Simulation and design analyses of turbulent combustion in Diesel engines

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Summary

Stringent legislation of EURO standards on emissions from diesel engines present a strong challenge to the engine designers who are forced to produce first prototypes with a design closer to that of the final engine. Hence it becomes crucially important to develop effective numerical tools.

A numerical procedure is described here with the objective of quantifying the generation and depletion of the pollutants, NO_x and particulate matter emission from diesel engines. The diesel fuel reaction mechanism included **43** species and **393** reactions. The ignition was treated as a homogeneous reaction and, for the combustion at later stages, the mechanism was reduced with Intrinsic Low Dimensional Manifolds **(**ILDM**)** technique. Balance equations are solved on a moving mesh with models of spray break-up and evaporation. The turbulence-chemistry reciprocity was based on the concept of the "time-layered ILDM". This model required a time scale from a **3**-D turbulent reacting flow, and is able to retrieve the corresponding local mean source values from a pre-processed data base. The main advantage of this method is to take into account non-equilibrium states of the combustion thermo-chemistry.

Introduction

With the advance of combustion technologies, use of Diesel engines rapidly spreads from its conventional use in heavy duty applications to light vehicles. Stringent regulations on the emissions of NO_x and soot, however, force the manufacturers to re-design the Diesel in-cylinder processes. Efforts along these directions have eventually led to new concepts, as for example, high swirl in-cylinder flows, high pressure injections, etc. Complex designs require complex models which are difficult to adapt to a wider ranges of design parameters. Attempts for **3**D simulation with global chemistry cannot capture the details of auto-ignition process and suffer from the lack of intermediate species, which proves to be very important for emission predictions. It appears that better modelling of turbulent mixing with reduced chemistry improves significantly the accuracy of the simulations. An important approach to trace chemistry of pollutant formation is to use Intrinsic Low Dimensional Manifolds **(**ILDM**)** technique as a reduction scheme. The key issue in turbulent combustion is to model turbulence-chemistry reciprocity: Transport of joint pdf models produces most accurate results but it is computationally expensive and nearly impossible to use in engine geometries. Therefore, presumed pdf methods are widely used in engineering calculations.

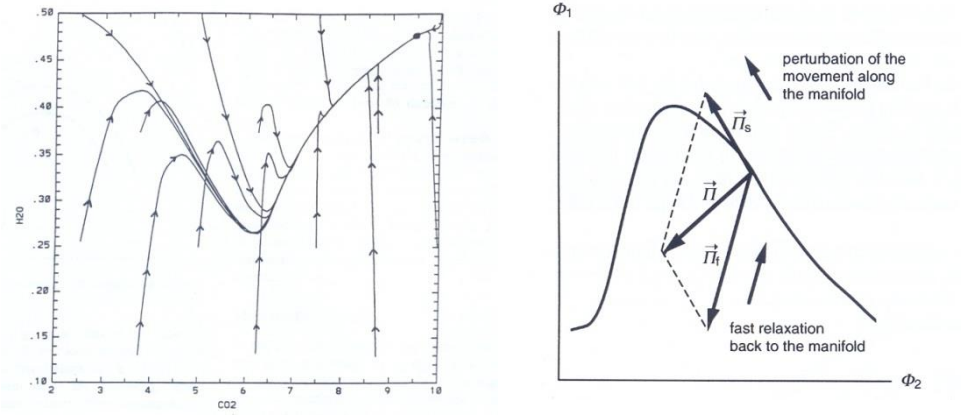


Figure **1**. Fast reactions are relaxed to manifold of slow reactions **[**U. Maas and S. B. Pope **(1992)]**.

From the system dynamics perspective, a chemical process with n_s species will be governed by n_s different time scales. ILDM, in principle, tries to find out the directions in which the chemical source term vector will rapidly reach a steady-state. If n_f fast processes are assumed in dynamic equilibrium, the system can be described by $n_r = n_s - n_f$ degrees of freedom by mixture fraction, pressure, enthalpy and n_r progress variables which parameterize the slow movement on the manifold. This reduces the chemical system in the composition space and the number of transport equations that need to be solved and, also, reduces the dimension of the probability density function that the reaction rate needs to be integrated over in turbulent flows.

