UNIVERSITÉ DE ROUEN

University of Brighton

EUROPEAN UNION

PROGRAMME EUROPEEN FRANCO-BRITANNIQUE INTERREG IIIA

FRANCO-BRITISH INTERREG EUROPEAN PROGRAMME

Les Sprays

Posters

1. ‘**Les Sprays**’. *Poster displayed permanently at the University of Brighton*
2. **‘Les Sprays’** S. Sazhin, M. Heikal, C. Crua, S. Martynov, E. Sazhina, M. Gorokhovski, and A. Chtab. *Poster presented at the INTERREG Showcase Event,* 1 March, 2006, Ashford.
3. **Modelling of Cavitation Flow in a Diesel Injection Nozzle** S. Martynov, D. Mason, Heikal and S. Sazhin. *Poster presented at UK national science week 2006. Annual Presentations by Britain Top Younger Scientists, Engineers and Technologists at the House of Commons*, 13 March 2006, London.
4. **Modelling of Droplet Heating, Evaporation and Break-up: Recent Developments** S. Sazhin, S. Martynov, I. Shishkova, C. Crua, K. Karimi, M. Gorokhovski, E. Sazhina and M. Heikal**.** *Poster presented at 13th International Heat Transfer Conference*, 13-18 August, 2006, Sydney.
5. **Modelling of Cavitation Flow in a Nozzle and its Effect on Spray Development** S. Martynov, D. Mason, M. Heikal, S. Sazhin and M. Gorokhovski. *Poster presented at 13th International Heat Transfer Conference***,**13-18 August, 2006, Sydney.
6. **Oscillating Jets and Sprays in Modern Technologies** S. Martynov, S. Sazhin, and M. Heikal. *Poster presented at the BISME conference, KTP*, 10-12 September, 2006, University of Brighton.
7. **CFD Modelling of Spray Processes** *Poster presented at the opening of the “Sir Harry Ricardo Laboratories”*, 14 November, 2006 and at *Brighton Science and Engineering Fair, University of Brighton*, 14 March, 2007.
8. **Advanced Models for Droplet Heating and Evaporation: Effect on the Autoignition of Diesel Fuel Sprays** S.S. Sazhin, C. Crua, S.P. Martynov, T. Kristyadi, and M. Heikal**.** *Poster presented at the Third European Combustion Meeting* ECM 2007, paper 15-2, 11-13 April, 2007, Crete.
9. **Autoignition of n-pentane in a Rapid Compression Machine: Experiment versus Modelling** M. Ribaucour, R. Minetti, E.M. Sazhina, S.S. Sazhin. *Poster presented at the Third European Combustion Meeting* ECM 2007, paper 1-1, 11-13 April, 2007, Crete.

FRANCO-BRITISH INTERREG IIIA PROGRAMME

LES SPRAYS

supported by the European Regional Development Fund (ERDF) and Ricardo Consulting Engineers Ltd (UK)

S. Sazhin[1], M. Heikal[1], C. Crua[1], S. Martynov[1], E. Sazhina[1], M. Gorokhovski[2], and A. Chtab[2]

[1] University of Brighton, U.K., [2]University of Rouen, France

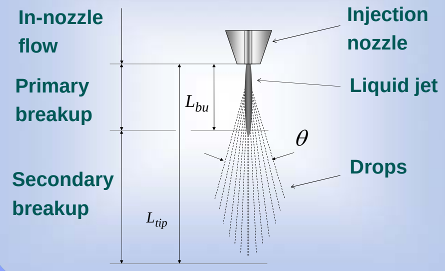
OBJECTIVES

- Development of a strategy for the calculation of high-speed atomisation
- Development of an atomisation model which takes into account the primary and secondary stages of spray breakup
- Application of this model for the calculation of sprays in diesel engine and other engineering and environmental applications

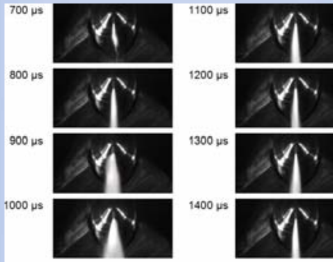
SPRAY MEASUREMENTS

- Application of high-speed video imaging, PDA and PIV measurements of fuel sprays for the validation of computational models of sprays
- Study of the transient behaviour of fuel sprays
- Imaging of jet breakup at the nozzle exit
- Measurements of the spray characteristics far from the nozzle

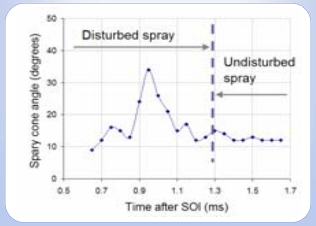
SPRAY STRUCTURE



HIGH-SPEED IMAGING OF DIESEL SPRAYS



- Oscillations of the spray angle are caused by the flow processes inside the injector during the first time after needle opening

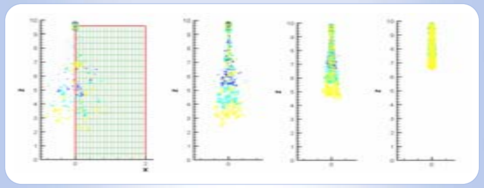


NUMERICAL MODELLING

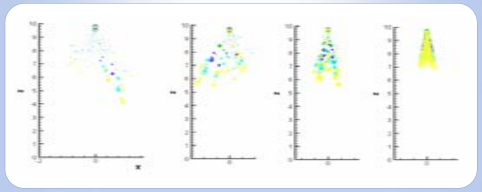
- Development of a strategy for the computation of liquid sprays
- Development of a new model of sprays dynamics
- Implementation of the new model into the code KIVA 2
- Validation of the models against experimental measurements
- Analysis of the influence of physical parameters on the spray characteristics

PRELIMINARY RESULTS OF CALCUALTIONS USING *KIVA 2* CODE

- Injection of undeformed droplets gives a narrow spray angle



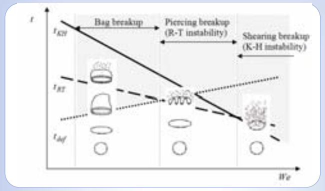
- Injection of deformed droplets gives a wider spray angle:



- The deformation of droplets is related to the effect of cavitation and turbulence

DROPLET BREAKUP REGIMES

A scheme of development of bag, piercing and shearing break-ups is suggested.



The scheme takes into account variation of the characteristic times t_{def}, t_{RT} and t_{KH} with Weber number.

t_{def}, t_{RT} and t_{KH} refer to the timescales of droplet deformation, development of the Rayleigh-Taylor and Kelvin-Helmgoltz instabilities, respectively

BRITISH INTERREG TEAM

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LES SPRAYS

Franco-British INTERREG IIIA program sponsored by the European Regional Development Fund (ERDF) and Ricardo Consulting Engineers Ltd (UK)

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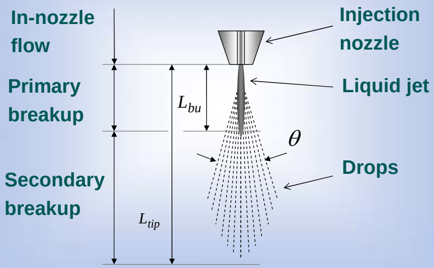
SPRAY STRUCTURE



SELECTED APPLICATIONS OF JETS AND SPRAYS

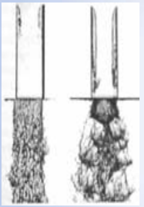
- Automotive industry – fuel injectors
- Environmental – aerosols and particle pollutions
- Agricultural – sprinkling and spraying
- Medical – drugs delivery

HOW CAN YOU BENEFIT FROM OUR STUDY?

