journal homepage: www.elsevier.com/locate/fuel

A multi-dimensional quasi-discrete model for the analysis of Diesel fuel droplet heating and evaporation

CrossMark

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Surrogate formulation – Using MDQDM

We have replaced the 40 components with the following 2 dominant quasi-components:

$C_{10.074}H_{22.15}$ with a molar fraction of 39.8%

$C_{11.633}H_{23.27}$ with a molar fraction of 34.8 %

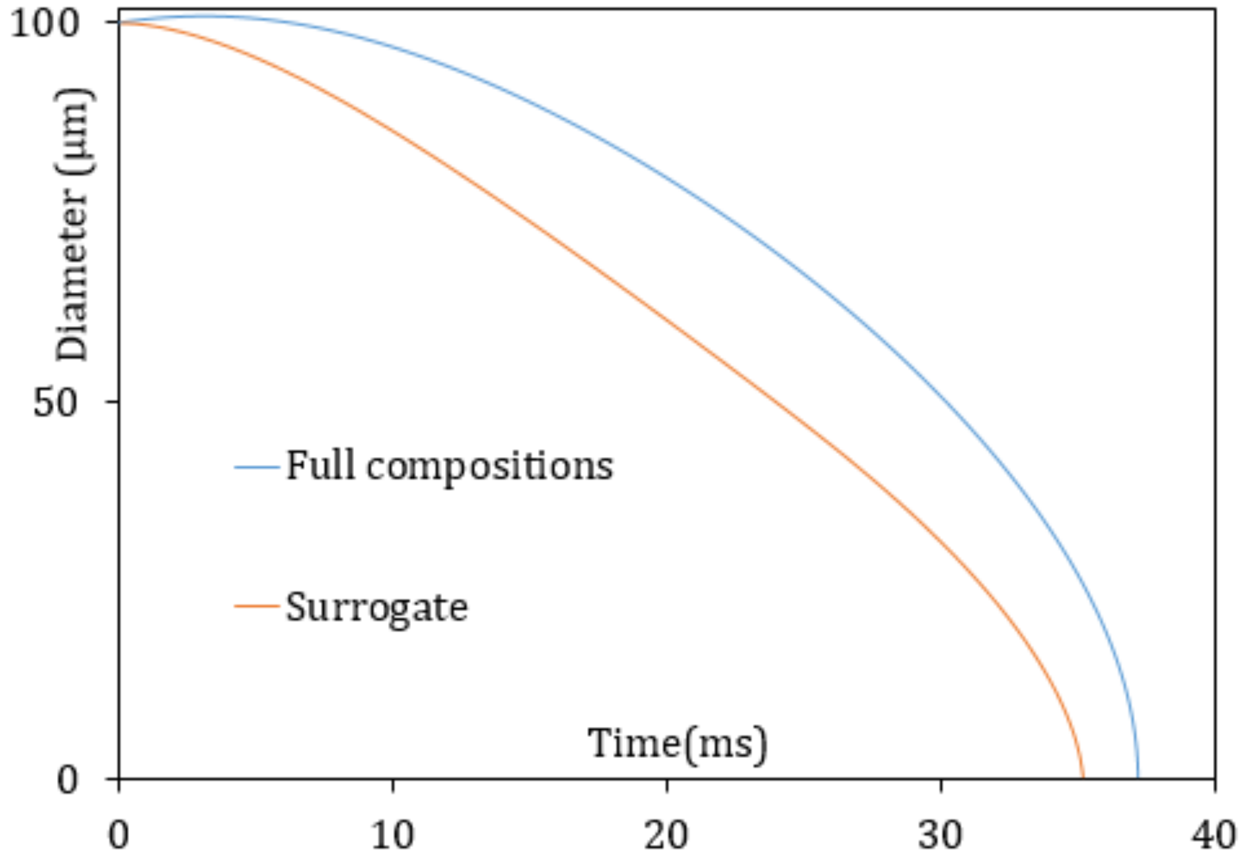
After molar-fraction normalization, and taking the representative integer value of the carbon number, the following compositions have been introduced and implemented into Ansys Fluent:

53.4% of $C_{10}H_{22}$

46.6% of $C_{12}H_{24}$

Surrogate formulation

The fuel surrogates have been compared with full composition of the fuel in terms of droplet lifetime, using the DCM.



Evaporation results

Input parameters:

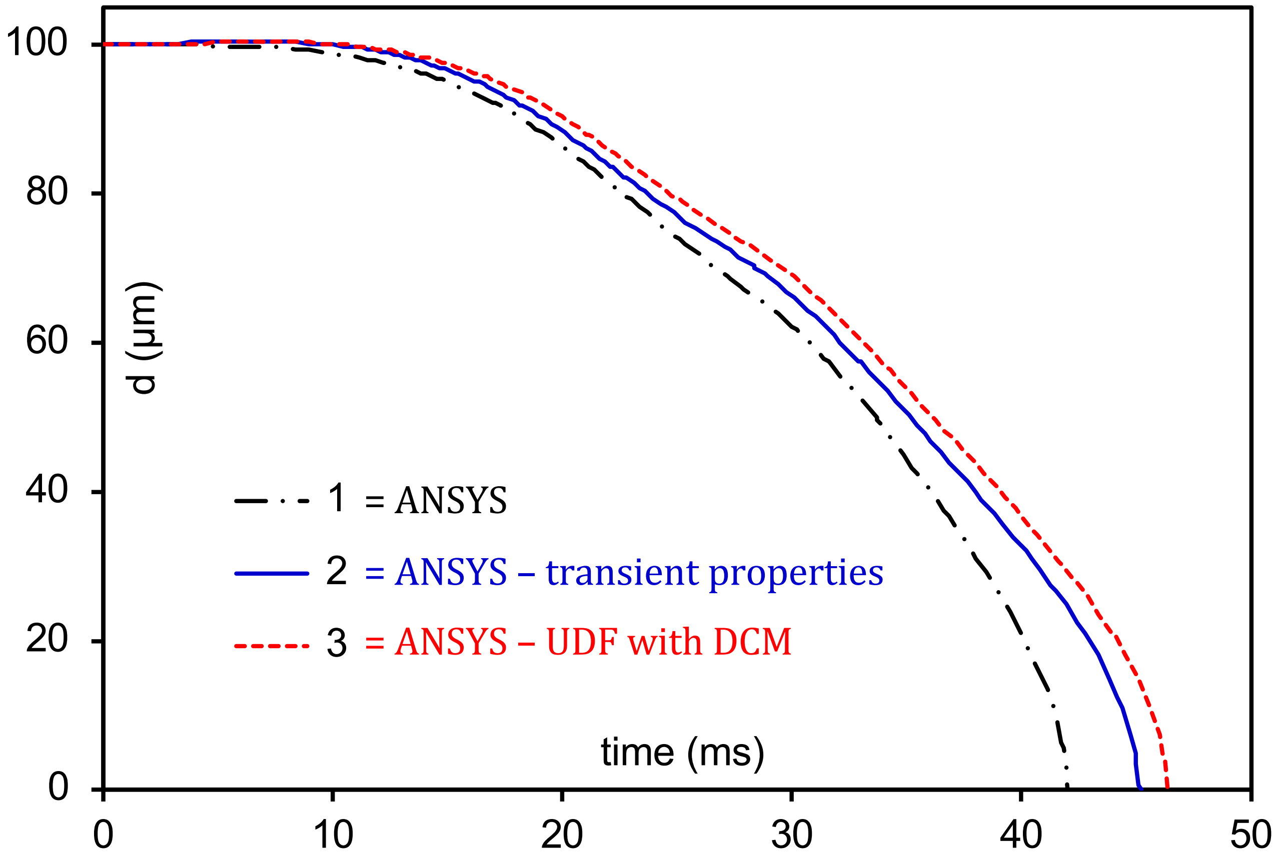
$D_d = 100\ \mu m$

$T_o = 375\text{ K}$

$T_g = 800\text{ K}$

$p_g = 4\text{ bar}$

$U_d = 1\text{ m/s}$

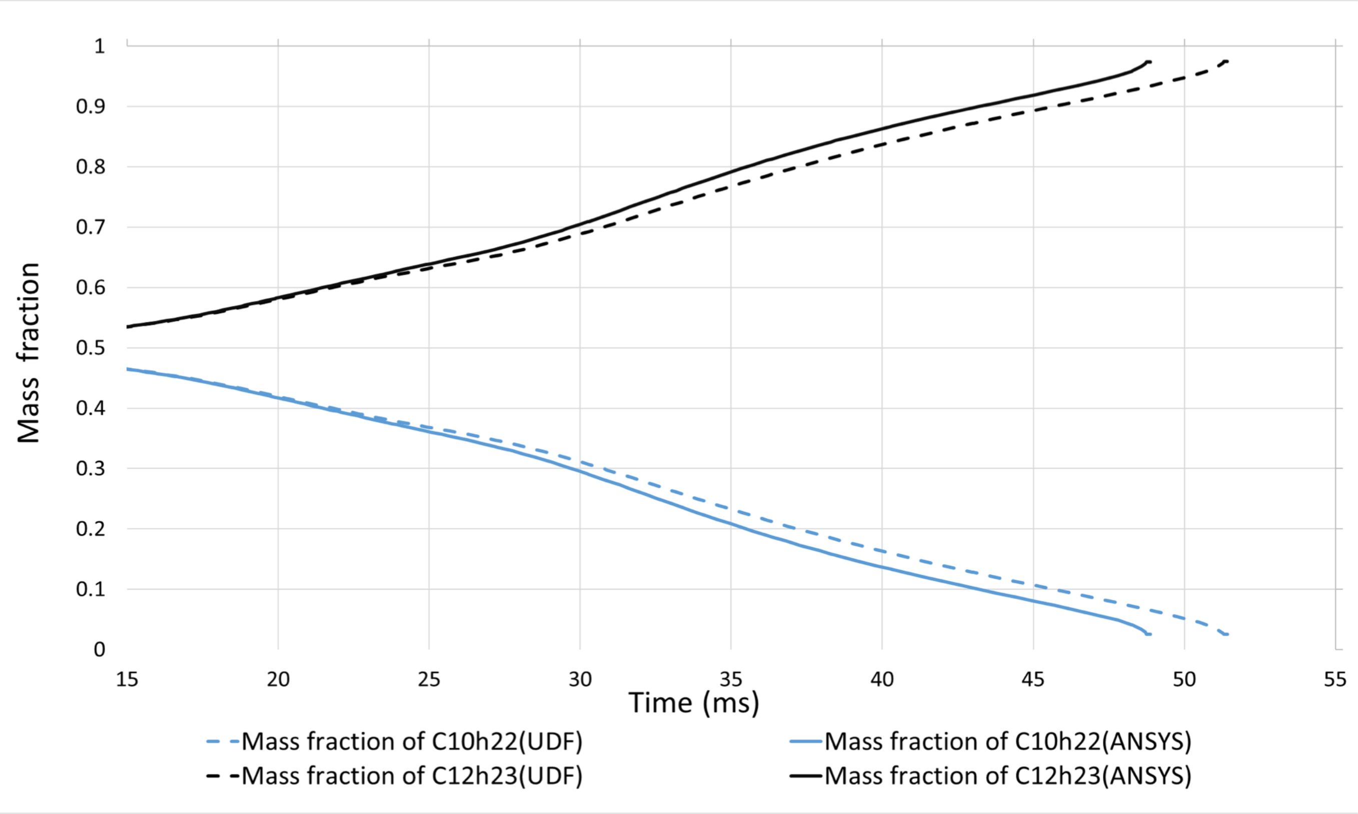