ALU **(**Arbitrary Lagrangian Eulerian**)** method is used to solve the equations expressing conservation of mixture mass, momentum, enthalpy expressed as,

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \right) = \overline{\dot{\rho}_i^{\mathrm{S}}}$$

$$\frac{\partial \bar{\rho} \tilde{\boldsymbol{u}}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \tilde{\boldsymbol{u}} \right) = \nabla \cdot \left(\underline{\underline{\sigma}} - \overline{\rho \boldsymbol{u}' \boldsymbol{u}'} \right) - \nabla \tilde{p} + \overline{\boldsymbol{F}^{\mathrm{S}}} + \nabla \left(2/3 \, \rho k \right)$$

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \tilde{E} \right) = -\tilde{p} \nabla \tilde{\boldsymbol{u}} - \nabla \cdot \left(\bar{\boldsymbol{J}}_q - \overline{\rho \boldsymbol{u}' E'} \right) + \bar{\rho} \tilde{\varepsilon} + \overline{\dot{Q}^{\mathrm{C}}} + \overline{\dot{Q}^{\mathrm{S}}}$$

where s refers spray and c chemistry-related terms. The equation for the mean mixture fraction,

$$\frac{\partial \bar{\rho} \tilde{\xi}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \tilde{\xi} \right) = \nabla \cdot \left(\bar{\rho} D_{\mathrm{T}} \nabla \tilde{\xi} \right) + \overline{\rho \dot{\xi}^{\mathrm{S}}}$$

is solved together with the equation for its variance.

$$\frac{\partial \bar{\rho} \overline{\xi''^2}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \overline{\xi''^2} \right) = \nabla \cdot \left(\bar{\rho} D_{\mathrm{T}} \nabla \overline{\xi''^2} \right) - 2 \bar{\rho} D_{\mathrm{T}} \left(\nabla \tilde{\xi} \right)^2 - 2 \rho \frac{\tilde{\varepsilon}}{\tilde{k}} \overline{\xi''^2} + \overline{\dot{\rho}^{\mathrm{S}} \xi''^2} \left(\frac{1 - 2 \tilde{\xi}}{\tilde{\xi}} \right)$$

For reaction progress variables, as for example CO_2, the transport is given as,

$$\frac{\partial \bar{\rho} \tilde{Y}_{\mathrm{CO_2}}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \tilde{Y}_{\mathrm{CO_2}} \right) = \nabla \cdot \left(\bar{\rho} D_{\mathrm{T}} \nabla \tilde{Y}_{\mathrm{CO_2}} \right) + \overline{\rho \dot{Y}_{\mathrm{CO_2}}^{\mathrm{C}}}$$

and its variance

$$\frac{\partial \bar{\rho} \overline{Y''^2_{\mathrm{CO_2}}}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{u}} \overline{Y''^2_{\mathrm{CO_2}}} \right) = \nabla \cdot \left(\bar{\rho} D_{\mathrm{T}} \nabla \overline{Y''^2_{\mathrm{CO_2}}} \right) - 2 \bar{\rho} D_{\mathrm{T}} \left(\nabla \tilde{Y}_{\mathrm{CO_2}} \right)^2 - 2 \rho \frac{\tilde{\varepsilon}}{\tilde{k}} \overline{Y''^2_{\mathrm{CO_2}}}$$

where averaged quantities are defined using,

$$\bar{\phi} = \frac{1}{N_{\mathrm{cyc}}} \sum_{n=1}^{N_{\mathrm{cyc}}} \phi_n \quad \text{and} \quad \tilde{\phi} = \frac{\overline{\rho \phi}}{\bar{\rho}}$$

The computational setup is designed to match FORD I**5**, a **5**-cylinder diesel engine with **3.2** lt cylinder volume, which was disretized in 184,487 cells as shown in Figure **2**,