- Full control of spray (parameters of dispersion phase, rate of penetration, evaporation, etc.)
- Efficient energy consumption
- Recommendations on configuration and setup of sprayers

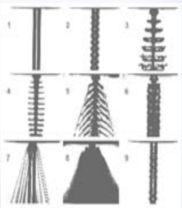
PHENOMENA WHICH AFFECT THE SPRAY

Flow inside the injector



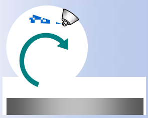
Snapshot of cavitation in 2D nozzle and spray (Sou, et al., 2005)

Flow oscillations



Shapes of oscillating jets (Chaves, et al., 2000)

Air motion



Swirling chamber in diesel combustion technology

COMPUTATIONAL MODEL OF SPRAY

Realistic 3D transient conditions

Visualised spray structure – droplet size spectra, velocities, temperature, spray penetration

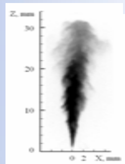
+ air motion and turbulence

+ evaporation and chemical reactions

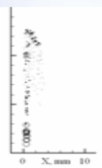
+ motion of droplets or particles

RESULTS: MEASUREMENTS AND COMPUTATIONS

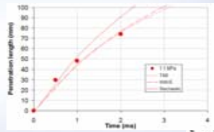
Calculations using KIVA-II CFD code – TAB, WAVE and Stochastic (Gorokhovski, 2003) models of spray breakup.

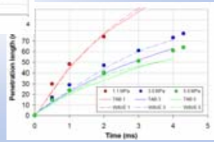


Experiment by C. Crua and K. Karimi, Univ. of Brighton



Spatial distribution of droplets predicted by stochastic breakup model (KIVA II)





Validation test (experiments by Hirouasu and Kadota, 1974)

RECENT PUBLICATIONS

- S. Sazhin (2006) Advanced models of droplet heating and evaporation, Progress in Energy and Combustion Science, v. 32, 162 – 214.
- S. Sazhin, T. Kristyadi, W. Abdelghaffar, and M. Heikal (2006) Models of fuel droplet heating and evaporation: comparative analysis. Fuel (in press).
- S. Martynov, D. Mason, M. Heikal, S. Sazhin and M. Gorokhovski. Modelling of cavitation flow in a nozzle and its effect on spray development, Submitted to the 13th International Heat Transfer Conference, Sydney, Australia.
- S. Sazhin, S. Martynov, I. Shishkova, M. Gorokhovski, E. Sazhina, M. Heikal. Modelling of droplet heating, evaporation and break-up: recent developments, Submitted to the 13th International Heat Transfer Conference, Sydney, Australia.
- S. Sazhin, S. Martynov, C. Crua, E. Sazhina, M. Heikal, A. Chtab, M. Gorokhovskii and D. Katoshevski. Modelling of the dynamics and break-up of jets and sprays - Submitted to the 6th Euromech Fluid Mechanics Conference, Sweden.

MODELLING OF CAVITATION FLOW IN A DIESEL INJECTION NOZZLE

S. Martynov, D. Mason, M. Heikal, and S. Sazhin

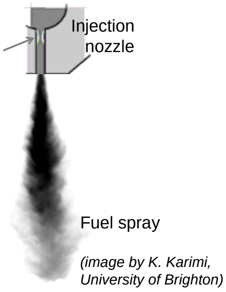
School of Engineering, Faculty of Science and Engineering, University of Brighton, Cockroft Building, Brighton BN2 4GJ, U.K.

Cavitation in fuel injector

- can improve break-up of the fuel jet,
- increases the hydraulic resistance of nozzle,
- produces instabilities in the flow, noise, vibration, and erosion wearing.

Main parameters of the flow:

- nozzle geometry,
- operating pressure,
- liquid viscosity and density,
- liquid quality (impurities and gas content).



(image by K. Karimi, University of Brighton)

Objectives of study

Development of a **mathematical model** of **hydrodynamic cavitation**, which:

- describes 3D viscous flows,
- takes into account bubbly nature of cavitation,
- is similarity consistent, and describes the geometry, viscous and liquid quality scale effects

Mathematical model of cavitation flow

The liquid-vapour flow is described using the **homogeneous mixture** concept. The phase content and mixture properties are described by the vapour **volume fraction** α.

Model for the volume fraction derived from the theory of bubble dynamics:

$$\frac{\partial \alpha}{\partial \tilde{t}} + \frac{\partial \alpha \tilde{u}_k}{\partial \tilde{x}_k} = C \cdot (1-\alpha)^{1/3} \alpha^{2/3} \cdot \sqrt{\left| CN^{-1} - \tilde{p} \right|} \cdot sign(p_v - p)$$

Hydrodynamic similarity criteria: $\mathrm{Re} = \frac{\rho_l U \cdot \ell_\infty}{\mu_l}$ $CN = \frac{p_1 - p_2}{p_2 - p_v}$

Radius and number density of cavitation bubbles give additional similarity criteria: R_o / ℓ_∞, $C = \ell_{cav} / \ell_\infty$

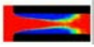
How to specify $C = \ell_{cav} / \ell_\infty$?

Model for the critical pressure

Conventional concept of the cavitation onset: $p < p_{cr} = p_v$

Alternative concept (Joseph, 1995):
in a flowing liquid cavitation onset depends on **maximum tension** $-p + 2\mu S_{ii}^{\max} \geq -p_v$

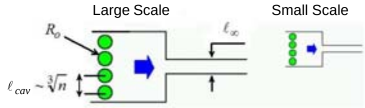
Experimental evidence:
Different cavitation pressure thresholds in liquids of *different* viscosity*:*

Flow	Authors	Liquid	Images of the flow	p_1 (bar)	p_2 (bar)	$p_1 - p_2$ (bar)
Inlet cavitation	Roosen, et al, (1996)	Water		80	21	59
	Winklhofer, et al. (2001)	Diesel fuel		100	43	57
Super-cavitation	Roosen, et al, (1996)	Water		80	11	69
	Winklhofer, et al. (2001)	Diesel fuel		100	34	66

Inlet cavitation: $p_1 - p_2 \sim 58$ *bar*

Super-cavitation: $p_1 - p_2 \sim 68$ *bar*

Model for the concentration of nuclei

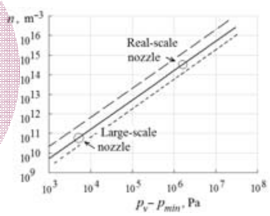


In **conventional** models the liquid quality and hydrodynamic scale effects are merged in parameter $n \sim \ell_{cav}^3$

In **our model** we decouple these effects by considering n as a function of liquid tension in cavitation region. A form for this function was derived to meet the similarity criterion: $C = \ell_{cav} / \ell_\infty = idem$

$$n = n_* \cdot \left(\frac{p_v - p_{\min}}{p_v} \right)^{3/2}$$

$p_v - p_{\min}$ = maximum tension in liquid
p_v = vapour pressure;
n_* = liquid-specific number density parameter.