1 = Standard ANSYS Fluent results, with constant properties.

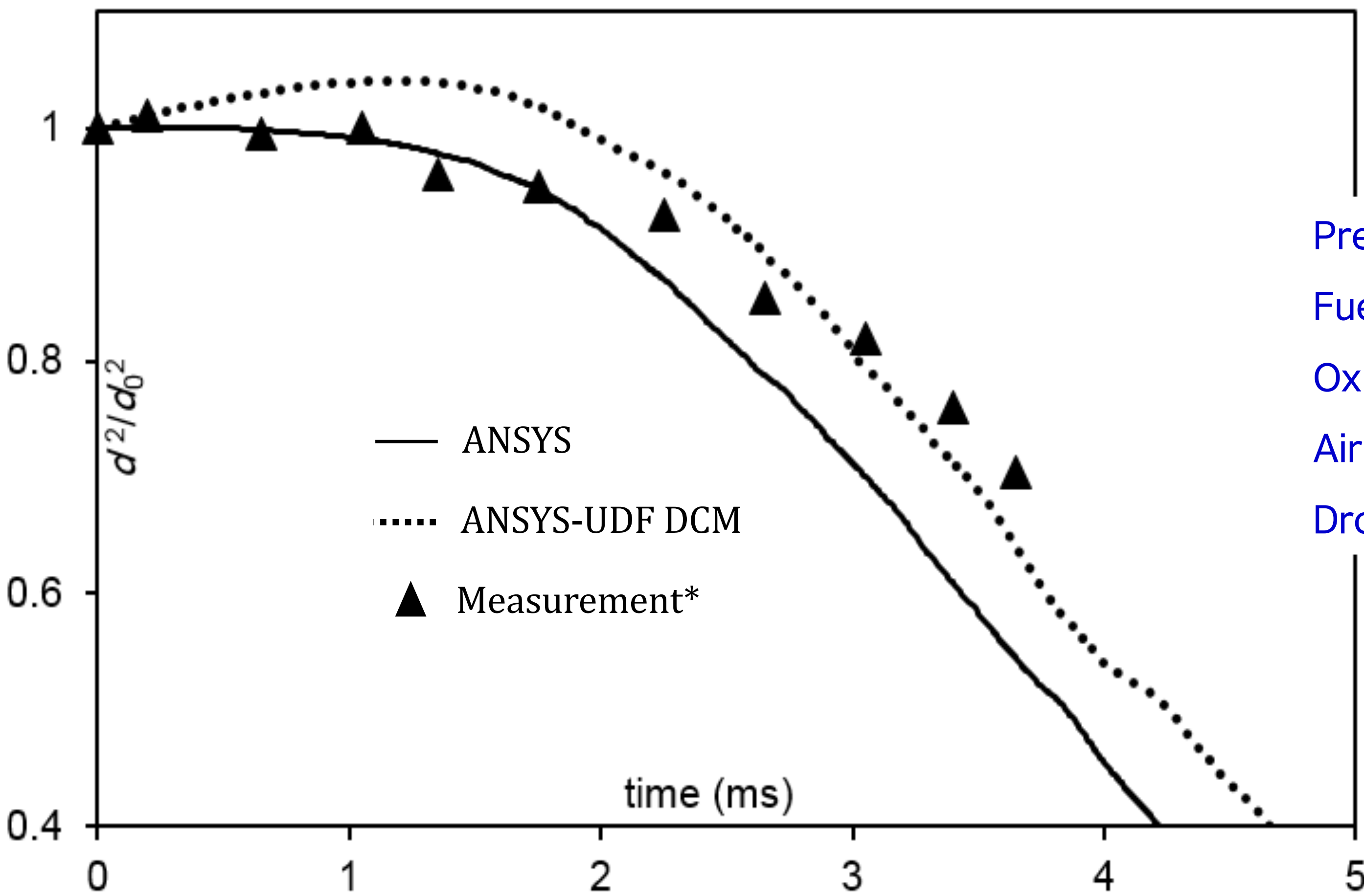
2 = ANSYS Fluent results, with transient properties using udf.

