POLITECNICO
MILANO 1863

Computational Techniques for Thermochemical Propulsion

Report: Assignement 3

Lagrangian Particle Tracking and thin liquid film.

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1 Introduction

1.1 Physics and quantities of interest

In this assignment, the simulation of fuel spray injection within a compressible fluid flow is conducted, building upon the baseline established in assignment 2.1. Additionally, a thin film model is incorporated at the interface with the side walls. Compared to previous simulations, this scenario is significantly more unsteady due to the rapid and sudden injection of the spray into the domain. To accurately capture the system's temporal evolution, smaller time steps are required. Consequently, the PISO algorithm is implemented, as it is more suitable for flow simulations characterized by rapid temporal changes. Although maintaining a Courant number below one inevitably increases the computational time, this effect is partially mitigated by implementing a single outer iteration.

The employment of a thin film model requires the subdivision of the problem into two domains, called regions, one for the solution of the fluid and the lagrangian particle tracking and one for the liquid film at the wall interface, the latter being ruled by its own set of equations. However the two systems are coupled with each other by means of the source terms inside the transport equations.

The main additional variables of interest are the mass fraction for each chemical species, which is integrated by means of the transport equations inside the fluid domain, the diameter of the particles, which decreases in time due to the evaporation and the local δ thickness of the thin film on the side walls.

2 Setup of the problem

2.1 Definition of the two regions

The presence of two different regions in the simulation implies the necessity of reorganizing the structure of the problem. The `fluid` and `film` regions are characterized by their own 0, constant and system folders. The only file that is shared by the two domains is the controlDict.

Due to limited space for the report only the most significant modifications will be presented.

2.2 extrudeToRegionMeshDict and blockMeshDict

The first file generates an extruded mesh on top of the original one at the interface of the wall on which the thin liquid film is desired. In order to properly use this function the `blockMeshDict` inside the `fluid` folder is modified: the name of the patch `sides` is changed in order to match the name in the dictionary for the extrusion of the mesh. Additionally the option type must be set to `mappedExtrudedWall`.

2.3 Fluid region

2.3.1 Boundary conditions and initial conditions

Considering the fields for the quantities which are in common with the previous compressible problem, the solution of a compressible precursor simulation is taken as the initial condition for this analysis, by means of the `mapFields` function. All the boundary conditions are maintained the same and the `p_rgh` field, the pressure quantity from which the idrostatic contribution is subtracted, is added before the remapping. Hence this quantity will is solved for in the transport equations instead of pressure and in order to do this also the name of the solver in the `fvSolution` is modified correspondingly.

Additionally the files for the initial condition of `N_2` and `O_2` mass fractions are required in the 0 folder. The uniform atmospheric composition is imposed for the internal field and the two inlets while at the walls with no film the `zeroGradient` BC is used. Regarding the `C7H16` species mass fraction arising from the evaporation of the fuel droplets, no file is generated inside the 0 folder because the field will be automatically generated during the simulation.

Finally in each 0 file the name of the patch at the wall interface with the liquid film must be changed according to the modifications in the previous section and the boundary conditions for velocity and temperature are set to `mappedValue` and `coupledTemperature` respectively, to connect the two regions.

2.3.2 physicalProperties and speciesThermo

The original `physicalProperties` file for the single-component compressible fluid flow problem is substituted ny the one from the `aacheBomb` OpenFOAM tutorial. In this new file the mixture is defined as `multiComponentMixture` and in order to retrieve the temperature from the specific enthalpy the coefficients for the polynomial expression of the c_p for each species needs to be specified. To do this the `thermo` option is set as `janaf` and the link to the speciesThermo input file is included inside the domain of `physicalProperties`.

Inside `speciesThermo` file the polynomial coefficients for the specific heat capacity at constant pressure can be found for each specie, among with other thermodynamic properties such as the molecular weight.

An additional important specification inside the`physicalProperties` input file is the imposition of C7H16 as liquid.

