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Les Sprays

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Diesel fuel spray penetration, heating, evaporation and ignition: modelling versus experimentation

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Introduction

Overview of the results of numerical and theoretical studies of processes in sprays.

The main focus is made on sprays found in technology of high-pressure atomisation in direct injection Diesel engine.

Structure of presentation

- Objectives
- Methods
- Results of numerical studies:
  - Penetration of “cold” sprays
  - Autoignition in Diesel sprays
- Conclusions

Objectives

- Development of advanced analytical and numerical models for in-cylinder processes in internal combustion (IC) engine
- Implementation of the models in KIVA II spray code
- Validation of the models against in-house measurements

Stages of research

Studies of dynamics of “cold” sprays (with a view of automotive, environmental, biomedical, etc applications). Modelling of processes of liquid injection, atomisation into droplets, gas-droplet momentum exchange, droplet collisions, dispersion, etc.

Studies of processes in “hot” sprays (Diesel engine). Modelling of gas-droplet heat and mass transfer, and fuel autoignition.

KIVA II - Methodology

- Eulerian (gas)/ Lagrangian (liquid) code for computation of flows with sprays and chemical reactions
- Liquid phase is represented by droplet parcels, characterising droplets of a given size, velocity and temperature
- Stochastic sampling technique is applied to describe droplet injection, collisions, breakup and turbulent dispersion

KIVA II customised version

- Advanced models of spray breakup (Patterson and Reitz, 1998; Gorokhovski and Saveliev, 2003)
- Effects of cavitation (Sarre and Kong, 1998)
- Advanced models for droplet heating and evaporation (Sazhin, 2006)
- Shell autoignition model (Halstead, 1977)

Stage 1 – Studies of "cold" sprays

- In-house measurements
- Results of studies:
  - Conventional spray breakup models
  - A new phenomenological breakup model
- Conclusions

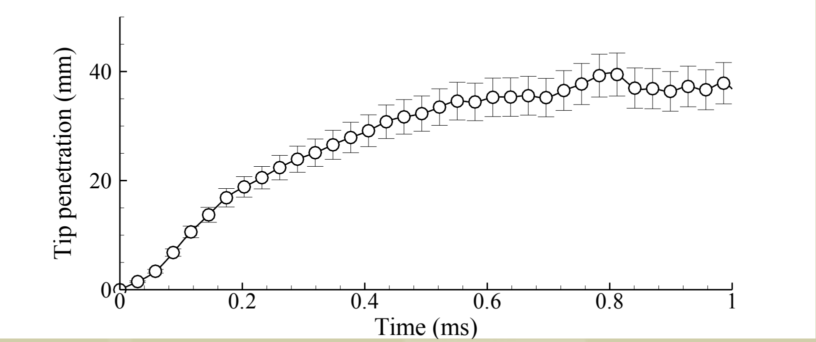
Experimental data. Validation test case

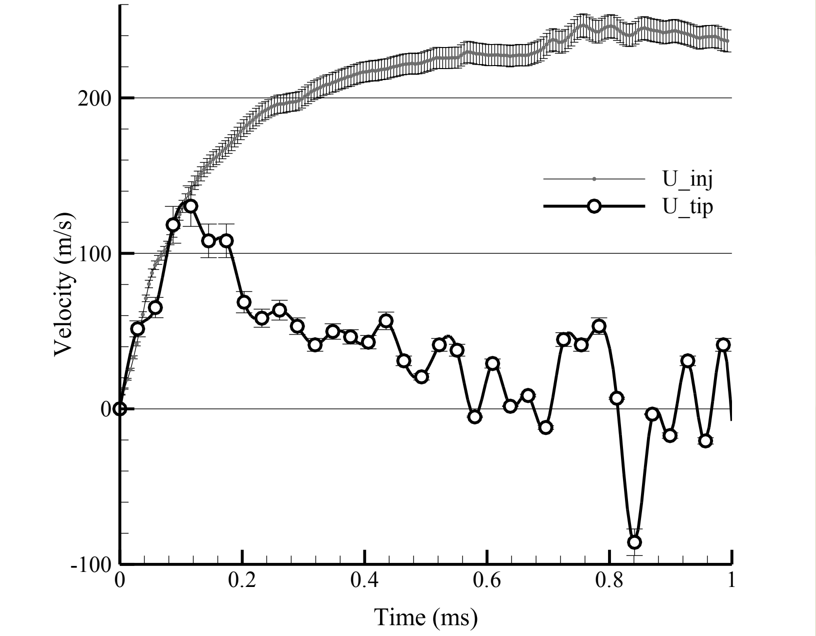
Measurements:

- Spray tip penetration (video recordings)
- Instantaneous rate of fuel injection (LUCAS rate tube)

Test case:

- 7-hole Diesel injector
- Nozzle diameter 0.135 mm
- Injection pressure 1600 bar
- In-cylinder pressure 20 bar