3 = ANSYS fluent results with the Discrete Component model using udf.

Species diffusion, using ANSYS-UDF DCM



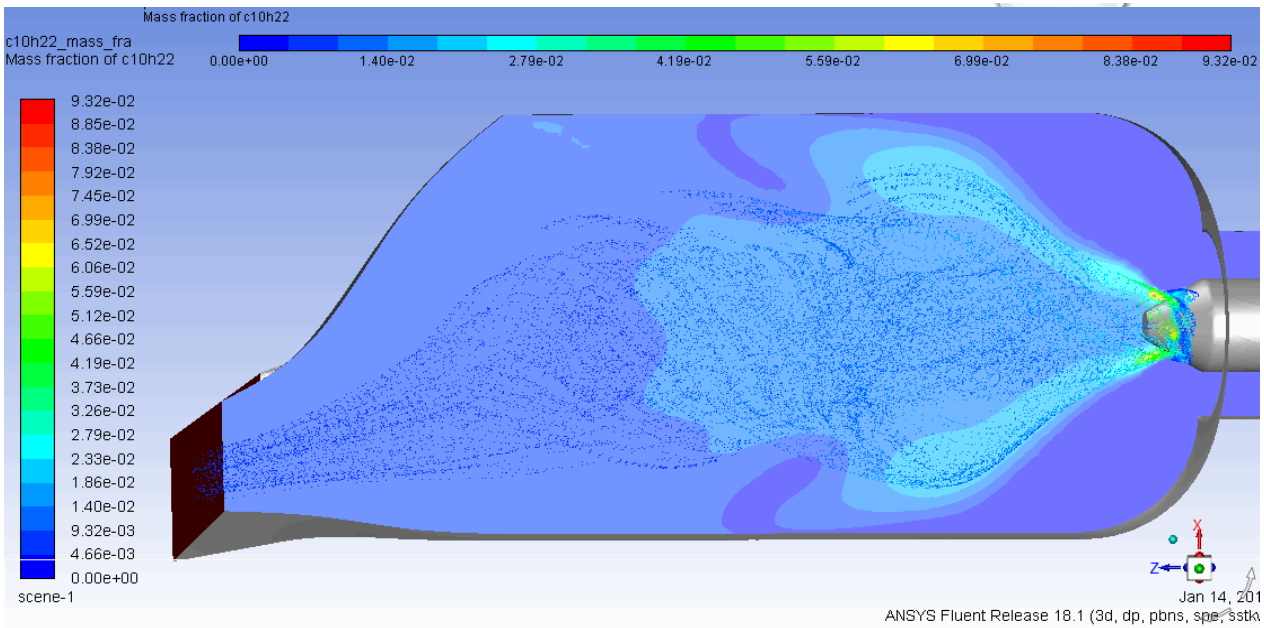
Validation



Pressure	0.1	MPa
Fuel temperature	298	K
Oxid temperature	573	K
Air flow rate	20	L/min
Droplet diameter	1.58	mm

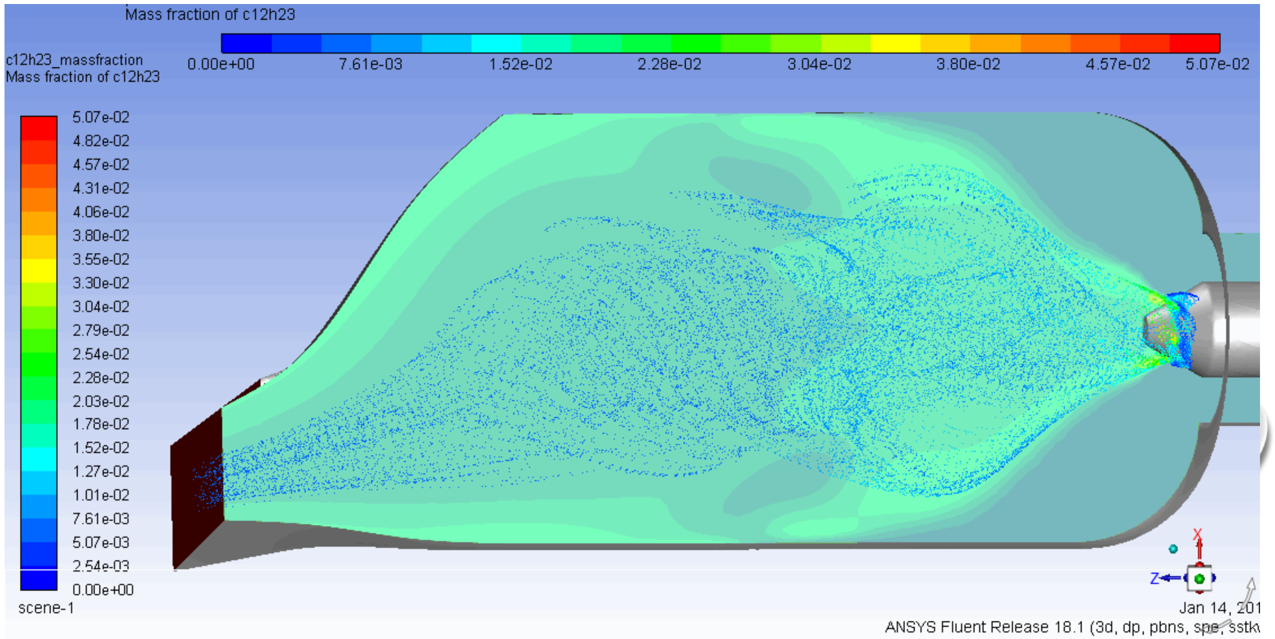
**Wang, F., et al., 2018. Fuel 211, 582–590.*