2.3.3 fvModels and cloudProperties

fvModels is a simple but important input file which is required to introduce the `cloud` spray model for the Lagrangian particle tracking. The `cloudProperties` from the aacheBomb OpenFOAM tutorial is taken as a baseline to characterize the fuel spray. However some modifications are needed. The settings that need to be properly imposed are:

- the total mass to be injected and the duration of the injection, which are imposed by the requirements to be 1e-4 kg and 0.1s respectively and can be changed via the `massTotal` and `duration` settings in the cloudProperties file;
- the number of parcels per second, which value is decreased to 400000 to reduce the computational effort;
- the table defining the `flowRateProfile`, hence for this problem a sinusoidal evolution of the spray is required. To do so the matrix was assembled on Matlab by means of a $Asin(\pi t/0.1)$ like function were the coefficient was iteratively computed in such a way that the intergral of the function along the first 0.1 seconds matches the total mass which needs to be expelled by the injector during the simulation;
- the position and the spray direction of the injector, represented by two vectors which are respectively set to (0 -0.259 0) and (0 1 0).
- The `ReitzKHRT` model is used for the breakup of the molecules due to aerdynamic forces.
- the surfaceFilmModel option is set to cloudFilmTransfer, to consider the interaction of the spray with the liquid film on the wall, and the relative settings are introduced.

2.4 Film region

2.4.1 Boundary conditions and initial conditions

The 0 folder for the film region is extracted directly from the `hotBoxes` tutorial and for this specific case it must contain four quantities: the `delta` thickness, the pressure, the temperature and the velocity. In each one of the input files the initial conditions and four boundary conditions are imposed, one for the interface with the internal fluid, one for the interface with side wall and two for the inlet and outlet patches. In order to communicate with the surrounding patches the mapped boundary conditions are needed;

- the `filmContactAngle` BC for `delta` in which a constant contact angle is given between the liquid and the wall;
- the `filmSurfaceVelocity` for U at the surface which provides the source term for the mass conservation equation;
- the `mappedFilmPressure` for p at the surface which represents the external forces in the momentum equation;
- the `coupledTemperature` BC for T at the surface to ensure the continuity in the heat balance.

All the remaining patches are characterized by a `zeroGradient` BC.

2.5 testCase2 and testCase3

Small modifications are needed for the following two test cases. For the second problem the `ReitzDiwakar` model is enabled instead of `ReitzKHRT` for the break up model, among with the respective tuning parameters and options. For the third testCase only the temperature at the inlet needs to be set to 450 K both for the main simulation and for the precursor one.

However for the following testcases also the number of injected parcels per second will be reduced to 200000, due to the significant amount of time that the first simulation required. The solution would be slightly affected in accuracy by this modification because the higher the number is, the smaller the amount of particles which are incorporated inside the parcel.

Additionally, since the results from the first two simulations are characterized by an evident discretization in the parcel distribution in the first instants as a solution to mitigate this effect the table for the spray mass flow rate profile in the last test case is modified by increasing the number of rows, which represents the time discretization.

3 Results

3.1 Post processing

The Figs. 3, 5 and 7 represent the contour of the fuel mass fraction in the gaseous domain and the liquid parcel distribution with a scaled proportional dimension and a coloring pattern which represents the velocity of each parcel. Additionally a scaled representation of the thin liquid film is plotted on the contour.

In this figures, due to the presence of significantly big parcels, it appears that the injection of fuel does not follow the semi-sinusoidal trace in time which was imposed. Hence the concentration of particles appears to be higher at the beginning and at the end of the injection, especially in the first case. This effect however is conterreacted by the velocity of the particles entering the domain. Hence it is believed that the `ReitzKHRT` model takes into account the dependence of the particle diameter from the jet inlet velocity and this can be observed inside the simulation at time 0.2s and 0.8s. It is experimentally observed that jets with high inlet velocity are characterized by a greater atomization of the liquid thanks to the enhanced aerodynamic instability at the interface with surrounding gas. The first particles to enter the domain are the biggest ones but at the same time the slowest. The following particles are entering the domain with higher velocity which increases the mass flow rate in the middle part of the simulation's time.

It can be noted that thanks to the temperature increase in the surrounding fluid the evaporation of the fuel is enhanced. In Fig. 1. the liquid penetration of the jet at 95% mass is showed. It is the distance in meters from the injector inlet for which 95% of the mass of the spray is still in the liquid phase. The first two testcases are characterized by a similar trace while the third simulation presents significantly lower values for this parameter.

Finally Fig. 2 represents the height of the liquid film on the wall located at the x = 0.12m coordinate while Fig. 4, 6 and 8 represent the parcel distribution.

