Effect of 4500bar injection pressure and super-critical phase change of surrogate and real-world fuels enriched with additives and powering Diesel engines on soot emissions reduction

Results

Project Information

IPPAD

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Project website

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Coordinated by
CITY UNIVERSITY OF LONDON
United Kingdom

CORDIS provides links to public deliverables and publications of HORIZON projects.

Links to deliverables and publications from FP7 projects, as well as links to some specific result types such as dataset and software, are dynamically retrieved from OpenAIRE.

Deliverables

Documents, reports (34)

Property measurements for fuels enriched with additives

The apparatus will be utilised for measuring 9 combinations of fuels: for each of the three base fuels, the effect of three additives (detergents, soot reducers and ignition improvers) on properties will be quantified.

DNS methodology for atomisation at supercritical conditions

Implementation of the SAFT EoS to interface tracking codes will be performed, in an effort to estimate the effect of supercritical conditions on near-nozzle atomisation. To account for the discontinuous nature of the phase interface, a one fluid approach will be followed, making property calculation a function of the liquid volume fraction. Dynamic grid refinement and advanced algorithms suppressing numerical diffusion of the gas/vapour-liquid interface will be employed. The computational model will address the issue of whether the fuel enters a supercritical state that allows it to readily mix with noncondensable gases (N2 + O2) or whether the fuel droplet has to vaporize before mixing as P-T conditions rapidly change.

Property measurements for non-additised fuels

Develop and commission a test rig for measuring fuel properties up to 3,000 bar and fuel's critical point; initially measurements of a surrogate, summer Diesel and low-quality Diesel will be measured.

Predictions with the above model in Diesel engines

Additional electronic structure calculations using VASP will allow surface thermo-kinetics on graphene layers to be considered. The detailed heterogeneous soot kinetic mechanism that will be developed for high temperature environments will include a wide variety of adsorbed species. The soot oxidation mechanisms in O2, O and OH will be unraveled to derive a closure of filtered source terms for oxidation in the sectional model. The developed model will be applied to cases of industrial interest, demonstrating the effects of selected fuel additives on soot.

EoS of additised fuels

Similar EoS model will be developed for the fuels enriched with additives. These models will also address the issue of whether the fuel droplets enter a supercritical state that allows them to readily mix with non-condensable gases (N2 + O2) or whether the fuel droplet has to vaporize before mixing as P-T conditions rapidly change.

Cavitation visualisation in true-scale optical Diesel injectors

High speed imaging of cavitation inside transparent nozzle tips will be performed safely at pressures up to 2,000bar, although higher ones will be tested. The clean tips will be manufactured from sapphire for withstanding high pressures while 3-D printing will be utilised for manufacturing enlarged nozzle replicas that will match geometries of aged injectors (both from field tests and from accelerated nozzle coking tests).

Heterogeneous soot oxidation kinetic mechanism

Molecular dynamics simulations using the ReaxFF code will be used to generate a database of soot structures from the combustion of different surrogate fuels under different thermochemical conditions. With respect to existing macroscopic pore modeling approach, this approach will allow to capture the interplay between boundary layer and surface chemistry inside the particle with mass transport, while capturing finely the structural changes of soot nanostructure and the interplay between neighboring pores during oxidation.

Nozzle flow for aged injectors exhibiting internal deposits

Predictions for the aged nozzles will then determine the differences in fuel delivery, injection temperature and vapour concentration for the aged injectors.

Soot measurements in metallic engines

The effect of high pressure injection, fuel properties and additive concentration will be tested in real engines. Tests will include surrogate fuels, summer Diesel and low-quality Diesel enriched with the additives under investigation.

Demonstration of technique in high pressure burner and optical engines

The developed techniques will be applied to liquid sprays in high pressure burner and optical engines in co-operation with ESR8 and ESR10.

Numerical predictions of soot emissions from engines

Subsequently, the CFD models to be developed as part of the work performed in WP2 and WP4 will be utilised to simulate the measured trends. The experimental data of ESRs 9, 10 and 11 will be used for validation of the combustion/emission simulations of ESR15.

Supercritical spray characterisation of non-additised fuels

Parallel to the near-nozzle studies, imaging and LIEF will characterise the macroscopic development and mixing under supercritical conditions for clean and aged injectors and for pressures up to 4,5000bar; initially measurements will be performed for the three base fuels.