$C_{10}H_{22}$

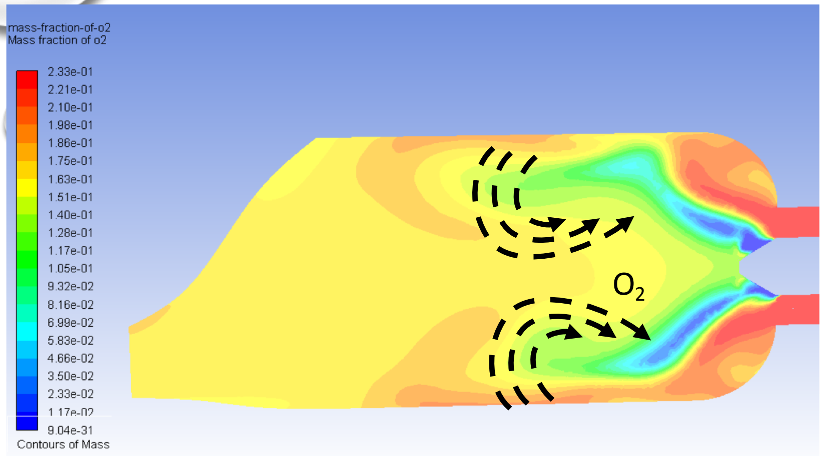


Bi-component mass fractions

$C_{12}H_{23}$

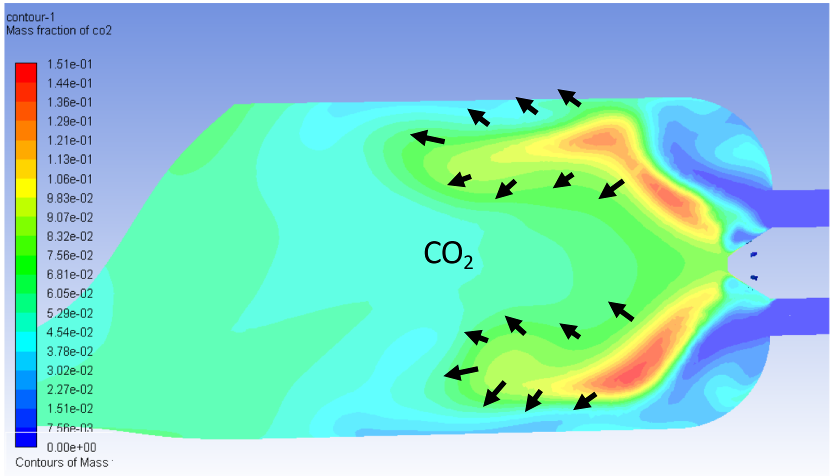


Combustion: Species distribution

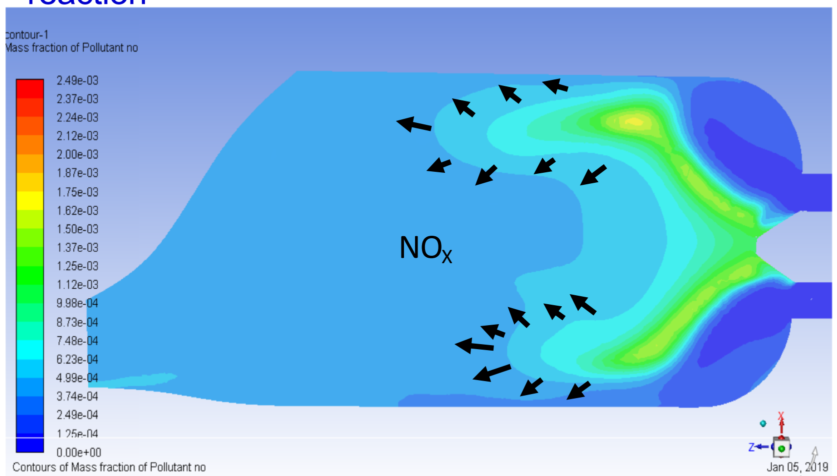