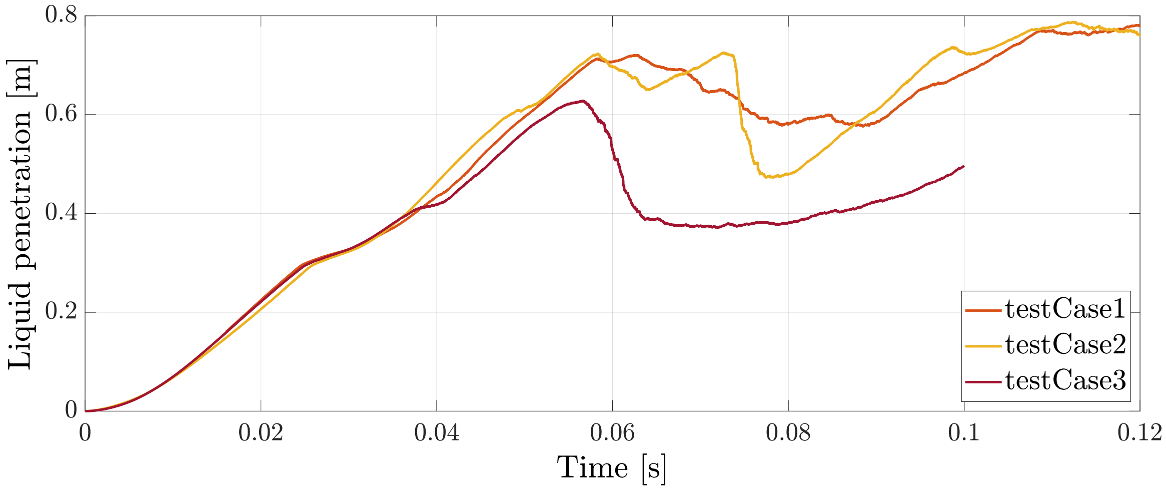


Figure 1: Liquid penetration parameter at 95% mass as function of time.

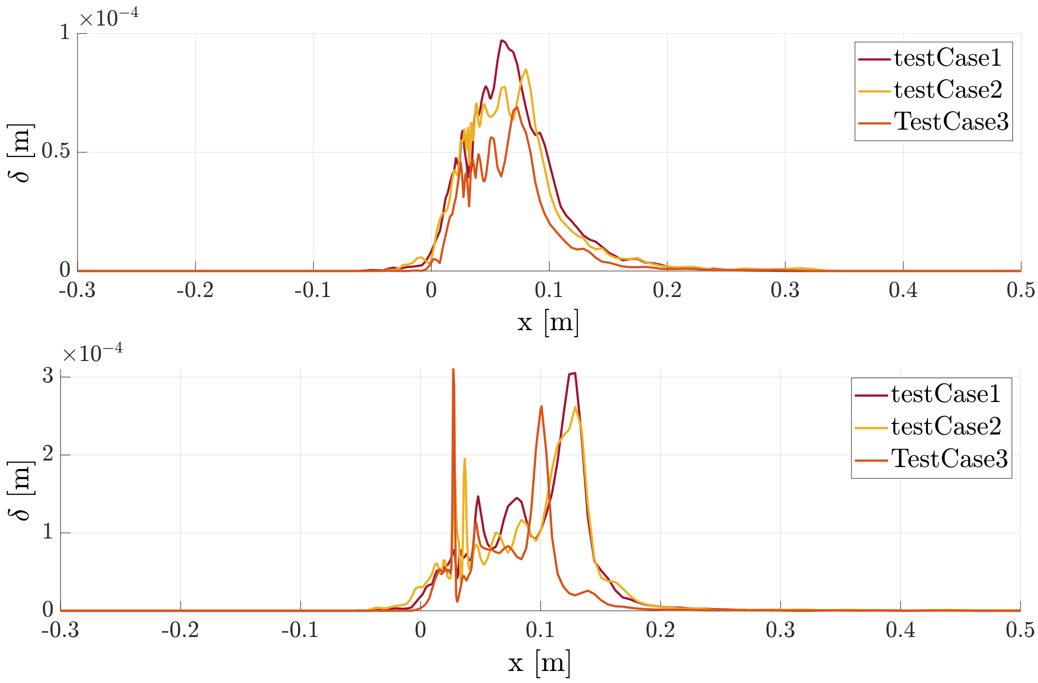


Figure 2: Liquid film thickness as function of y coordinate at x = 0.12m for t = 0.5s and 0.8s respectively (no film is present at t=0.2s).