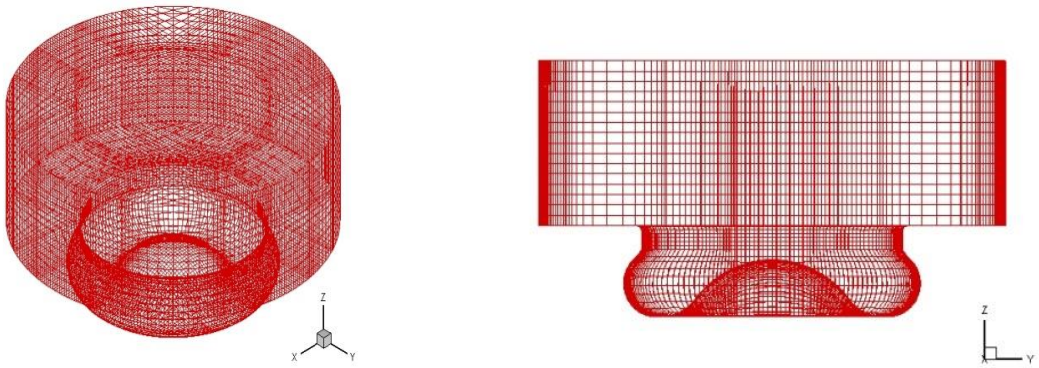


Figure 2. Computational domain.

The spray injection profile is shown in Figure **3**.