Mass fraction distribution of O2: Charge from dilution hole

Mass fraction distribution of CO: generated in the flame and reaction

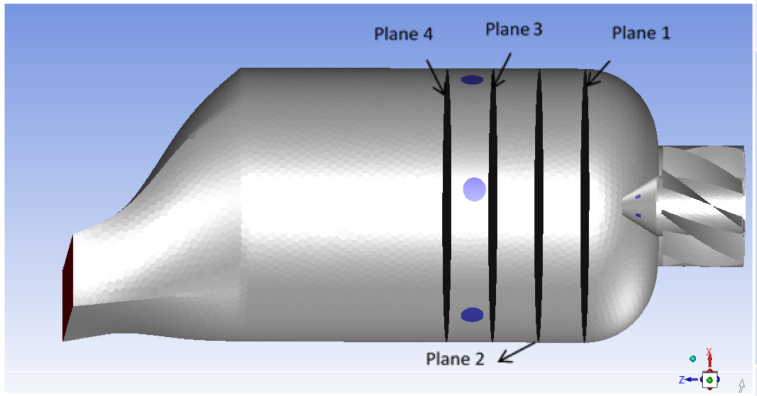


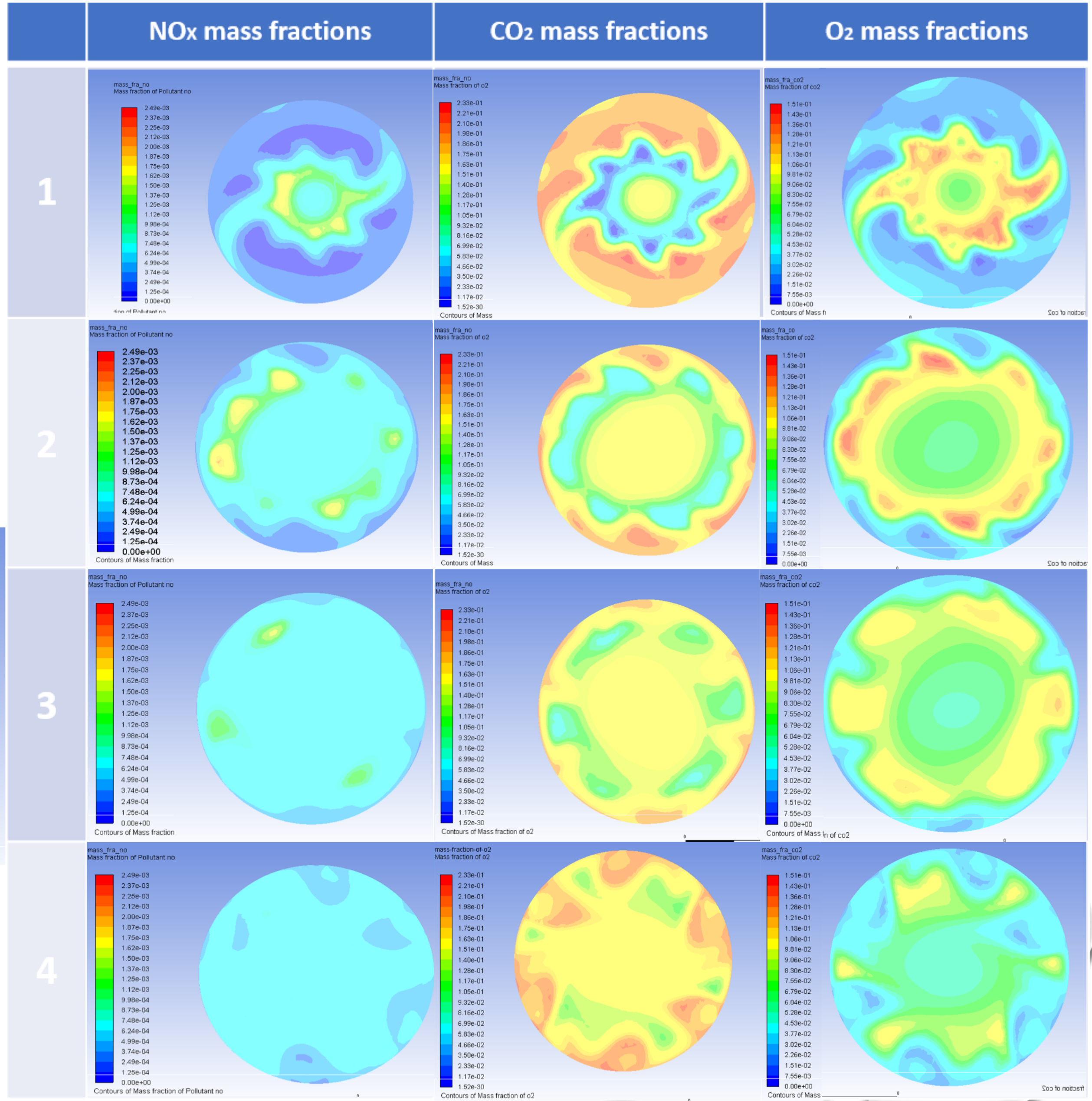
Mass fraction distribution of CO2: generated during the reaction