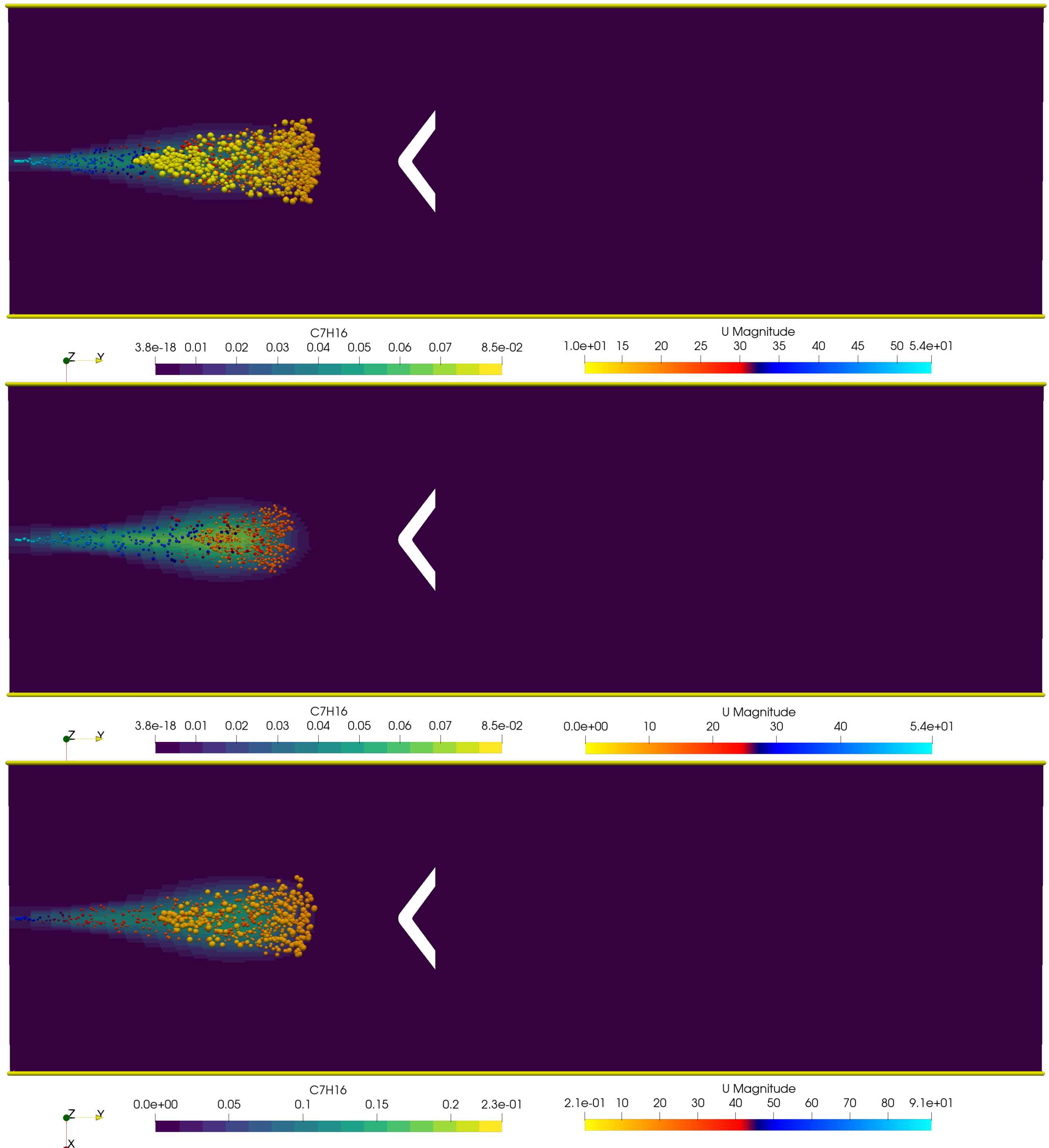
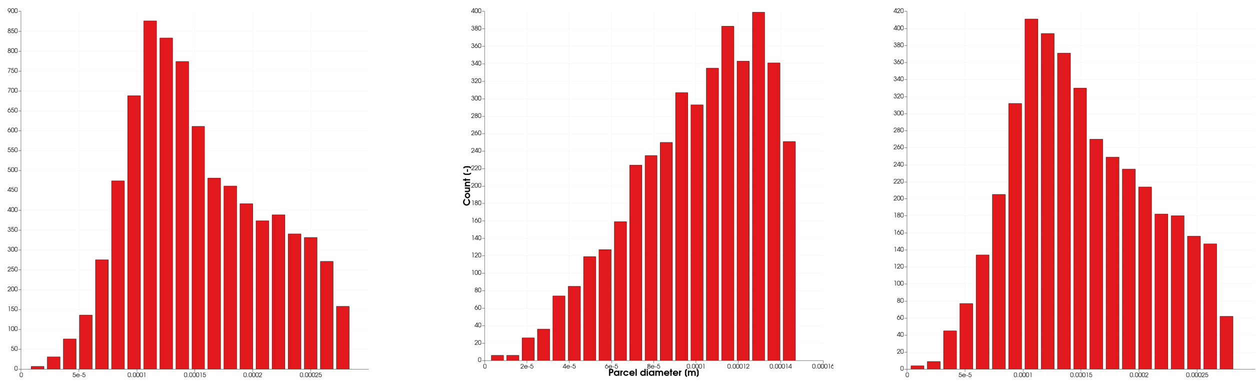