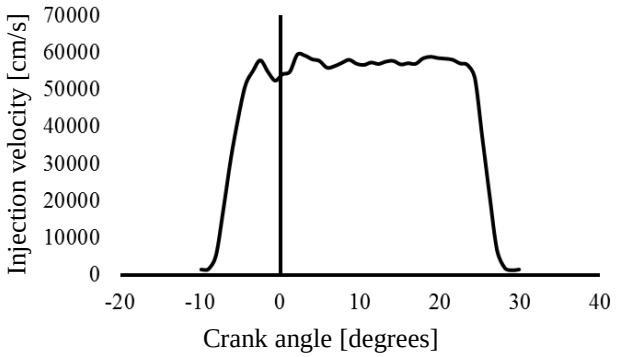
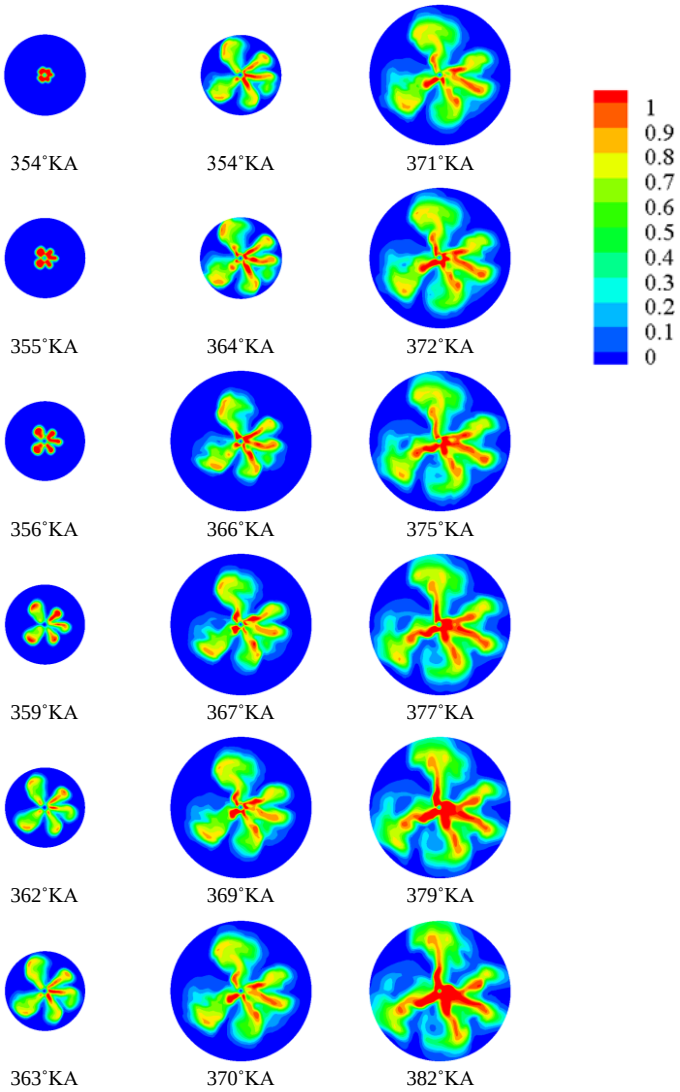
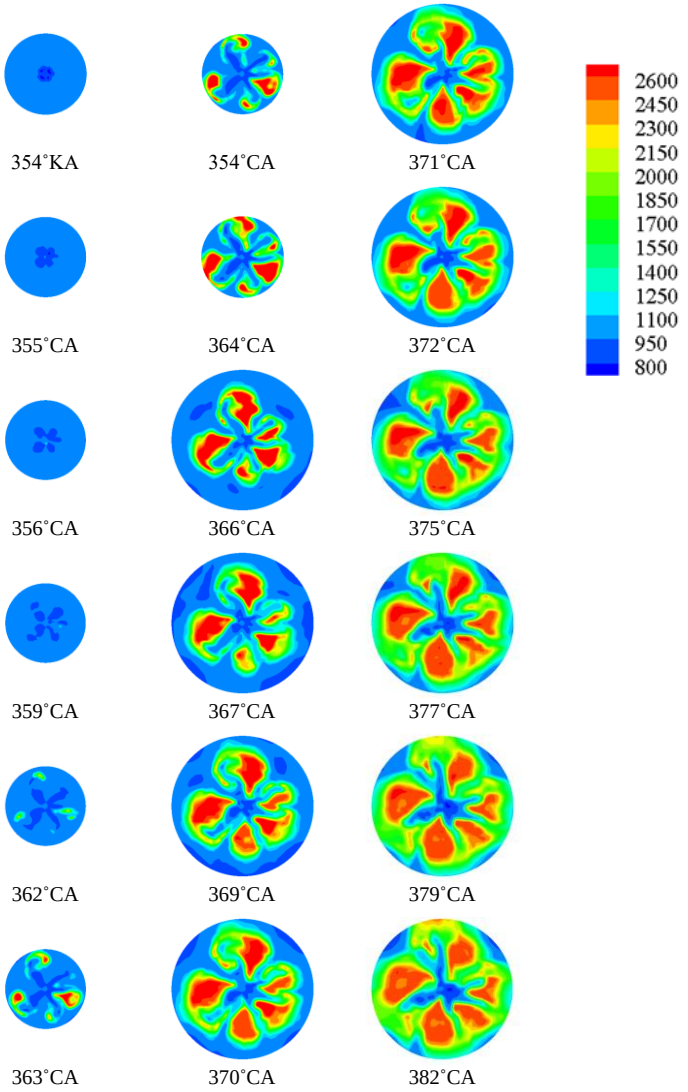