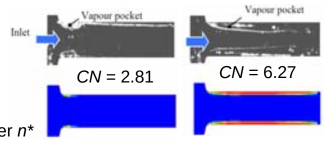
Parameter n* can be adjusted for a given liquid and applied for another conditions and geometry of the flow.

Results

Cavitation of a low viscosity fluid

Measured vapour-liquid field (Roosen et al., 1996)

Numerical predictions using the same parameter *n**



Cavitation of a high viscosity fluid

Measured vapour-liquid field (Winklhofer et al., 2001)

Numerical predictions:

Conventional concept:

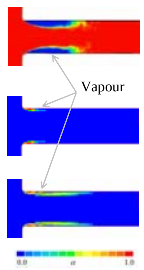
$p_{cr} = p_v$ $n = 1.6 \cdot 10^{19} (\mathrm{m}^{-3})$

Higher *n* **did not** change cavitation

Our model:

$$p_{cr} = p_v + 2\mu \cdot \left(1 + C_t \frac{\mu_t}{\mu} \right) \cdot S$$

$C_t = 10$
$n = 1.6 \cdot 10^{19} (\mathrm{m}^{-3})$



Computational method

The governing equations were solved numerically using the CFD package PHOENICS (*Cham Ltd*). The model of cavitation was implemented into the code. Discretisation of the void fraction equation was performed using the "super-bee" convection scheme.

Main features of the model developed

- The model accounts for the bubbly nature of cavitation,
- The model is similarity consistent (scalable),
- Concentration of the bubble nuclei is a function of liquid tension,
- The liquid quality is described by an adjustable parameter,
- The effect of viscous shear stress on the cavitation pressure threshold is considered.

Publications

- S. Martynov (2005) Numerical Simulation of the Cavitation Process in Diesel Fuel Injectors. Ph.D. thesis, University of Brighton, U.K.
- S. Martynov, D. Mason, and M. Heikal (2005) Hydrodynamic similarity of cavitation flows in nozzles. Proc. of the 5th Int. Symposium on Multiphase Flow, Heat Mass Transfer and Energy Conversion. Xi'an, China 3-6 July 2005.
- S. Martynov, D. Mason, and M. Heikal (2006) Numerical simulation of cavitation flows based on their hydrodynamic similarity. To be published in the Int. J. Engine Research.
- S. Martynov, D. Mason, M. Heikal, S. Sazhin and M. Gorokhovski. (2006) Modelling of cavitation flow in a nozzle and its effect on spray development. Submitted to the 13th Int. Heat Transfer Conf., Sydney, Australia.

Acknowledgements

The authors are grateful to the European Regional Development Fund Franco-British ***INTERREG IIIa (Project Ref. 162/025/247)*** for partial financial support of this study.

MODELLING OF DROPLET HEATING, EVAPORATION AND BREAK-UP: RECENT DEVELOPMENTS

S.S. Sazhin[1], S.B. Martynov[1], I.N. Shishkova[2] , C. Crua[1], K Karimi[1], M. Gorokhovski[3], E.M. Sazhina[1], M.R. Heikal[1]

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Models for heating and evaporation of droplets

Liquid phase (convective)

- Constant droplet temperature
- ***Infinite liquid thermal conductivity***
- Conduction limit
- ***Effective conductivity***
- Vortex model of droplet heating
- Navier-Stokes solution

Sirignano, W. A. Fluid Dynamics and Transport of Droplets and Sprays, CUP, 1999.

Gas phase (convective)

Seven models using various approximations for Nu and Sh

Simplified radiation term

The power generated in unit volume inside the droplet due to external radiation:

$$P(R) = 3\cdot 10^6 a\sigma R_{d(\mu m)}^{b-1}\left(T_{ext}^4 - \overline{T}^4\right)$$

$$\approx 3\cdot 10^6 a\sigma R_{d(\mu m)}^{b-1} T_{ext}^4,$$

$\overline{T}$ is the average droplet temperature ($\overline{T} << T_{ext}$)

$R_{d(\mu m)}$ is the droplet radius, μm;

a, b are polynomials of external temperature (quadratic functions in the first approximation).

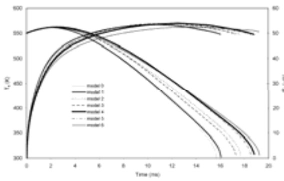
Dombrovsky, L.A., Sazhin, S.S, Sazhina, E.M, Feng, G., Heikal, M.R., Bardsley, M.E.A. and Mikhalovsky, S.V. (2001) Heating and evaporation of semi-transparent Diesel fuel droplets in the presence of thermal radiation. Fuel, 80 (11), 1535 -1544.

Sazhin, S.S., Abdelghaffar, W.A., Sazhina, E.M., Mikhalovsky, S.V., Meikle, S.T. and Bai, C. (2004) Radiative heating of semi-transparent diesel fuel droplets, ASME J Heat Transfer, 126, 105-109. Erratum (2004) 126, 490-491.

Numerical algorithms

- ***Numerical algorithm based on the analytical solution (analytical solution at the end of the time step is considered as the initial condition for the next time step)***
- Numerical solution of the discretised heat conduction equation (fully implicit approach)
- Numerical solution based on the parabolic model (surface temperature is calculated from the average droplet temperature at each time step)
- Numerical solution based on the assumption of no temperature gradient inside the droplet (conventional approach currently used in CFD codes)

Results



Plots of T_s and R_d versus time for the initial gas temperature T_{g0}= 880K, gas pressure p_{g0}=3 MPa, droplet temperature T_{d0}= 300 K, radius R_{d0}=50 μm and velocity v_{d0}=1 m/s.

The overall volume of injected liquid fuel was taken equal to 1 mm³, and the volume of air, where the fuel was injected, was taken equal to 883 mm³.

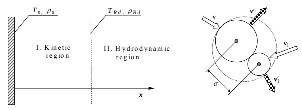
The results were obtained based on the effective thermal conductivity (ETC) model, the analytical solution of the heat conduction equation, and using seven gas phase models. T_{ext}=2000K

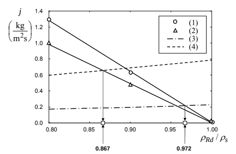
Conclusions (Heating and evaporation models)

Among liquid phase models, the analysis is focused on the model based on the assumption that the liquid thermal conductivity is infinitely large, and the so called effective thermal conductivity model. Seven gas phase models are compared. It is pointed out that the gas phase model, taking into account the finite thickness of the thermal boundary layer around the droplet, predicts the evaporation time closest to the one based on the approximation of experimental data. In most cases, the droplet evaporation time depends strongly on the choice of the gas phase model. In the absence of droplet break-up, the dependence of this time on the choice of the liquid phase model is weak. On the other hand, the droplet surface temperature at the initial stage of heating and evaporation does not practically depend on the choice of the gas phase model, while the dependence of this temperature on the choice of the liquid phase model is strong. In the presence of droplet break-up processes, the evaporation time and the total ignition delay depend strongly on the choice of both gas and liquid phase models.