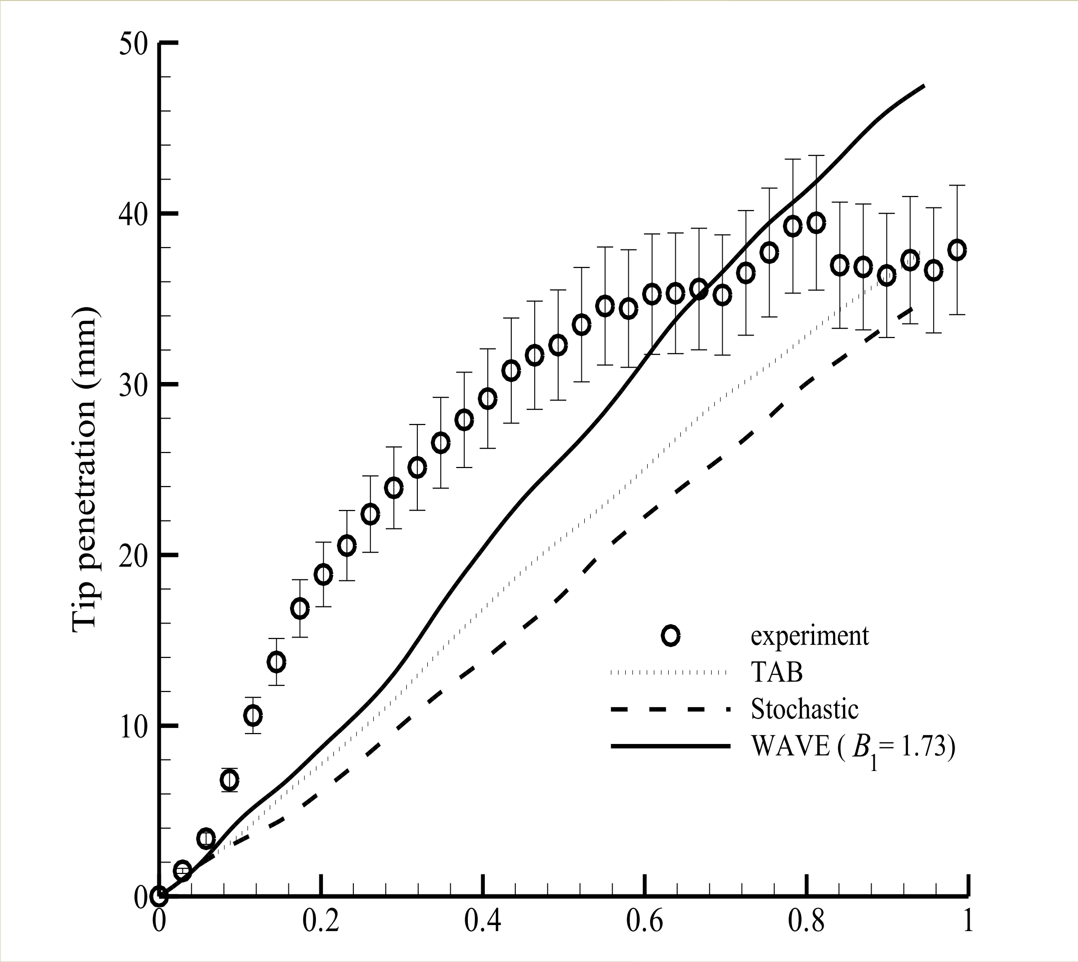
Conventional models of breakup

- Taylor Analogy Breakup model (O' Rourke and Amsden, 1987)
- Wave breakup model (Reitz, 1987)
- Stochastic breakup model (Gorokhovski and Saveliev, 2003)

All these models assume *quasi-steady-state* nature of breakup. The breakup time can be defined as:

$$\tau_{bu} = B_1 \frac{R}{U}\sqrt{\frac{\rho_l}{\rho_g}} \qquad (B_1 = \sqrt{3}\,..\,100)$$

Results of computations



Effects of cavitation

- Effects of cavitation are described using the dimesionless criterion – “cavitation number” CN.
- Parameters of injected parcels (diameter and velocity) are modified depending on CN.

Diesel fuel spray
(photograph by K. Karimi,
University of Brighton)

Phenomenological model of breakup in transient sprays

Experimental facts:

- At the start of injection the fuel is highly accelerated, and
- spray penetration rate is close the rate of injection.

Conventional models:

- An adjustable breakup time constant
- Do not take into account for a finite thickness of the boundary layer (BL) in the gas phase around the jet

However:

- Flow acceleration promotes thicker BL in the gas phase
- Thicker BL makes the liquid-gas inter-phase more stable

New model for the breakup time constant

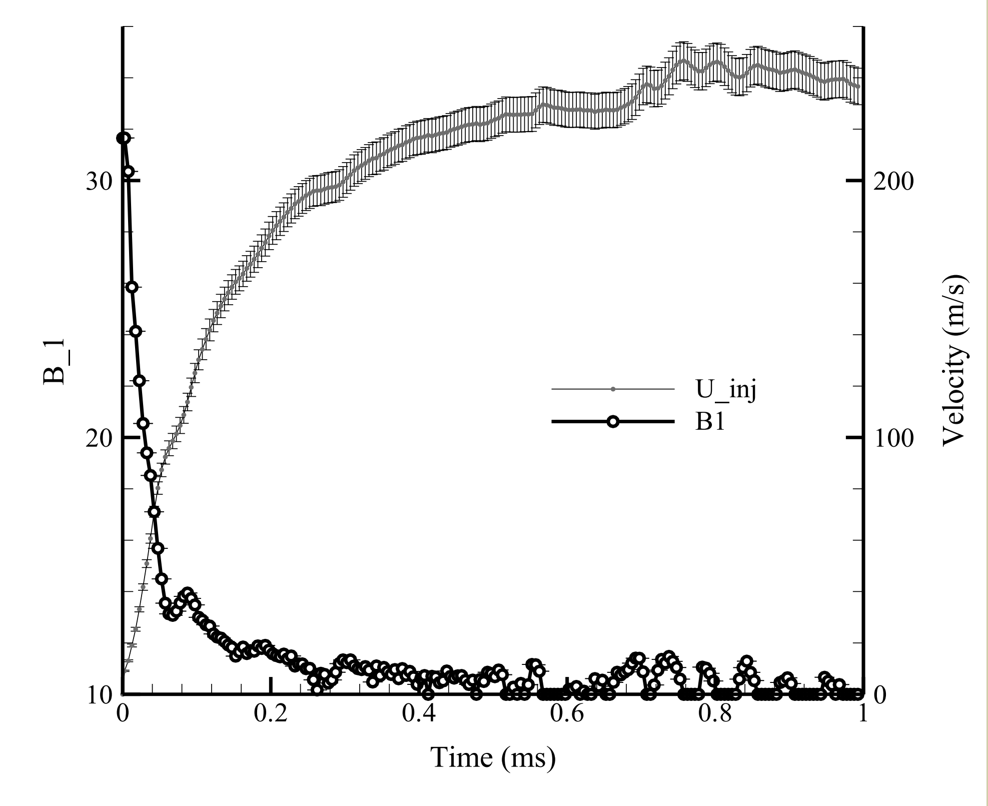
Basic concept – Wave breakup model (Reitz, 1987; Patterson and Reitz, 1998)