Figure 3. Injection timing.

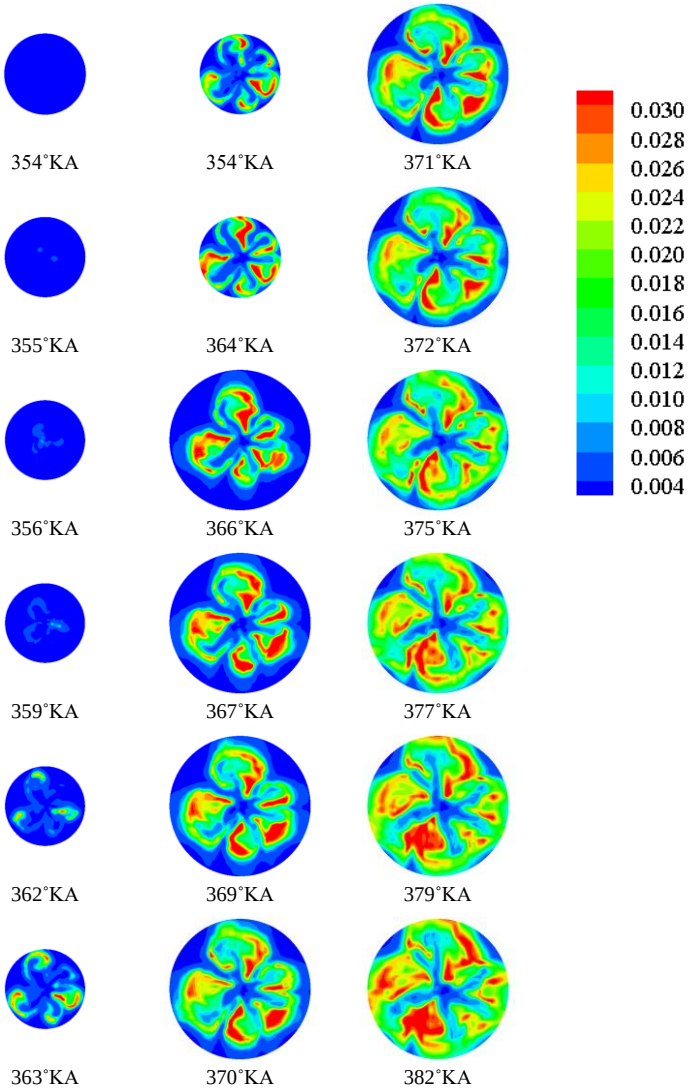
Results; Mixture fraction



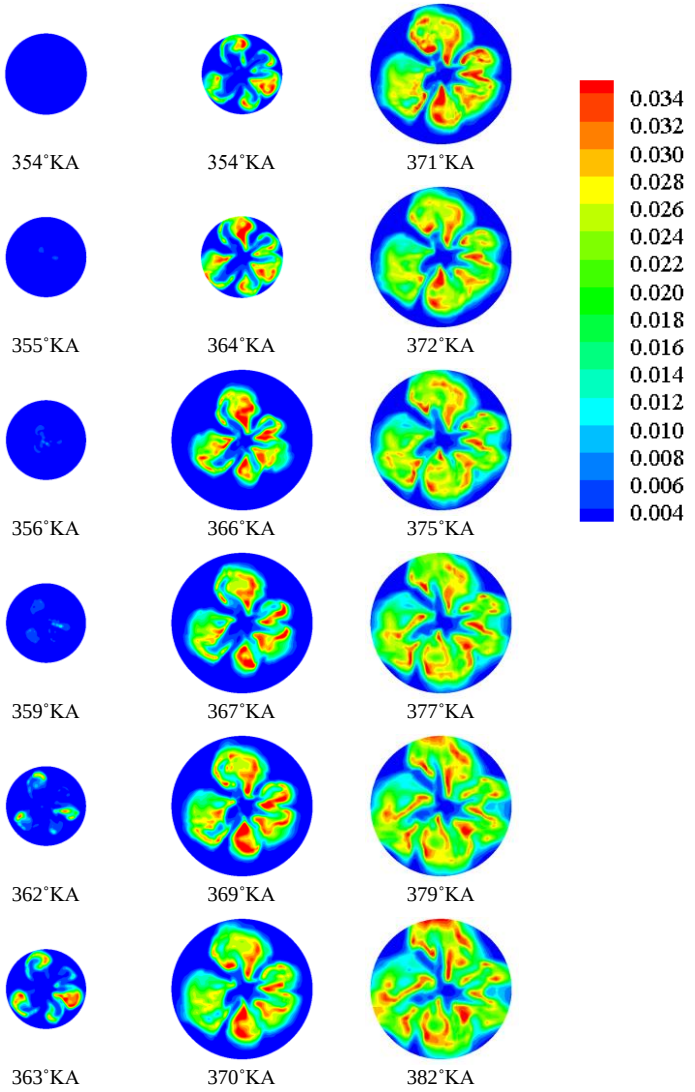
Results; Temperature