Sazhin, S.S., Kristyadi, T., Abdelghaffar, W.A. and Heikal, M.R. (2006) Models for fuel droplet heating and evaporation: comparative analysis, Fuel, 85(12-13), 1613-1630.

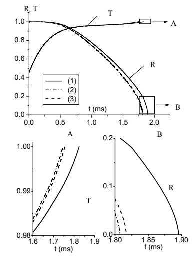
Kinetic effects





Lines (1) and (2) refer to j_{Rd} for R_{d0}=20 μm and R_{d0}=5 μm respectively.
Curves (3) and (4) refer to j diff for R_{d0}=20 μm and R_{d0}=5 μm respectively. T_s=600 K. The intersection points between j_{Rd} and j_{diff}, corresponding to the same values of R_{d0}, give the values of $j_{Rd} = j_{diff}$ and the corresponding values of ρ_{Rd}.
In the case shown in this figure:

- for R_{d0}=20 μm: $j_{Rd} = j_{diff}$ =0.217 kg/(m2s) and ρ_{Rd} = 0.972 ρs;
- for R_{d0}=5 μm: $j_{Rd} = j_{diff}$ = 0.657 kg/(m2s) and ρ_{Rd} = 0.867 ρs.



Plots of R= R_d/R_{d0} and T= T_s/T_{cr} versus time as predicted by the

- rigorous kinetic model (1),
- hydrodynamic model (2),
- simplified kinetic model with β=1 (3).

The total pressure is 30 bar, the initial droplet temperature is 300K, R_{d0}= 5 μm, T_g=750 K and T_{cr}=659K. The contribution of air in the kinetic region is taken into account.

Conclusions (Kinetic effects)

A numerical algorithm for kinetic modelling of droplet evaporation processes is suggested. This algorithm is focused on the direct numerical solution of the Boltzmann equations for two gas components: vapour and air. The distribution of molecular velocities after collisions is found based on the assumption that the total impulse and energy of colliding molecules are conserved. The numerical algorithm is applied to the analysis of the evaporation of a diesel fuel droplet into a high pressure air. The difference of masses and radii of vapour and air molecules is taken into account. The kinetic effects predicted by the numerical algorithm turned out to be noticeable if the contribution of air in the Knudsen layer is taken into account.

Shishkova, I.N. and Sazhin, S.S. (2006) A numerical algorithm for kinetic modelling of evaporation processes, J Computational Physics, 218 (2), 607-634 .

Conclusions (Dynamic decomposition technique)

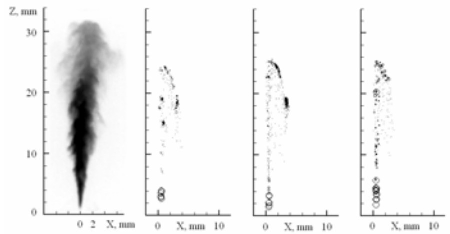
New decomposition technique for a system of ordinary differential equations is suggested, based on the geometrical version of the integral manifold method. This is based on comparing the values of the right hand sides of these equations, leading to the separation of the equations into 'fast' and 'slow' variables. The hierarchy of the decomposition is allowed to vary with time. Equations for fast variables are solved by a stiff ODE system solver with the slow variables taken at the beginning of the time step. The solution of the equations for the slow variables is presented in a simplified form, assuming linearised variation of these variables for the known time evolution of the fast variables. This can be considered as the first order approximation for the fast manifold. This technique is applied to analyse the explosion of a polydisperse spray of diesel fuel. Clear advantages are demonstrated from the point of view of accuracy and CPU efficiency when compared with the conventional approach widely used in CFD codes. The difference between the solution of the full system of equations and the solution of the decomposed system of equations is shown to be negligibly small for practical applications. It is shown that in some cases the system of fast equations is reduced to a single equation.

Bykov, V., Goldfarb, I., Gol'dshtein, V., Sazhin, S., Sazhina, E. (2006) System decomposition technique for spray modelling in CFD codes, Computers and Fluids

Droplet breakup effects

- Models of breakup: TAB (O'Rourke and Amsden 1987), WAVE (Reitz, 1987), and Stochastic (Gorokhovski and Saveliev, 2003)
- Application:

VCO type diesel injector with three nozzle holes of 200 μm in diameter. The injection pressure was 600 bar, the in-cylinder pressure was 20 bar, and the in-cylinder gas temperature was 570 K.



(a) (b) (c) (d)

Patterns of diesel spray observed at t = 0.5 ms after the start of injection (a), and predicted by the KIVA-2 CFD code using the TAB (b), WAVE (c) and stochastic (d) models of spray break-up. Only the right half of the spray is shown for the results of computations.

Conclusions (breakup effects)

The lengths of the spray tip penetration and the cone angles of the spray predicted by all three models are close. The stochastic model predicts wider spectra of droplets in the spray region, and longer break-up length compared to the TAB and WAVE models. Also, the TAB and WAVE models predict the fastest atomization of the spray and the smallest size of droplets at the spray tip. Large droplets in the vicinity of the spray tip appear as a result of coalescence. The largest droplets at the spray tip are predicted by the stochastic model.

Acknowledgements

The authors are grateful to the European Regional Development Fund Franco-British INTERREG IIIa (Project Ref 162/025/247) for financial support of the work on this project.

MODELLING OF CAVITATION FLOW IN A NOZZLE AND ITS EFFECT ON SPRAY DEVELOPMENT

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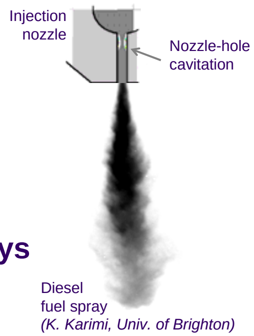
[2] Univertity of Rouen, Site Universitaire du Madrillet – BP12, 76801 Saint Etienne du Rouvray Cedex, France

High-pressure atomisation in diesel fuel combustion technology

- injection pressures up to 2000 bar,
- small injection durations ~1 ms,
- small diameter of nozzle holes ~0.1mm.



Cavitation in nozzles

- can enhance spray break-up,
- increases the hydraulic resistance of nozzle,
- produces instabilities in the flow,
- causes noise, vibration, and erosion wearing.

Lagrangian models of sprays

- jet and droplet breakup,
- gas-droplet interaction,
- droplet collisions,
- droplet heating and evaporation

Stages of spray breakup

Primary break-up of aerodynamic nature, caused by relative velocity between the liquid jet and ambient gas, enhanced by turbulent fluctuations and cavitation in the nozzle.