$$\tau_{bu} = B_{1,st} \frac{R}{U} \sqrt{\frac{\rho_l}{\rho_g}} \qquad B_{1,st} = 10$$

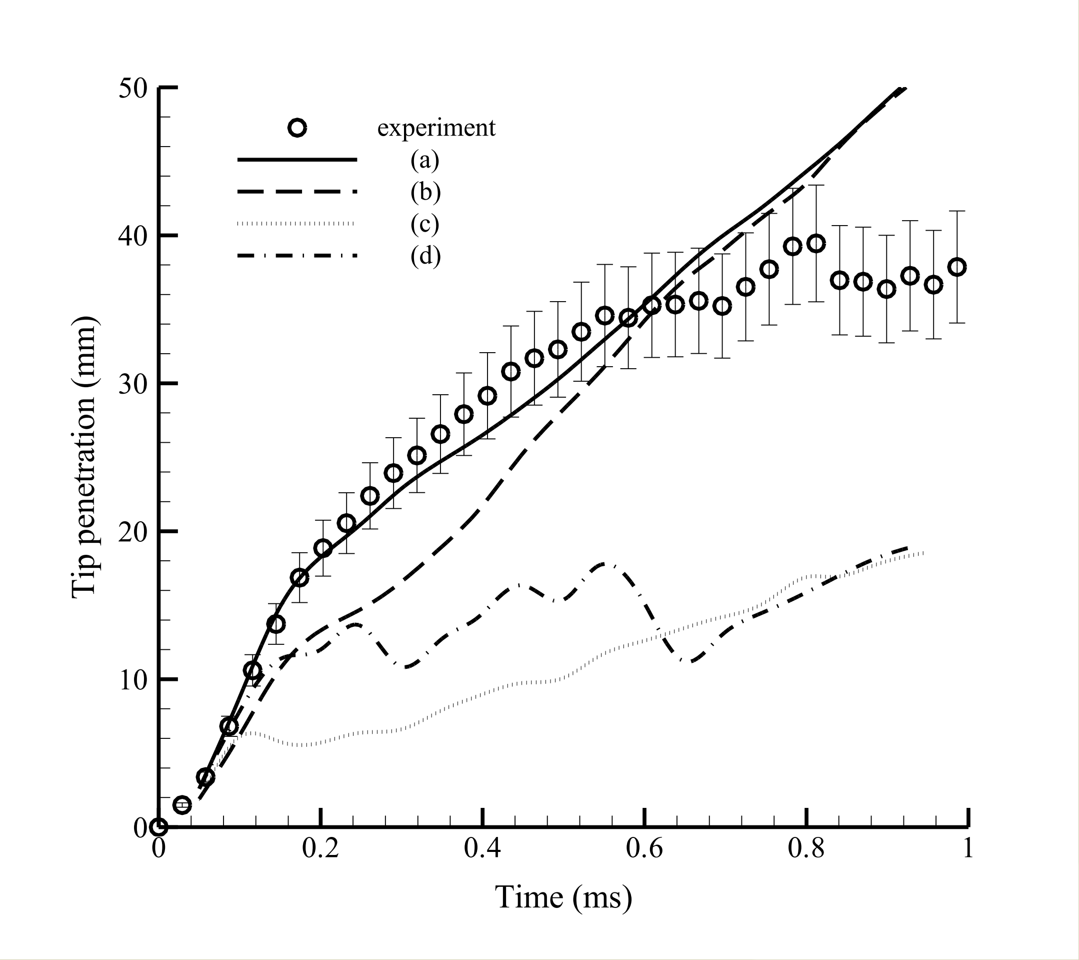
Phenomenological equation for the breakup time constant, taking into account for an effect of injection acceleration:

$$B_1 = B_{1,st} + c_1 \cdot \left(a^+\right)^{c_2}$$

$$a^+ = \sqrt{\mathrm{Re}} \frac{D}{U_{inj}^2} \cdot \frac{dU_{inj}}{dt}$$



Results – new model: spray tip penetration and breakup length

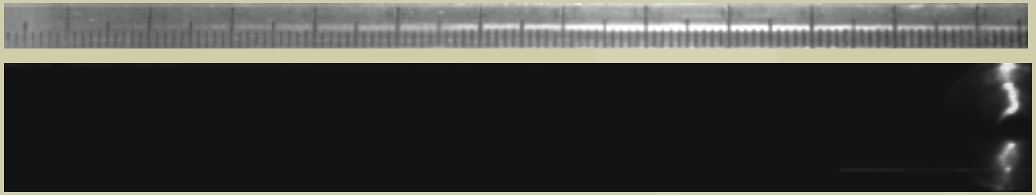


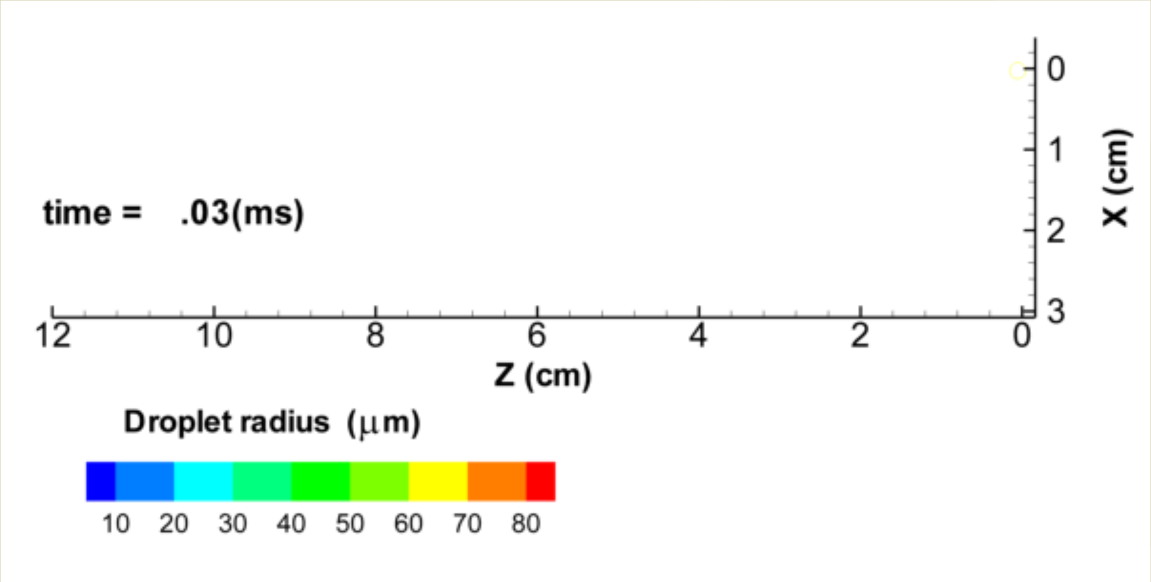
$c_1 = 0.5$

$c_2 = 0.2$

$R_{core}/R_o = 0.5$

Comparison with spray video

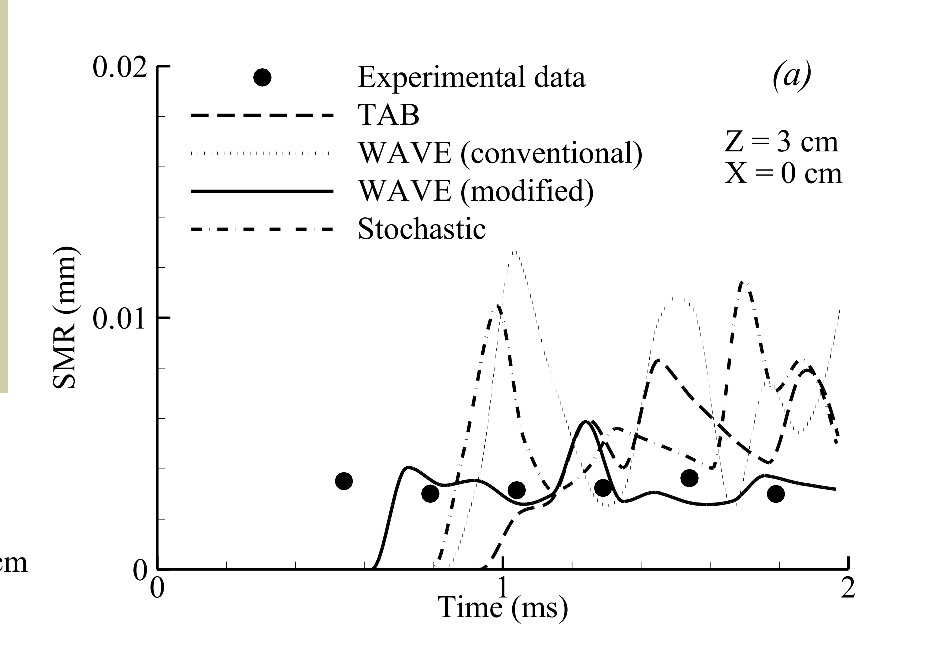


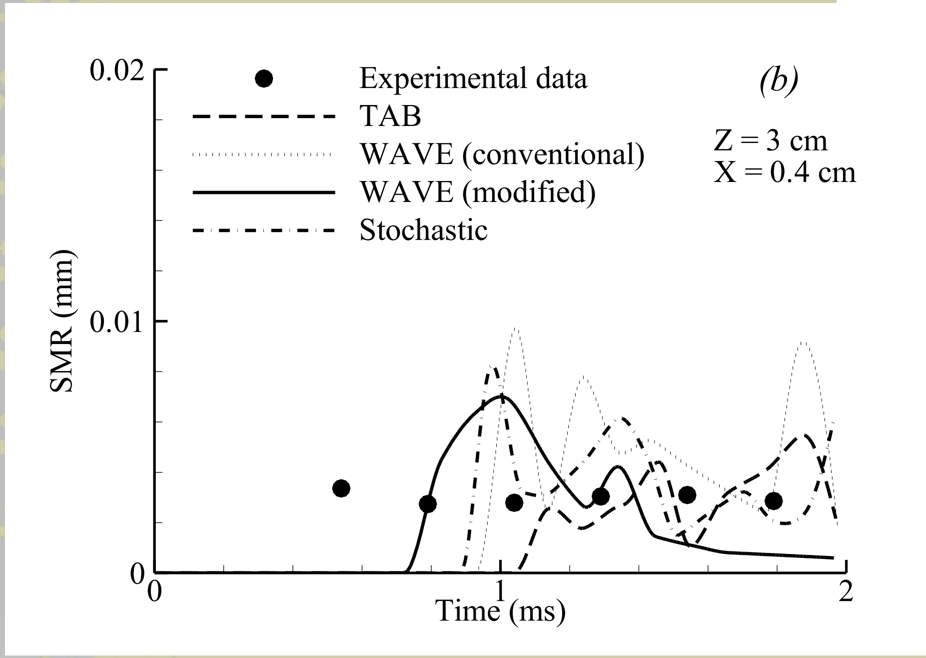


Comparison for the Sauter Mean Radius (SMR) of droplets

Measurements (Lacoste, 2005)

- Single-hole Diesel injector
- Nozzle diameter 0.2mm
- Injection presure 1600 bar
- In-cylinder pressure 40 bar





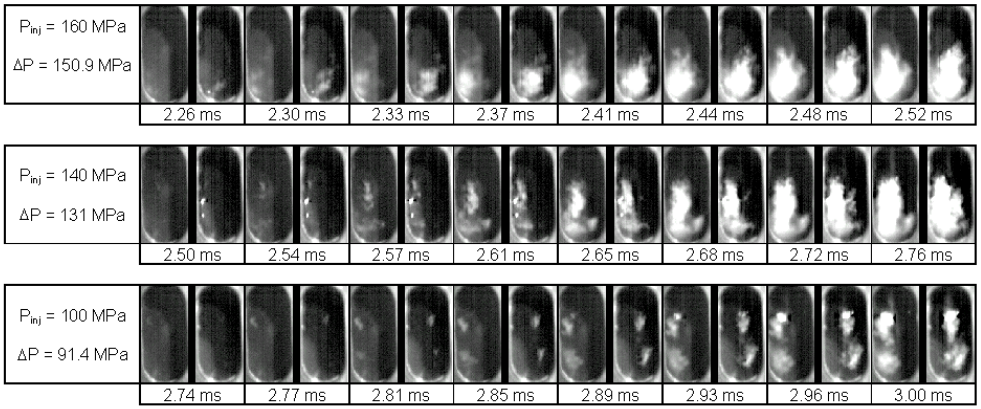
Conclusions. “Cold” sprays

- Several models of spray breakup has been implemented in KIVA code and validated against the in-house measurements of Diesel sprays