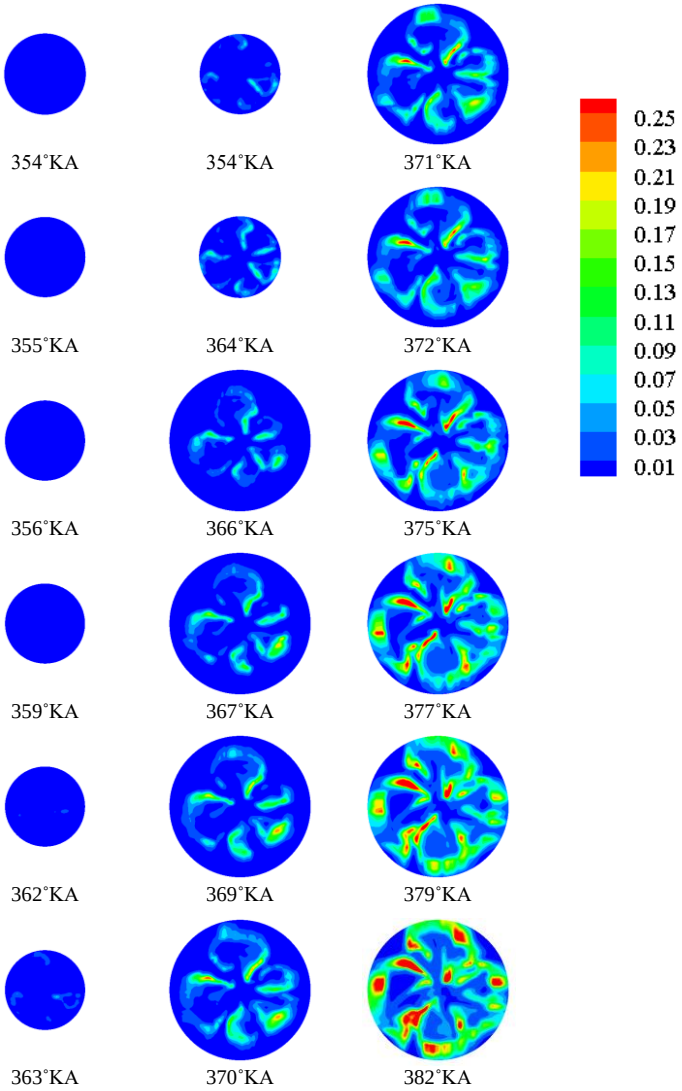
Results; CO_2 Mass fraction



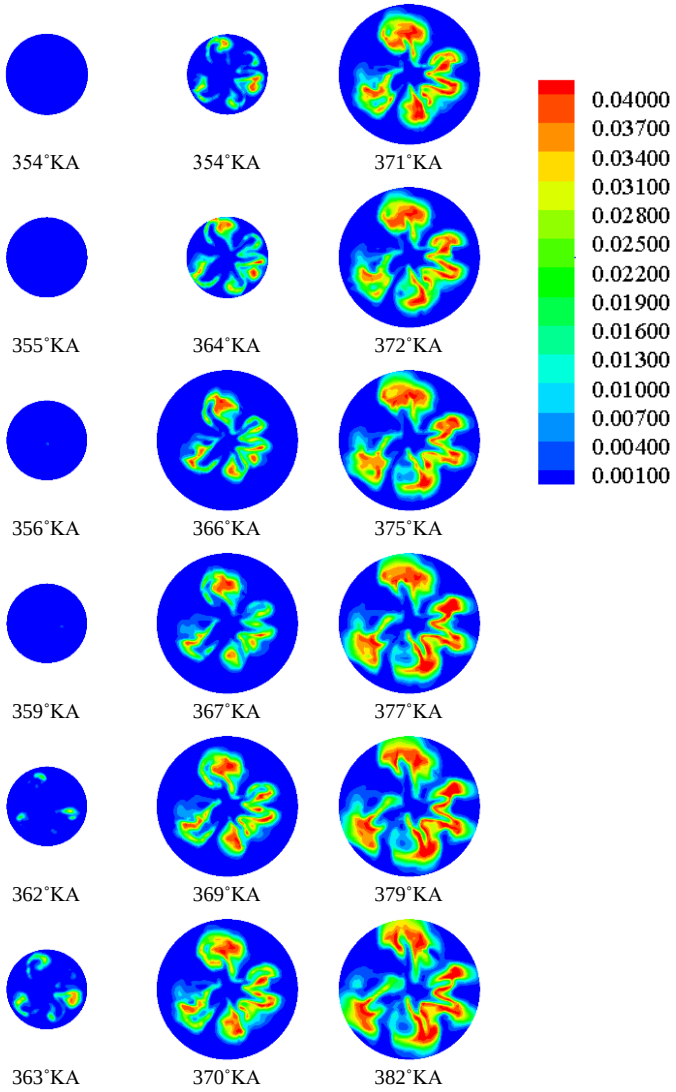
Results; H_2O Mass fraction



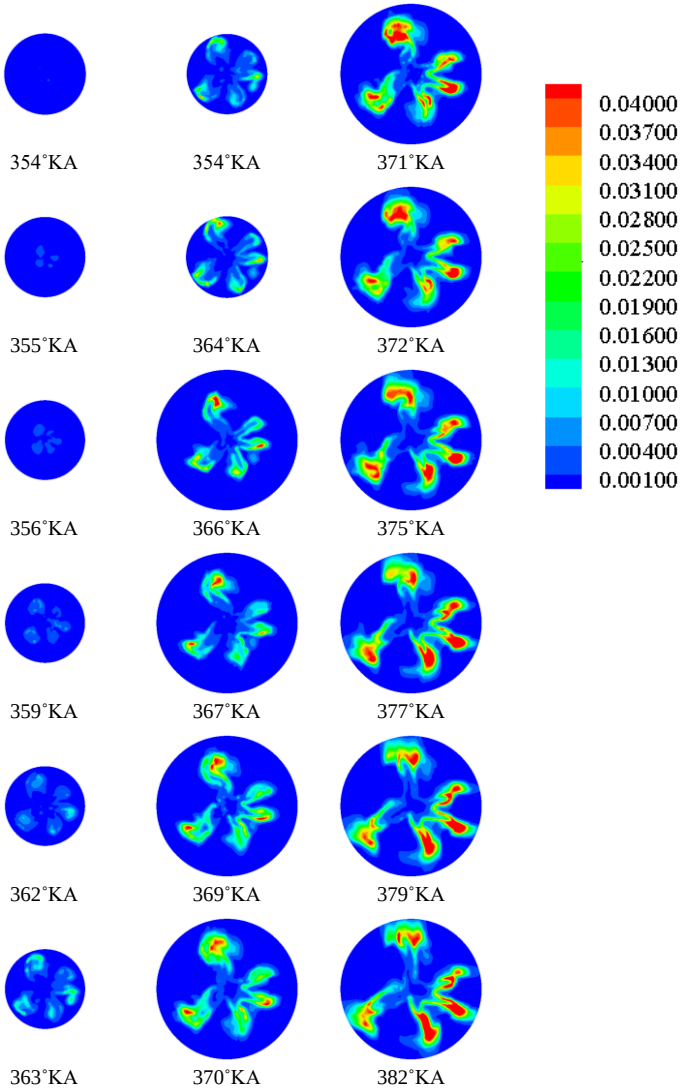