Secondary break-up of droplets and ligaments via bag, stripping and catastrophic scenarios.

Models of spray breakup

Deterministic models describe the breakup in terms of size and number density of product droplets, assuming an equilibrium distribution.

A **stochastic** model of breakup (Gorokhovski and Saveliev, 2003) describes the evolution of a droplet probability distribution function during the breakup. The model naturally accounts for the spectra of droplets injected from the nozzle, which can be recalculated from the spectrum of nozzle-flow disturbances caused by cavitation bubbles and turbulent motion.

The work is focused on the prediction of cavitation in the injection nozzles and its effects on the spray break-up.
A single-fluid model of cavitation, which takes into account the liquid quality and viscous shear stress effects, is proposed.

Similarity of cavitation flows

Similarity criteria

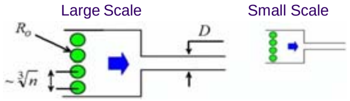
Reynolds number: $\mathrm{Re} = \dfrac{\rho_l U \cdot D}{\mu_l}$

cavitation number: $\mathrm{CN} = \dfrac{p_1 - p_2}{p_2 - p_v}$

Strouhal number: $\mathrm{Str} = \dfrac{f \cdot D}{U}$

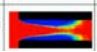
Scale effects

Cavitation bubble nuclei:



Radius and number density of cavitation bubbles give additional similarity criteria: $R_o/D;\ \sqrt[3]{n}/D$

Viscous scale effect:

Flow	Authors	Liquid	Images of the flow	p_1 (bar)	p_2 (bar)	$p_1 - p_2$ (bar)
Inlet cavitation	Roosen, et al, (1996)	Water		80	21	59
	Winklhofer, et al. (2001)	Diesel fuel		100	43	57
Super-cavitation	Roosen, et al, (1996)	Water		80	11	69
	Winklhofer, et al. (2001)	Diesel fuel		100	34	66

Inlet cavitation: $p_1 - p_2 \sim 58\ bar$
Super-cavitation: $p_1 - p_2 \sim 68\ bar$

Model of hydrodynamic cavitation

Volume fraction equation

The liquid-vapour flow is described using the **homogeneous mixture** concept. The phase content and mixture properties are described by the vapour **volume fraction** α., governed by the transport equation:

$$\frac{\partial \alpha}{\partial t} + \frac{\partial u_j \alpha}{\partial x_j} = \frac{(1-\alpha)\rho_l}{\rho} \cdot \frac{n}{1 + n\frac{4}{3}\pi R^3} \frac{d}{dt}\left(\frac{4}{3}\pi R^3\right)$$

$$\alpha = \frac{n\frac{4}{3}\pi R^3}{1 + n\frac{4}{3}\pi R^3}$$ – volume fraction of vapour;

$$\frac{dR}{dt} = \sqrt{\frac{2}{3}\frac{|p_v - p_l|}{\rho_l}} \cdot sign(p_v - p_l)$$ -rate of the bubble growth/ collapse (Rayleigh, 1917);

n – concentration of cavitation bubble nuclei, which has to be specified for particular cavitation flow, 1/m³.

The model was implemented into the CFD code PHOENICS. Discretisation of the void fraction equation was performed using the "super-bee" convection scheme (Hirsch, 1990).

Model for the concentration of bubble nuclei

A model for the parameter *n* has been derived to meet the similarity criterion: $C = \sqrt[3]{n}/D = idem$

$p_v - p_{\min}$ = maximum tension in liquid, Pa;
p_v = vapour pressure, Pa;
n^* = adjustable liquid-specific number density parameter, 1/m³.

$$n = n^* \cdot \left(\frac{p_v - p_{\min}}{p_v}\right)^{3/2}$$

Model for the cavitation pressure threshold

Cavitation onset in a **static** liquid: $p < p_{cr} = p_v$

In a flowing liquid cavitation onset depends on **maximum tension** (Joseph, 1995): $-p + 2\mu S_{ii}^{\max} \geq -p_v$

$S_{ii}^{\max}$ = maximal rate of strain, 1/s;
μ = dynamic viscosity of liquid, Pa s;
μ_t = turbulent viscosity, Pa s;
C_t = adjustable coefficient.

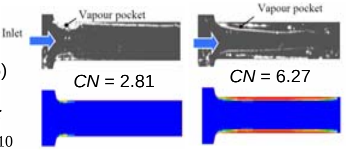
$$p < p_{cr} = p_v + 2\mu \cdot \left(1 + C_t \frac{\mu_t}{\mu}\right) \cdot S_{ii}^{\max}$$

Results

Cavitation of a low viscosity fluid

Measured vapour-liquid field: (Roosen et al., 1996)

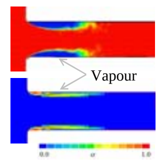
Numerical predictions: $n = 4.4 \cdot 10^{14}\,(\mathrm{m}^{-3});\ C_t = 10$



Cavitation of a high viscosity fluid

Measured vapour-liquid field: (Winklhofer et al., 2001)

Numerical predictions: $n = 2 \cdot 10^{18}\,(\mathrm{m}^{-3});\ C_t = 10$



Conclusions

- A homogeneous-mixture model of cavitation flow, based on the theory of bubble dynamics, has been extended in order to describe the liquid quality and viscous shear stress effects on cavitation flow.
- Assuming hydrodynamic similarity of cavitation flows, an algebraic model for the number density of active cavitation nuclei is suggested.
- The influence of viscous shear stress on cavitation flow has been clarified, and described in the model for the cavitation pressure threshold.
- The model was adjusted to describe sub-cavitation and super-cavitation flows in real-scale models of diesel injectors.

Acknowledgements

The authors are grateful to the European Regional Development Fund Franco-British INTERREG IIIa (Project LES SPRAYS Ref 162/025/247) for financial support of this work.

Publications

- Gorokhovski, M.A. and Saveliev, V.L., (2003). Analysis of Kolmogorov's model of breakup and its application into Lagrangian computation of liquid sprays under air-blast atomisation. Physics of Fluids, **15** (1), pp. 184-192.
- S. Martynov (2005) Numerical Simulation of the Cavitation Process in Diesel Fuel Injectors. Ph.D. thesis, University of Brighton, U.K.
- S. Martynov, D. Mason, and M. Heikal (2006) Numerical simulation of cavitation flows based on their hydrodynamic similarity. Int. J. Engine Research, **7** (3), pp. 283-296.

OSCILLATING JETS AND SPRAYS IN MODERN TECHNOLOGIES

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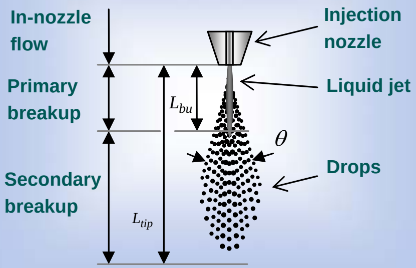
SPRAY STRUCTURE



SELECTED APPLICATIONS OF JETS AND SPRAYS

- **Automotive industry – fuel sprays**
- **Environmental – aerosols and pollutions**
- **Agricultural – sprinkling and spraying**
- **Medical – drugs delivery**

HOW CAN YOU BENEFIT FROM OUR STUDY?