EoS of non-additised fuels

Based on the fuel property measurements, a SAFT-based EoS approach will be developed for predicting fuel thermodynamic and transport properties that occur in high pressure FIE for Diesel engines. Properties will include internal energy, heat capacity, viscosity, density, thermal conductivity, surface tension and enthalpy of vaporisation of a surrogate fuel, summer Diesel and low quality Diesel.

Soot measurements in optical engines for various fuels/injectors

The developed soot measurements will be obtained in optical Diesel engines fuelled with the three reference fuels and the selected additives both for clean and aged injectors.

Nozzle flow simulations for clean injectors

SAFT EoS for the three base fuels and the additive combinations will be implemented in the CFD code of CITY in order to determine friction-induced heating, cavitation and boiling effects occurring during realistic injection events. The initial task will be validation against the experimental data of ESR2 for clean injectors.

DNS studies for surfactant activity

Identification of physically sound constituent laws (surfactant-surface-tension relation) for realistic fuel compositions and additives and formulation of numerical models for surfactant transport at the vapor-liquid interface, numerical validation for simple gas-bubbles in liquid, followed by formulation of surface tension models with a generalized-Riemann-solver framework for conservative interface-interaction models, and validation for single-bubble growth and collapse configurations.

Journal publications

Conference publications

Supercritical spray development under engine driving conditions

Predictions will be performed utilising real-world operating conditions in realistic Diesel engine geometries.

Supercritical atomisation visualisation for pilot injection events

High energy X-rays at ANL will characterise initially the liquid/vapour distribution inside the nozzle's sac volume for different fuels/additives both for clean and aged injectors with deposits. High speed imaging in CVC will then characterise the liquid atomisation near the nozzle exit for pilot injection events, aiming to link the amorphous ligaments formed at the nozzle exit with the nozzle geometry/flow.

Supercritical atomisation visualisation for main injection events

Near-nozzle atomisation will be then characterised with high magnification/speed imaging for main injection events under supercritical conditions. Injection pressures as high as 4,500bar will be tested.

Supercritical spray development in idealised configurations

The developed models of ESR7 and ESR12 will be utilised in the framework of a commercial CFD software for estimating the effect of nozzle geometry (being function of injector aging and operating conditions) on spray formation under supercritical conditions initially in a CVC environment.

Simulation of soot emissions from Diesel engines/environmental assessm

As a follow-up, the heterogeneous soot mechanism of ESR14 will be utilised for predictions of soot under real-world driving scenario, allowing an environmental assessment of the integrated activities of the programme. Model validation will be performed against the measurements of ESR9, 10 and 11.

LES methodology coupled in-nozzle flow and spray formation

The SGS models of ESR5 and ESR6 will be implemented into the developed code for estimating fuel atomisation under 4,500 injection pressure and SCF conditions.

SGS model for the effect of fuels/additive on atomisation

The developed model will be used to compare the effect of fuel and additive properties on the atomisation process.

Development of soot measurement technique in high pressure

Soot diagnostics (such as extinction, laser-induced incandescence (LII) and elastic light scattering) for high pressure and optically dense environments will be co-developed with ESR8. Measurements will be initially performed in simplified flame configurations. These data will assist ESR14 in the development of the relevant simulation model.

Simulation of integrated technologies on combustion

The model of ESR13 will be further extended under the framework of a commercial CFD to account initially the effects of fuels and additives on combustion in Diesel engines.

mCT measurements in transparent nozzle replicas

mCT will be performed in all transparent tips for quantifying the cavitation volume fraction as function of nozzle geometry and fuel composition.

CGS model for the effect of fuels/additives on primary atomisation

Direct numerical simulations with adaptive multi-resolution scheme and scale-separation approach for the interface (identification of under-resolved interface structures) of collapsing single bubbles and bubble clouds for different configurations: away from free surfaces and near free surfaces. The developed surface tension SGS closure model will be communicated to ESR6 working on LES.

Supercritical spray characterisation of additised fuels

Similar measurements will be performed for additised fuels.