- A model for the breakup of accelerating sprays has been developed
- Further studies are needed to identify the range of application of the model

Stage 2 – “Hot” Diesel sprays

- Experimental observations
- Models of droplet heating and evaporation
- Shell model of autoignition
- Results of numerical studies

Measurements of autoignition delay time in Diesel sprays (Crua, 2002)



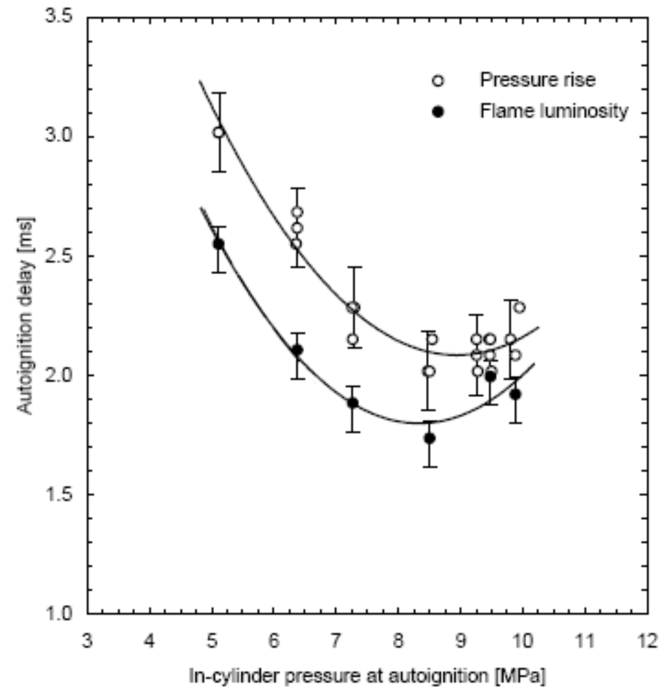


Figure 5-7. Comparison between autoignition delays detected by in-cylinder pressure rise, and by flame luminosity (100 MPa injection pressure, 720 K in-cylinder temperature). Times are relative to start of injection (when droplets are first seen leaving the nozzle). The injector nozzle shuts at 3.1 ms.