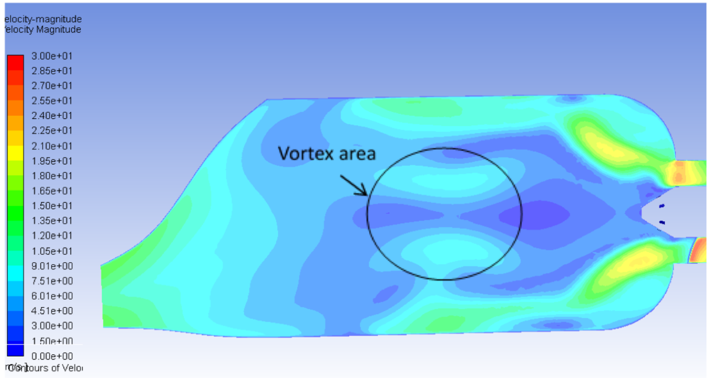
Mass fraction distribution of NOX: discharged to the ambient vapor

Combustion: Species distribution

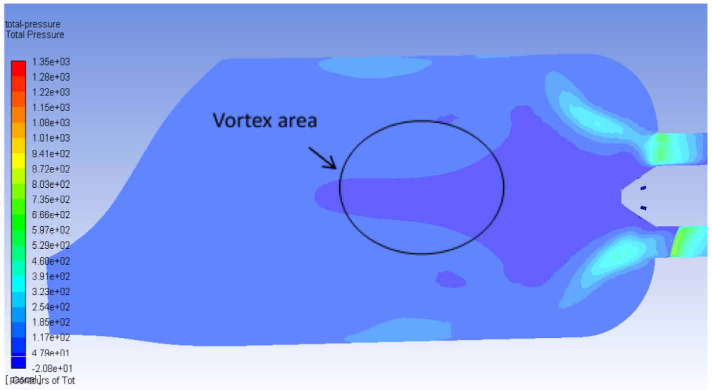




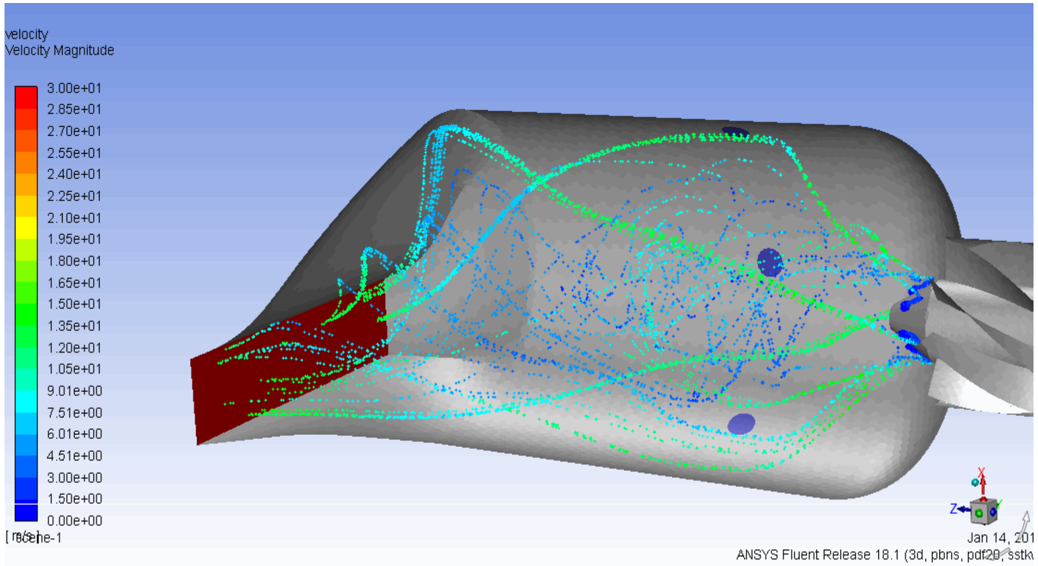
Flow structure



The velocity distribution an the symmetry plane

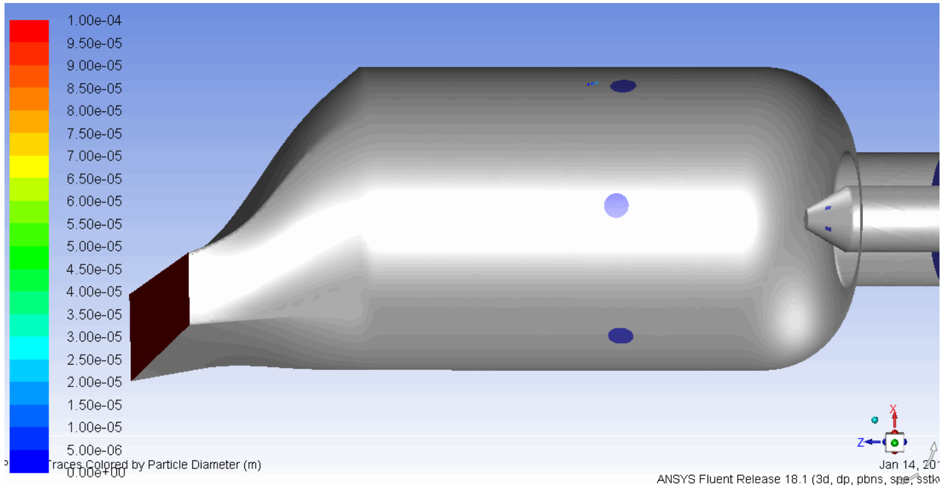


The Pressure distribution an symmetry plane

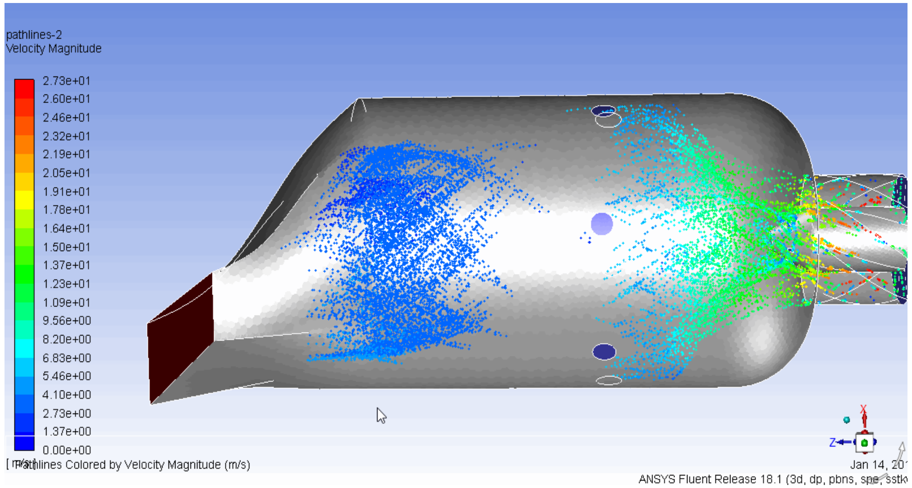


- Vortex leads to the lower pressure zone
- Decrease the velocity
- Enhance the species mixture

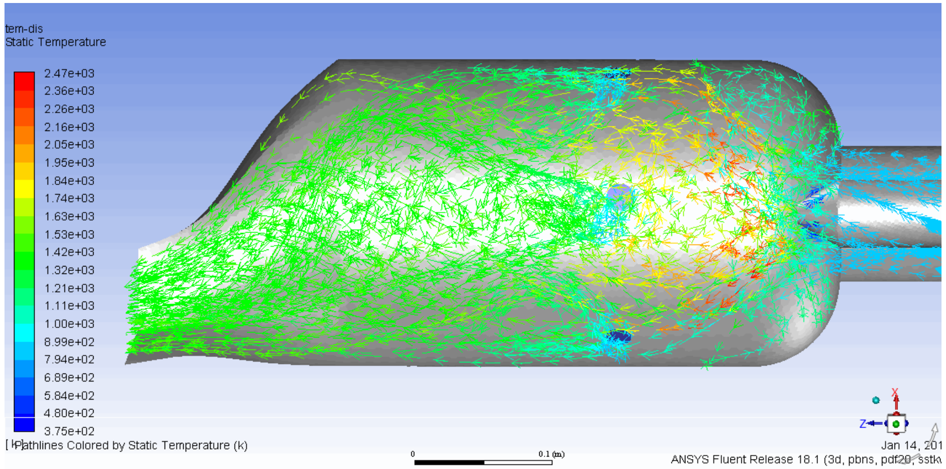
Flow characteristics



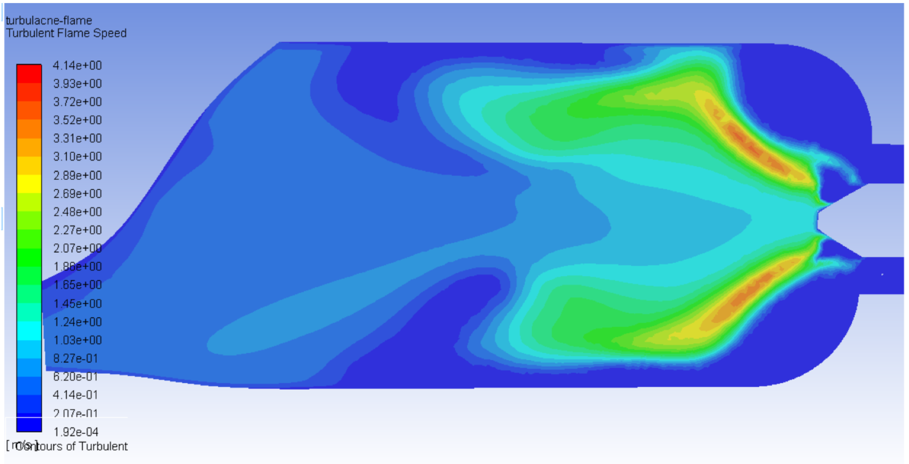
Particle diameter (m), droplet evaporation



Velocity magnitude (m/s)



Temperature of the stream (K)



Turbulent Flame Speed

Conclusions

- Multi component kerosene fuel droplet heating, evaporation and combustion is investigated using:
  - CFD model (ANSYS-Fluent) for the hydrodynamic region
  - The DCM for the droplet evaporation and species diffusion in liquid phase
  - Chemkin mechanism for reaction pathways
- The kerosene fuel composition is reduced to 2 surrogates using the MDQD model.
- The heating and evaporation of kerosene fuel droplet are investigated using the DC model.
- The DC model implementation into ANSYS-fluent shows good agreement with the in-house code and the experimental data.

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