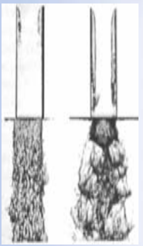
- **Full control of spray (e.g. parameters of dispersed phase, rate of penetration, evaporation)**
- **Efficient energy consumption**
- **Recommendations on configuration and setup of sprayers**

PHENOMENA WHICH AFFECT THE SPRAY

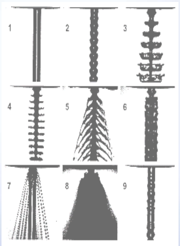
Flow inside the injector

Flow oscillations

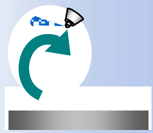
Air motion



Snapshot of cavitation in 2D nozzle and spray (Sou, et al., 2005)



Shapes of oscillating jets (Chaves, et al., 2000)



Swirling chamber in diesel combustion technology

WE HAVE DEVELOPED COMPUTATIONAL MODEL OF SPRAY

Realistic 3D transient conditions

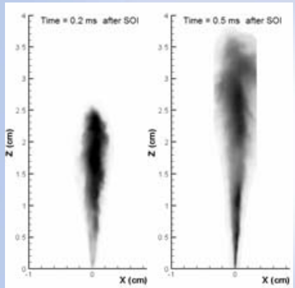
Visualised spray structure – droplet size spectra, velocities, temperature, spray penetration

+ air motion and turbulence

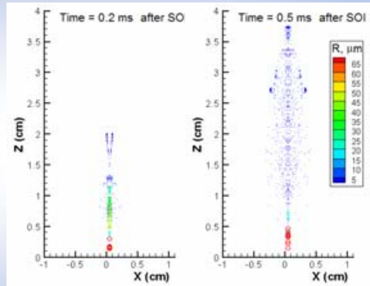
+ evaporation and chemical reactions

+ motion of droplets or particles

RESULTS OF COMPUTATION OF TRANSIENT SPRAYS



Spray images by C. Crua and K. Karimi, Univ. of Brighton



Results of calculations using our spray model in KIVA-II CFD code

ACKNOWLEDGEMENTS

Franco-British INTERREG IIIA program LES SPRAYS is sponsored by the European Regional Development Fund (ERDF) and Ricardo Consulting Engineers Ltd (UK)

CFD MODELLING OF SPRAY PROCESSES

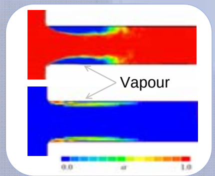
UNIVERSITÉ DE ROUEN
University of Brighton
ICEG
RICARDO
EUROPEAN UNION European Regional Development Fund
Interreg IIIA

Cavitation Flow in Diesel Injectors

A model for the cavitation flow in nozzles has been developed using the homogeneous mixture approach. The model takes into account the fluid quality and viscous scale effects. The model has been implemented into the PHOENICS CFD code.

Photograph of cavitation flow *(Winklhofer, et al, 2001)*:

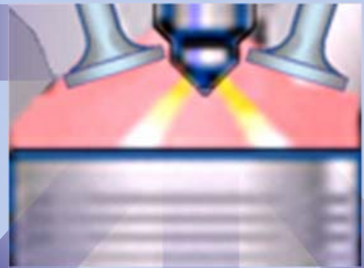
Results of computations:



Nozzle height = 0.3 mm
Nozzle length = 1 mm
Diesel fuel
P_{inj} = 100 bar
P_g = 34 bar
U_{inj} = 116 m/s

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

• S. Martynov, D. Mason, and M. Heikal (2006) Numerical simulation of cavitation flows based on their hydrodynamic similarity. Int. J. Engine Research, 7 (3), 283-296.
• Martynov, S., Mason, D., Heikal, M., Sazhin, S., Gorokhovski, M. (2006) Modelling of cavitation flow in a nozzle and its effect on spray development. Proceedings of 13th International Heat Transfer Conference , Sydney, Australia. Paper JET-08.



Objectives

- Development of advanced analytical/asymptotic and numerical models for in-cylinder processes in internal combustion (IC) engine
- Validation of the models against in-house measurements
- Prediction of operational characteristics of IC engines

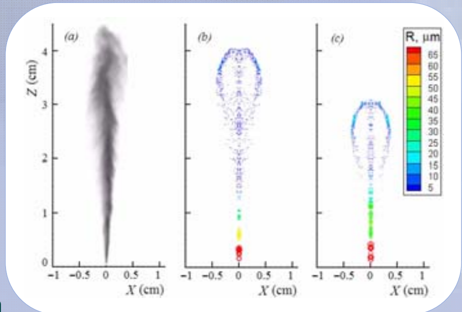
Spray Penetration and Breakup

A model for the primary breakup taking into account the effect of acceleration has been developed and implemented into KIVA-II spray code.

Martynov, S., Sazhin, S., Gorokhovski, M., Chtab A., Karimi, K., Crua C., Heikal M. A modified WAVE model for transient liquid sprays. International Journal of Heat and Fluid Flow. (Submitted).

A transient spray penetration model based on the momentum conservation of the injected fuel mass, has been developed.

Karimi, K., Sazhina, E., Abdelghaffar, W. Crua, C., Cowell, T., Heikal, M., Gold, M. (2006) Development in diesel spray characterisation and modelling. THIESEL Conference, Valencia, Spain, 13-15 September. Paper A1-2.



Snap-shot from the video record of the Diesel fuel spray *(a)* in comparison with the calculated spatial distributions of droplets using the new breakup model *(b)* and the conventional WAVE breakup model *(c)*, at 0.7 ms after the start of injection.

Dynamic Decomposition

A dynamic decomposition technique for the solution of a system of ordinary differential equations (ODE) for droplets, gas exchange and autoignition, has been suggested.

It is shown that this method:

- reduces stiffness of the ODE system
- allows coupled solution of the ODE system for all the droplet parcels and gas phase

Bykov, V., Goldfarb, I., Gol'dshtein, V., Sazhin, S., Sazhina, E. (2006) System decomposition technique for spray modelling in CFD codes, Computers and Fluids. (in press).

Droplet Heating and Evaporation

Substantial decrease in the droplet evaporation time and ignition delay due to finite temperature gradient inside the droplets has been shown.

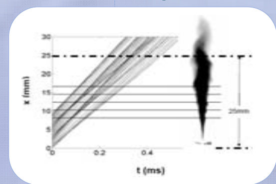
Sazhin, S.S., Kristyadi, T., Abdelghaffar, W.A. and Heikal, M.R. (2006) Models for fuel droplet heating and evaporation: comparative analysis, Fuel, 85 (12-13), 1613-1630.

A comparative analysis of hydrodynamic and kinetic approaches to the problem of diesel fuel droplet evaporation has been performed.