Figure 3: Fuel mass fraction contour for the three testCases and visualization of parcel distribution and liquid film thickness for timestep 0.2s.



(a) testCase1 (b) testCase2 (c) testCase3

Figure 4: Velocity contour at last iteration, t = 0.2s.

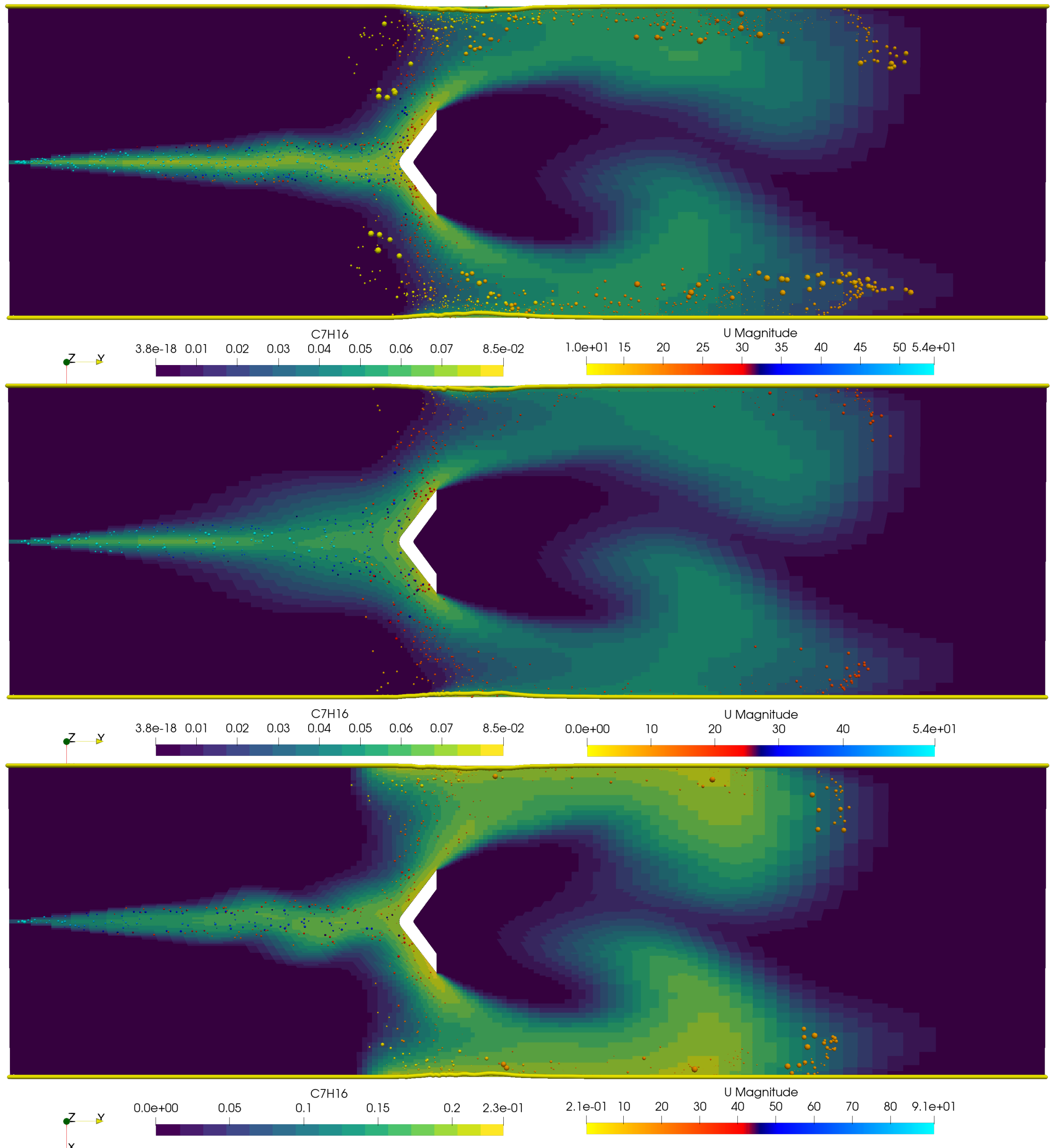
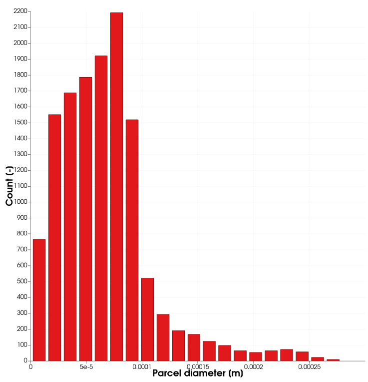
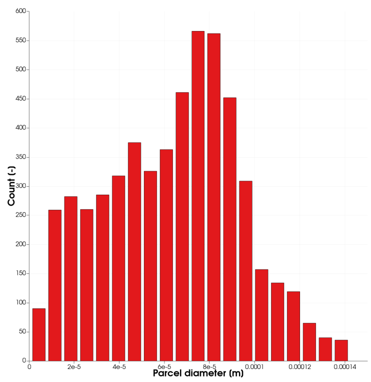