Total autoignition delay time comprises of the

- *chemical* ignition delay of the vapour fuel, and
- *physical* delay time, spent on liquid breakup, evaporation and mixing processes

Key processes in modelling of autoignition in Diesel sprays

- Liquid atomisation into droplets
- Droplet heating
- Droplet evaporation and vapour diffusion
- Autoignition of the air/ fuel mixture

Models of droplet heating and evaporation

Models of heat and mass transfer from evaporating droplets has been reviewed (Sazhin, 2006)

- Due to high diffusivity of the gas phase thermal conductivity can be considered steady-state for the gas, and transient for the liquid
- Heat transfer in the liquid and gas phases are modelled separately
- Preliminary study have shown that in presence of breakup choice of the liquid-phase model can have significant effect on the predicted rate of fuel evaporation

This study investigates the effects of heat-mass transfer on evaporation and ignition for realistic transient 3D Diesel sprays

Liquid phase models

- Infinite thermal conductivity (ITC) model – based on the assumption that there is no temperature gradient inside droplets
- Effective thermal conductivity (ETC) model – taking into account both finite liquid thermal conductivity and the re-circulation inside droplets via the introduction of a correction factor to the liquid thermal conductivity

Gas phase models

- Conventional KIVA describes the heat and mass transfer from the droplet surface using approximations for Nusselt and Sherwood numbers:

$$Sh_o = 2\left(1 + 0.3\,\mathrm{Re}_d^{1/2}\,Sc_d^{1/3}\right)$$
$$Nu_o = 2\left(1 + 0.3\,\mathrm{Re}_d^{1/2}\,\mathrm{Pr}_d^{1/3}\right)$$

- Abramzon and Sirignano (1998) have suggested more accurate approximations, taking into account finite thickness of thermal boundary layer around droplet, effects of variable properties, Lewis number, and the Stefan flow on heat and mass transfer between the droplet and the gas

Shell model (Halstead, 1977)

- Describes the autoignition chemistry using reduced mechanism of eight-step chain branching reactions between the fuel, O_2, products (H_2O, CO, CO_2), radicals (R), branching (B) and intermediate (Q) agents
- Originally was designed for autoignition in premixed fuels
- Later adopted for computation of autoignition in Diesel sprays (Sazhina et al, 1999). The rate of production of Q has been modified to: $A_{f4} = (3 - 6) \cdot 10^{6}$ The main challenge is 3D nature of spray
- Now implemented into KIVA II code (University of Rouen) and applied to describe experimental data collected at the University of Brighton (Crua, 2002)

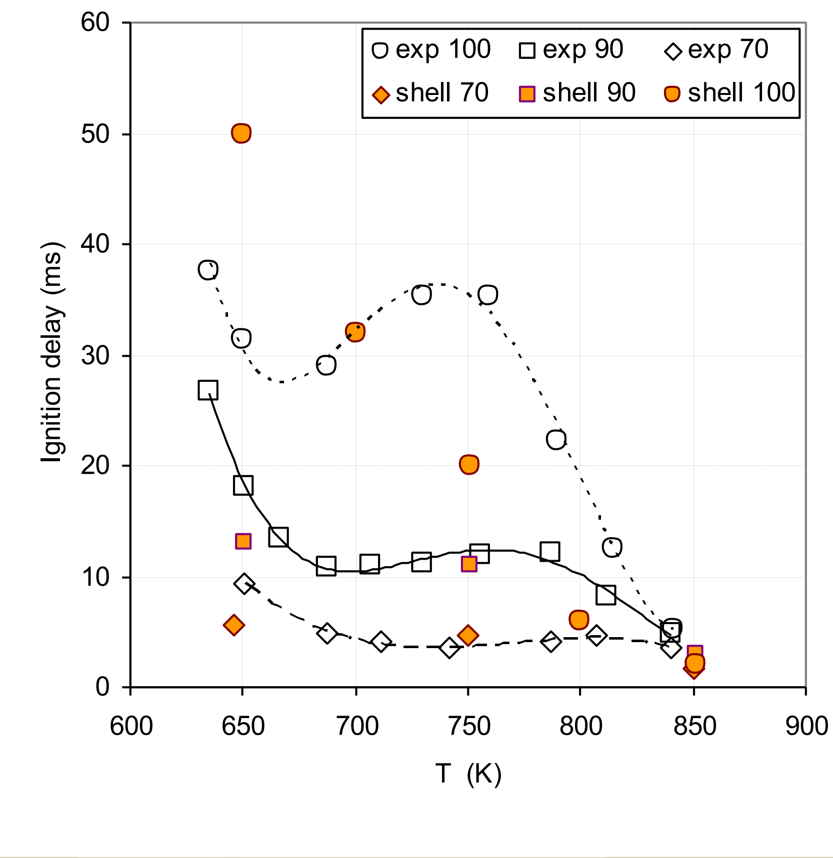
Basic validation case – autoignition in premixed fuel (Halstead, 1977)

Test conditions:

- Research octane number fuels:
  RON70, RON90, RON100
- Equivalence fuel/air ratio = 0.9
- Temperatures (TDC) = 650–850 K
- Pressures (TDC) = 17–23 bar

KIVA results:

- Mixture at TDC
- Shell autoignition model



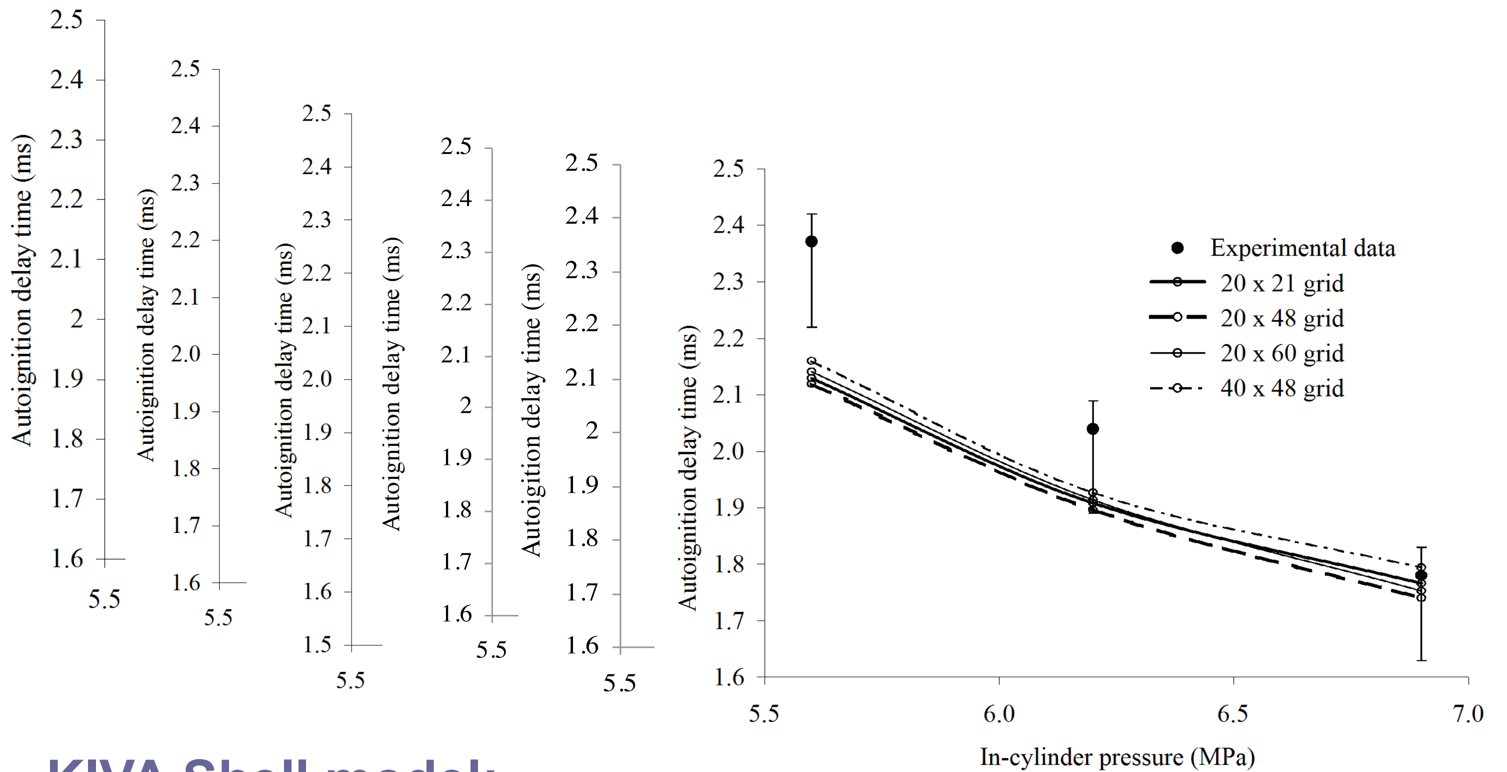
Computational studies of autoignition process in Diesel sprays

Test cases:

- Single-hole injector of nozzle diameter 0.2 mm;
- Injection pressure 1600 bar;
- Fuel temperature at injector 350-400 K (estimated).

In-cylinder temperatures at TDC (K)	832	847	852
In-cylinder pressure at TDC (bar)	56	62	69
Autoignition delay time (ms)	2.37	2.04	1.78

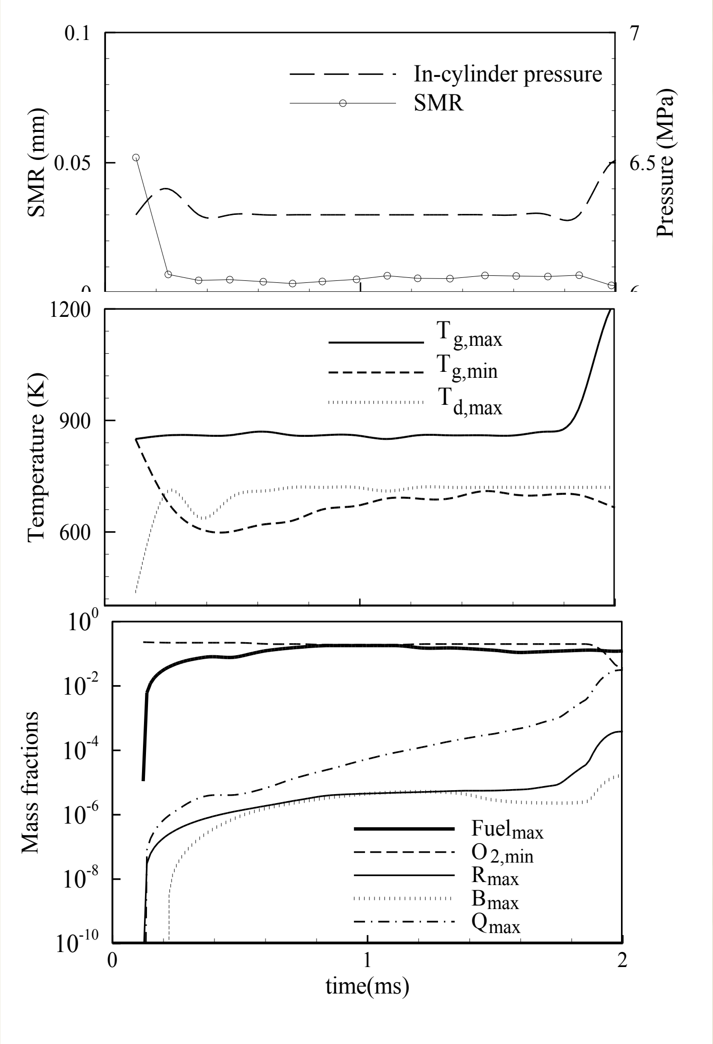
Results – ignition delay time



KIVA Shell model:

- Kinetic parameters - fuel RON 70
- $A_{f4} = 3 \cdot 10^{6}$.