Shishkova, I.N. and Sazhin, S.S. (2006) A numerical algorithm for kinetic modelling of evaporation processes, J. Computational Physics, 218 (2), 607-634.

Droplet Grouping

A model for droplet clustering has been developed.



Experimentally observed diesel spray (right) and the predicted droplet trajectories (left). *Time* = 2.ms ASOI; $P_{inj.}$= 160MPa; P_g= 6 MPa; T_g =590K.

Sazhin, S., Martynov, S., Crua, C., Sazhina, E., Heikal, M., Chtab, A., Gorokhovskii, M. and Katoshevski, D (2006) Modelling of the dynamics and break-up of jets and sprays. The 6th Euromech Fluid Mech. Conference, KTH- Royal Institute of Technology, Stockholm.

Acknowledgements

- Ricardo Consulting Engineers Ltd (UK)
- European Regional Development Fund (Franco-British INTERREG Project "Les Sprays" – Ref 162/025/247)
- EPSRC grants GR/S98368101, GR/P02745/01 EP/C527089/1, EP/D002044/1.

ADVANCED MODELS FOR DROPLET HEATING AND EVAPORATION: EFFECT ON AUTOIGNITION OF DIESEL FUEL SPRAYS

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Models for heating and evaporation of droplets

Liquid phase (convective)

- Constant droplet temperature
- ***Infinite liquid thermal conductivity***
- Conduction limit
- ***Effective conductivity***
- Vortex model of droplet heating
- Navier-Stokes solution *(Sirignano, 1999)*

Gas phase (convective)

Seven models using various approximations for the Nusselt and Sherwood numbers

Simplified radiation term

The power generated in unit volume inside the droplet due to external radiation:

$$P(R) = 3\cdot 10^6 a\sigma R_{d(\mu m)}^{b-1}\left(T_{ext}^4 - \bar{T}^4\right)$$
$$\approx 3\cdot 10^6 a\sigma R_{d(\mu m)}^{b-1} T_{ext}^4,$$

$\bar{T}$ is the average droplet temperature $(\bar{T} << T_{ext})$

$R_{d(\mu m)}$ is the droplet radius, μm;

a, b are polynomials of external temperature (quadratic functions in the first approximation).

Spray breakup models

- TAB (O'Rourke and Amsden 1987),
- WAVE KH-RT (Patterson and Reitz, 1998),
- Stochastic (Gorokhovski and Saveliev, 2003)
- The modified version of the WAVE model, which takes into account the damping effect of injection acceleration on the break-up rate constant:

$$B_1 = B_{1,eq} + 3.8\cdot\left(a^+\right)^{0.2}, \qquad a^+ = \mathrm{Re}^{3/2}\frac{v_g}{U_{jet}^3}\frac{dU_{jet}}{dt}$$

where $B_{1,eq}$ = 10 is the break-up time of the conventional WAVE model, and a^+ is a dimensionless acceleration parameter. This empirical equation has been shown to provide a better description of the highly transient initial stage of spray penetration.

Numerical algorithms

- ***Numerical algorithm based on the analytical solution (analytical solution at the end of the time step is considered as the initial condition for the next time step)***
- Numerical solution of the discretised heat conduction equation (fully implicit approach)
- Numerical solution based on the parabolic model (surface temperature is calculated from the average droplet temperature at each time step)
- Numerical solution based on the assumption of no temperature gradient inside the droplet (conventional approach currently used in CFD codes)

Implementation into the KIVA code

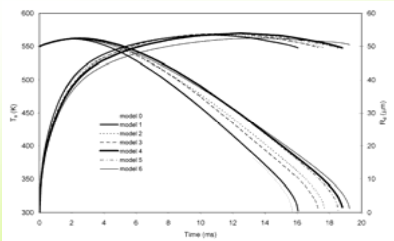
The models for droplet heating and evaporation were implemented into a customised version of the KIVA-II code, alongside the Taylor-analogy break-up (TAB) model (the default model in KIVA-II), and the conventional and modified version of the WAVE break-up model. In all cases, the blob injection method was used.

In the Shell autoignition model (Halstead, et al, 1977), the pre-exponential constant for the reaction rate for the production of the branching agent was set to value $A_{f4} = 3\ 10^6$.

Experimental setup

- VCO type Diesel single-hole injection nozzle of 200 μm in diameter;
- Injection pressures 60 – 160 MPa,
- In-cylinder pressures 5 – 9 MPa,
- In-cylinder gas temperature 750 – 800 K.

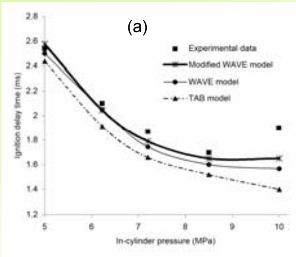
Results

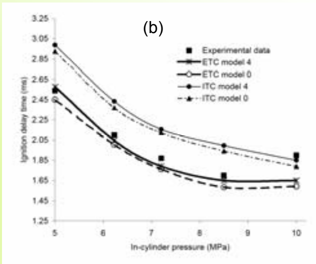


Plots of T_s and R_d versus time for the initial gas temperature T_{g0} = 880K, gas pressure p_{g0} = 3 MPa, droplet initial temperature T_{d0} = 300 K, radius R_{d0} = 50 μm and velocity v_{d0}=1 m/s.

The overall volume of injected liquid fuel was taken equal to 1 mm^3, and the volume of air, where the fuel was injected, was taken equal to 883 mm^3.

The results were obtained based on the effective thermal conductivity (ETC) model, the analytical solution of the heat conduction equation, and using seven gas phase models. T_{ext} = 2000K





Predicted and experimentally measured ignition delay times versus in-cylinder pressure: (a) effect of breakup model (ETC liquid phase model and gas model 4 (Abramzon and Sirignano, 1989)), (b) effect of heating and evaporation models (spray breakup described using the conventional WAVE model). 1000 droplet parcels with initial droplet temperature 375 K were injected at 100MPa into a cylinder with initial temperature 750 K.