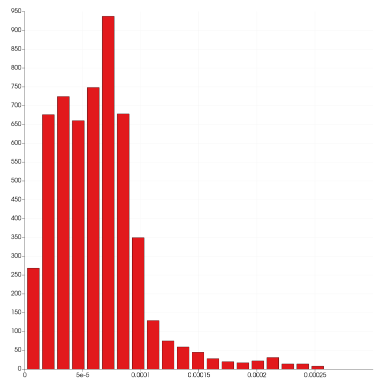
Figure 5: Fuel mass fraction contour for the three testCases and visualization of parcel distribution and liquid film thickness for timestep 0.5s.



(a) testCase1



(b) testCase2



(c) testCase3

Figure 6: Velocity contour at last iteration, t = 0.5s.

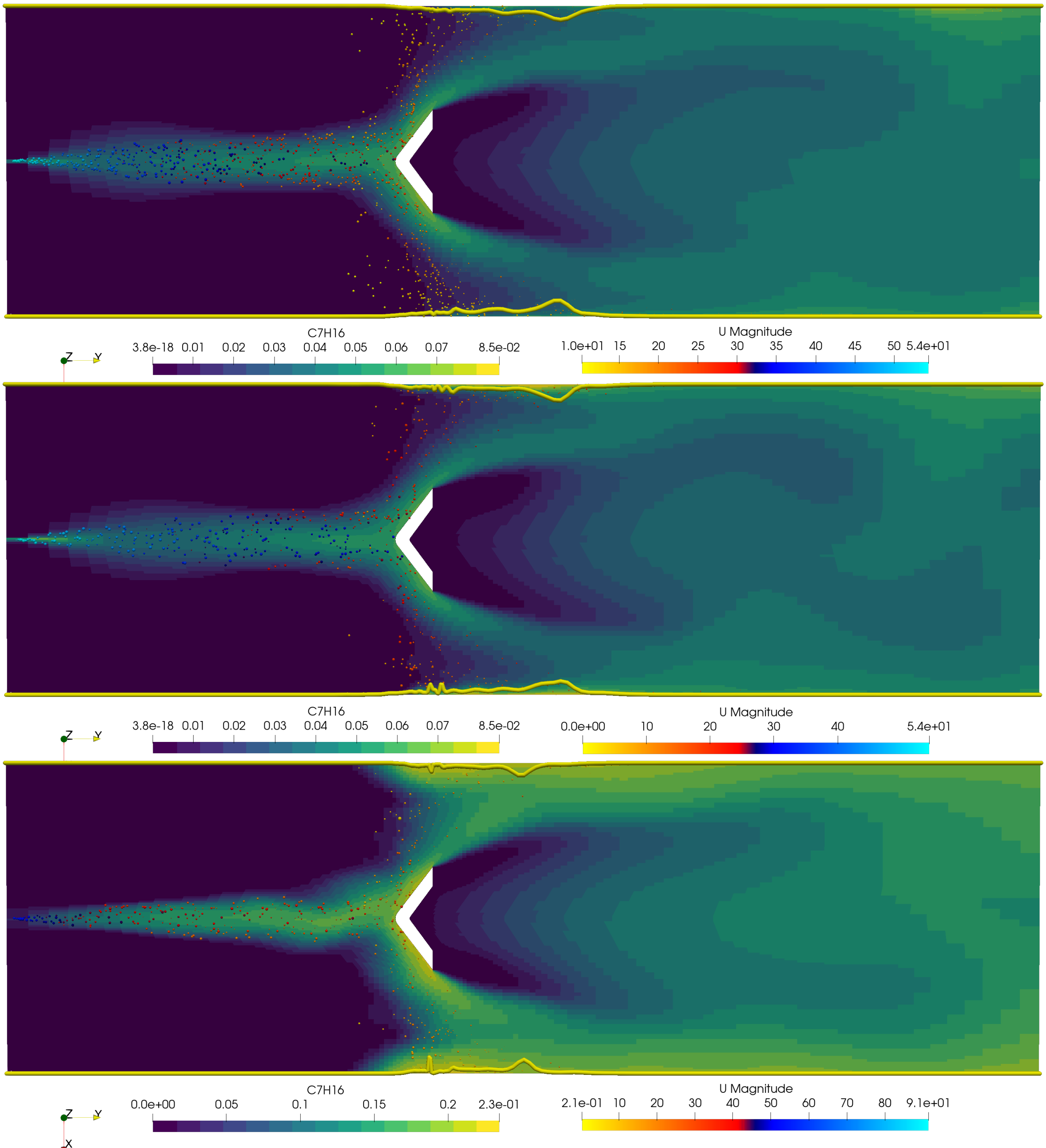
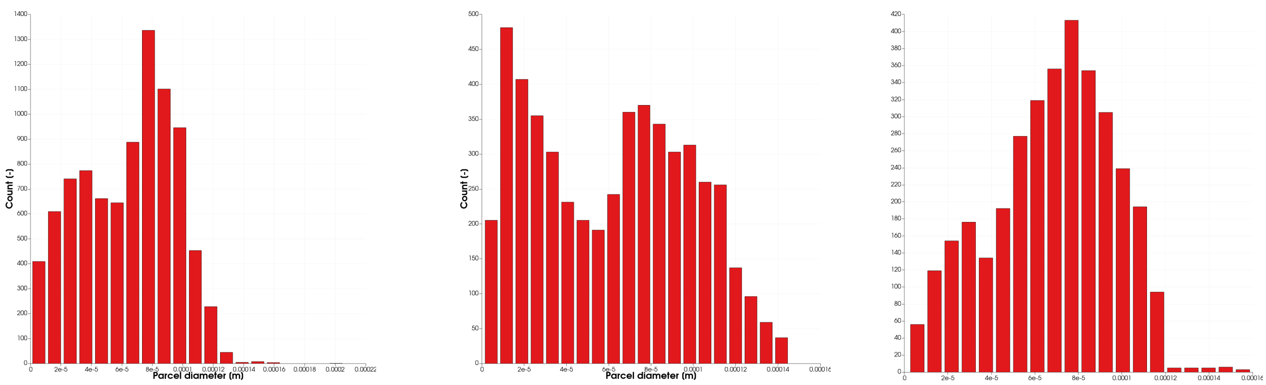


Figure 7: Fuel mass fraction contour for the three testCases and visualization of parcel distribution and liquid film thickness for timestep 0.28s.



(a) testCase1 (b) testCase2 (c) testCase3

Figure 8: Velocity contour at last iteration, t = 0.8s.