Results – pre-ignition spray

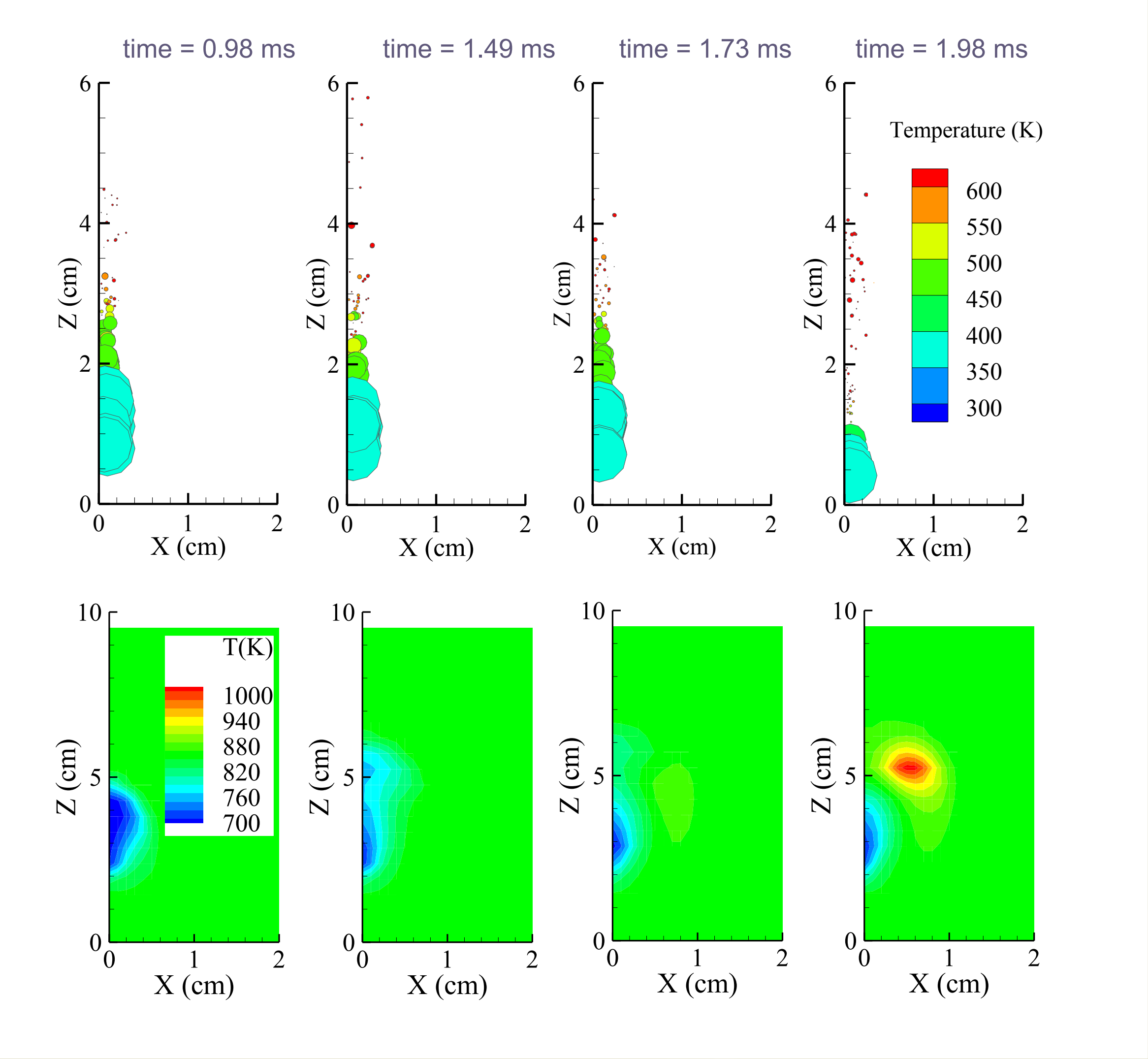


Integral properties of an autoigniting spray

Contribution of the spray processes to the ignition delay time:

- Spray breakup
- Droplet heating and evaporation
- Autoignition

Results – pre-ignition spray



Conclusions. “Hot” sprays

- Stages of autoignition have been quantified
- Ignition delay time has been shown to be sensitive to the choice of liquid-phase model and predicted gas temperature (turbulence model)
- Specifics of initial stage of breakup has negligible effect on ignition for “single-pulse” sprays considered, but can be important for pilot and split injection schemes

Summary

- A modified Wave breakup model has been developed and applied to predict Diesel sprays
- Several heating and evaporation models has been implemented in KIVA code
- Shell model implemented into KIVA code has been applied to predict autoignition in Diesel sprays
- The results of studies are summarised in two papers prepared for publication

Directions for future studies

- Theoretical studies:
  - stability and breakup of transient jets and sprays
- Experimental studies:
  - breakup length in transient sprays
- Modelling and numerical analysis:
  - time constant for the primary atomisation in stochastic breakup model
  - computation of heat-mass transfer at supercritical in-cylinder temperatures and pressures
  - analysis of the limiting phases (kinetics and diffusion) of autoignition using Shell model
  - fuel combustion and soot formation models in KIVA

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Thank you ☺