Publications

- *Crua, C. (2002) Combustion processes in a diesel engine. PhD thesis, University of Brighton.*
- *Dombrovsky, L.A., Sazhin, S.S, Sazhina, E.M, Feng, G., Heikal, M.R., Bardsley, M.E.A. and Mikhalovsky, S.V. (2001) Heating and evaporation of semi-transparent Diesel fuel droplets in the presence of thermal radiation. Fuel, 80 (11), 1535 -1544.*
- *Sazhin, S.S. (2006) Advanced models of fuel droplet heating and evaporation, Progress in Energy and Combustion Science, 32 162-214.*
- *Sazhin, S.S., Abdelghaffar, W.A., Krutitskii, P.A., Sazhina, E.M., Heikal, M.R. (2005) New approaches to numerical modelling of droplet transient heating and evaporation, Int. J Heat Mass Transfer, 48. 4215-4228.*
- *Sazhin, S.S., Abdelghaffar, W.A., Sazhina, E.M., Heikal, M.R. (2005) Models for droplet transient heating: effects on droplet evaporation, ignition, and break-up, Int. J Thermal Science, 44, 610-622.*
- *Sazhin, S.S., Abdelghaffar, W.A., Sazhina, E.M., Mikhalovsky, S.V., Meikle, S.T. and Bai, C. (2004) Radiative heating of semi-transparent diesel fuel droplets, ASME J Heat Transfer, 126, 105-109. Erratum (2004) 126, 490-491.*
- *Sazhin, S.S., Kristyadi, T., Abdelghaffar, W.A., Begg, S., Heikal, M.R., Mikhalovsky, S.V., Meikle, S.T., Al-Hanbali, O. (2007) Approximate analysis of thermal radiation absorption in fuel droplets. ASME J Heat Transfer (in press).*
- *Sazhin, S.S., Kristyadi, T., Abdelghaffar, W.A. and Heikal, M.R. (2006) Models for fuel droplet heating and evaporation: comparative analysis, Fuel, 85(12-13), 1613-1630.*
- *Sazhin, S.S., Krutitskii, P.A., Abdelghaffar, W.A., Sazhina, E.M., Mikhalovsky, S.V., Meikle, S.T., Heikal, M.R. (2004) Transient heating of diesel fuel droplets, Int. J Heat Mass Transfer, 47. 3327-3340.*
- *Sazhina, E.M., Sazhin, S.S., Heikal, M.R., Babushok, V.I., Johns, R.A. (2000) A detailed modelling of the spray ignition process in Diesel engines. Combustion Science and Technology, 160, 317-344.*

Conclusions

- Among liquid phase models, the analysis is focused on the model based on the assumption that the liquid thermal conductivity is infinitely large, and the so called effective thermal conductivity model.
- Seven gas phase models are compared. It is pointed out that the gas phase model, taking into account the finite thickness of the thermal boundary layer around the droplet, predicts the evaporation time closest to the one based on the approximation of experimental data. In most cases, the droplet evaporation time depends strongly on the choice of the gas phase model.
- In the absence of droplet break-up, the dependence of this time on the choice of the liquid phase model is weak. On the other hand, the droplet surface temperature at the initial stage of heating and evaporation does not practically depend on the choice of the gas phase model, while the dependence of this temperature on the choice of the liquid phase model is strong.
- In the presence of droplet break-up processes, the evaporation time and the total ignition delay depend strongly on the choice of both gas and liquid phase models.
- The models of droplet heating and evaporation have been implemented into zero-dimensional and 3-dimensional spray codes (KIVA-II). To describe the breakup in the accelerated Diesel fuel sprays, the WAVE breakup model has been modified.
- The results of computations using KIVA code show a reasonably good agreement with in-house experimental data referring to autoignition delay. It was confirmed that the effective thermal conductivity model predicts smaller ignition delay than the infinite thermal conductivity model. Both models predict decreasing ignition delay with increasing in-cylinder pressure, in agreement with experimental measurements at pressures less than 8.5 MPa.

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AUTOIGNITION OF *n*-PENTANE IN A RAPID COMPRESSION MACHINE: EXPERIMENT *versus* MODELLING

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Ignition and cool flame delay times of stoichiometric *n*-pentane/'air' mixtures were measured in a rapid compression machine with pressures at top dead centre (TDC) between 4 and 11 bar.

A so-called weighted temperature $T_w = 0.75T_m + 0.25T_c$ was calculated from the mean gas temperature T_m (deduced from the perfect gas law) and the core gas temperature T_c at the end of compression. The dependence of the delay times on these temperatures was investigated.

A customised version of the Shell model, taking into account convective and radiative heat losses, was used to predict the ignition features.

A good agreement with experimental data was obtained both for ignition and cool flame delay times using the same rate constants and a value of 10 for the scaling factor of the convective heat losses.

The Shell model (Halstead *et al*, 1977)

Initiation:	$RH + O_2 \rightarrow 2R^*$
Propagation:	$R^* \rightarrow R^* + P$
	$R^* \rightarrow R^* + B$
	$R^* \rightarrow R^* + Q$
	$R^* + Q \rightarrow R^* + B$
Branching:	$B \rightarrow 2R^*$
Termination:	$R^* \rightarrow out$
	$2R^* \rightarrow out$

where ***RH*** represents the hydrocarbon fuel (C_nH_{2m}),
R* is a radical, ***B*** is a branching agent,
Q is an intermediate product, and ***P*** is the final product, consisting of ***CO, CO₂***, and ***H₂O***.

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Rate of temperature rise

$$\frac{dT}{dt} = \frac{Q_K - Q_L - Q_R}{C_v n_{tot}}$$

where C_v is the molar heat capacity at constant volume,
n_{tot} is the total number of moles,
Q_K is the chemical heat release rate,
Q_L and Q_R are the convective and radiative heat loss rates respectively.

The radiative heat loss rate: $Q_R = \varepsilon A(T^4 - T_w^4)$

where ε is the emissivity of the gaseous mixture.

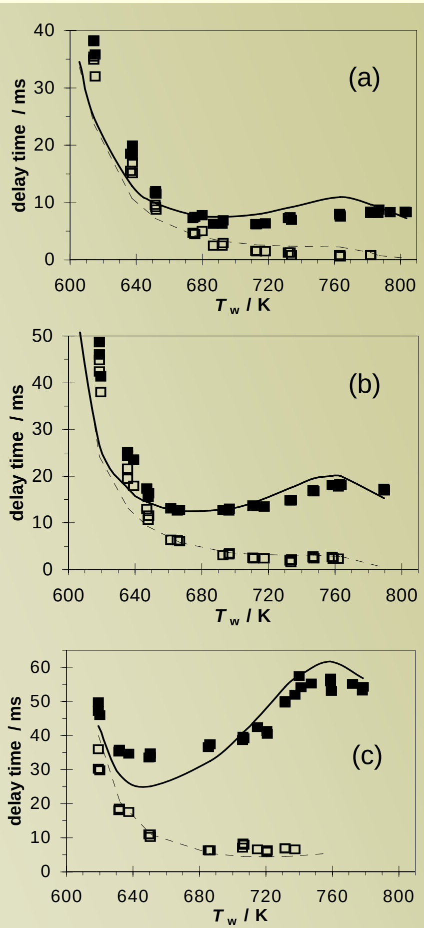
The convective heat loss rate: $Q_L = hA(T - T_w),\quad h = \alpha k_{gas}/L$

where convective heat transfer coefficient *h* is taken with the convective scaling coefficient α varying between 1 – 10 for a parametric study

The chemical heat release rate: $Q_K = k_p q V [R^*]$

where ***q*** is the molar internal energy release of combustion per fragment CH_2, and ***V*** is the volume of the combustion chamber at Top Dead Centre of RCM.
The value of ***q*** is taken equal to the absolute value of the standard enthalpy of reaction at 298 K:
$q = 383$ **kJ·mol⁻¹** for ***n-pentane.***

Results



Experimental (symbols) and calculated (curves) ignition delay times for P_o= 400 torr(a), 300 torr (b), and 200 torr (c). Calculations were performed for α = 10.
Solid lines – total ignition delays, dashed lines – cool flames.

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