Soot formation in vapour fuel burners

A Diesel fuel vaporiser and burner will be initially designed, allowing for quantification of ‘soot reducer’ additives to be quantified independently, as atomisation, phase-change and mixing processes will be bypassed. Soot measurements will be performed using LII, wide-angle light scattering, SMPS and TEM.

Implementation of real fluid EoS into IFPEN code

sub-critical atomisation, will be extended on the basis of the SAFT EoS for the liquid phase and real-gas EoS for the air/vapour phases to multi-component fuels with/without additives at supercritical conditions.

Measurements for late-cycle soot oxidation in optical engines

Further tests will examine the spray behaviour and cycle-to-cycle vatiation inside the cylinder of an optical light-duty engine, focusing on formation and late-cycle oxidation of soot.

Blackbody emission imaging and LII for spray combustion

Following, high speed-video blackbody emission imaging and LII will be developed and utilised for quantifying soot in liquid spray flames in cooperation with ESR9, utilising fuels enriched with the same additives.

Other (4)

Supervisory Board of the Network

Mid-term review meeting

Progress report

Draft Periodic Report

Websites, patent fillings, videos etc. (1)

Project website
Project website is created and upa nd running.

Publications

Conference proceedings (11)

The liquid penetration of diesel substitutes
Author(s): Lukas Weiss, Sebastian Riess, Javad Rezaei, Andreas Peter, Michael Wensing
Published in: Proceedings ILASS–Europe 2017. 28th Conference on Liquid Atomization and Spray Systems, 2017, ISBN 9788-490485804
Publisher: Universitat Politècnica València
DOI: 10.4995/ILASS2017.2017.4764

Towards a multicomponent real-fluid fully compressible two-phase flow model
Author(s): Songzhi Yang, Chaouki Habchi, Yi Ping, Rafael Lugo
Published in: Proceedings of the 14th International Conference on Liquid Atomization and Spray Systems, 2018
Publisher: University of Illinois at Chicago

Investigation of Phase Change Mechanisms of n-Alkanes Injected in sub-and Supercritical Conditions
Author(s): Javad Rezaei, Sebastian Reis, Andreas Peter, Michael Wensing
Published in: Proceedings of the 14th International Conference on Liquid Atomization and Spray Systems, 2018
Publisher: University of Illinois at Chicago

Effect of realistic multicomponent diesel surrogates on predicted in-nozzle flow and cavitation
Author(s): Vidal Roncero A., Gavaises M., Koukouvinis P., Rodriguez C.
Published in: Proceedings of the 14th International Conference on Liquid Atomization and Spray Systems, 2018
Publisher: University of Illinois at Chicago

On the effect of realistic multicomponent diesel surrogates on cavitation and in-nozzle flow
Author(s): Vidal Roncero A. , Koukouvinis F., Gavaises, M.
Published in: Proceedings of the IMechE Fuel systems engines: Inject your ideas, Fuel your technology, 2018
Publisher: IMechE

Simulation of transcritical Diesel jets using the PC-SAFT EoS
Author(s): Rodriguez C., Vidal A., Koukouvinis P. and Gavaises M.
Published in: Proceedings of the 14th International Conference on Liquid Atomization and Spray Systems, 2018
Publisher: University of Illinois at Chicago

CFD simulation of pseudo-diesel injections at high-load conditions employing the PC-SAFT EoS and VLE calculations
Author(s): Rodriguez C., Rokni H. B. Koukouvinis P. , Gupta, A. and Gavaise M.
Published in: Proceedings of the 29th European Conference on Liquid Atomization and Spray Systems, 2019
Publisher: Sorbonne University

Numerical analysis of droplets subcritical evaporation and transcritical mixing using a tabulated real-fluid thermodynamics method coupled to a homogeneous equilibrium model
Author(s): Yi Ping, Sajad Jafari, Songzhi Yang, Chaouki Habchi
Published in: Proceedings of the 29th European Conference on Liquid Atomization and Spray Systems, 2019
Publisher: Sorbonne University

Effect of Diesel injection pressures up to 450MPa on in-nozzle flow using realistic multicomponent surrogates
Author(s): Vidal Roncero A. , Koukouvinis P. and Gavaises M.
Published in: Proceedings of the 29th European Conference on Liquid Atomization and Spray Systems, 2019
Publisher: Sorbonne University