Results; NO Mass fraction

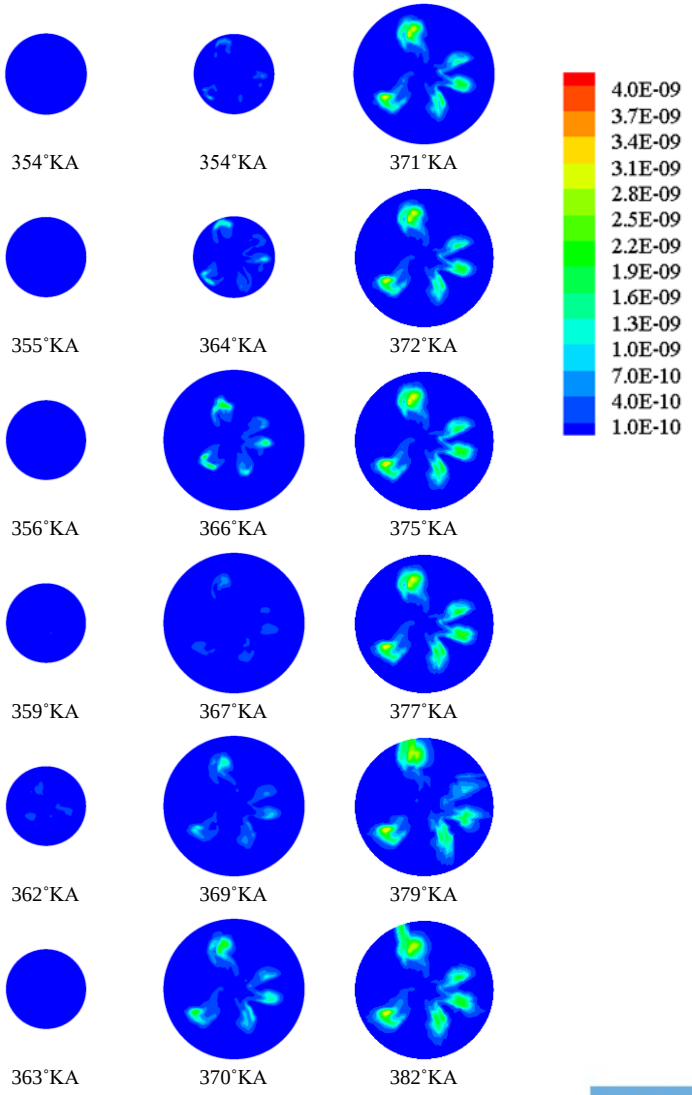


Results; CO Mass fraction



Results; Soot precursor & soot volume fraction





Results; Soot vs crank angle

N_s [1/cm^3]