A multi-component real-fluid two-phase flow solver with high-order finite-difference schemes
Author(s): Jianhang Wang, Songzhi Yang, Chaouki Habchi, Xiangyu Hu, Nikolaus Adams
Published in: Proceedings of the 29th European Conference on Liquid Atomization and Spray Systems, 2019
Publisher: Sorbonne University

Supercritical and transcritical real-fluid mixing using the PC-SAFT EOS
Author(s): Carlos Rodriguez, Alvaro Vidal, Phoevos Koukouvinis, Manolis Gavaises
Published in: Proceedings ILASS–Europe 2017. 28th Conference on Liquid

Atomization and Spray Systems, 2017, ISBN 9788-490485804
Publisher: Universitat Politècnica València
DOI: 10.4995/ILASS2017.2017.5000

Peer reviewed articles (16)

Air entrainment and mixture distribution in Diesel sprays investigated by optical measurement techniques
Author(s): Sebastian Riess, Lukas Weiss, Andreas Peter, Javad Rezaei, Michael Wensing
Published in: International Journal of Engine Research, 2017, Page(s) 146808741774252, ISSN 1468-0874
Publisher: Professional Enjineering Publishing Ltd.
DOI: 10.1177/1468087417742527

Purely predictive method for density, compressibility, and expansivity for hydrocarbon mixtures and diesel and jet fuels up to high temperatures and pressures
Author(s): Houman B. Rokni, Ashutosh Gupta, Joshua D. Moore, Mark A. McHugh, Babatunde A. Bamgbade, Manolis Gavaises
Published in: Fuel, Issue 236, 2019, Page(s) 1377-1390, ISSN 0016-2361
Publisher: Elsevier BV
DOI: 10.1016/j.fuel.2018.09.041

High-Temperature, High-Pressure Viscosities and Densities of n -Hexadecane, 2,2,4,4,6,8,8-Heptamethylnonane, and Squalane Measured Using a Universal Calibration for a Rolling-Ball Viscometer/Densimeter
Author(s): Aaron J. Rowane, Rajendar R. Mallepally, Ashutosh Gupta, Manolis Gavaises, Mark A. MHugh
Published in: Industrial & Engineering Chemistry Research, Issue 58/10, 2019, Page(s) 4303-4316, ISSN 0888-5885
Publisher: American Chemical Society
DOI: 10.1021/acs.iecr.8b05952

Fluid properties at high pressures and temperatures: Experimental and modelling challenges
Author(s): Rajendar R. Mallepally, Babatunde A. Bamgbade, Aaron J. Rowane, Houman B. Rokni, Matthew S. Newkirk, Mark A. McHugh
Published in: The Journal of Supercritical Fluids, Issue 134, 2018, Page(s) 33-40, ISSN 0896-8446
Publisher: Elsevier BV
DOI: 10.1016/j.supflu.2017.12.003

Entropy scaling based viscosity predictions for hydrocarbon mixtures and diesel fuels up to extreme conditions

Author(s): Houman B. Rokni, Joshua D. Moore, Ashutosh Gupta, Mark A. McHugh, Manolis Gavaises
Published in: Fuel, Issue 241, 2019, Page(s) 1203-1213, ISSN 0016-2361
Publisher: Elsevier BV
DOI: 10.1016/j.fuel.2018.12.043

Partial characteristic decomposition for multi-species Euler equations

Author(s): Jian-Hang Wang, Shucheng Pan, Xiangyu Y. Hu, Nikolaus A. Adams
Published in: Computers & Fluids, Issue 181, 2019, Page(s) 364-382, ISSN 0045-7930
Publisher: Pergamon Press Ltd.
DOI: 10.1016/j.compfluid.2019.01.023

General method for prediction of thermal conductivity for well-characterized hydrocarbon mixtures and fuels up to extreme conditions using entropy scaling

Author(s): Houman B. Rokni, Joshua D. Moore, Ashutosh Gupta, Mark A. McHugh, Rajendar R. Mallepally, Manolis Gavaises
Published in: Fuel, Issue 245, 2019, Page(s) 594-604, ISSN 0016-2361
Publisher: Elsevier BV
DOI: 10.1016/j.fuel.2019.02.044

A split random time-stepping method for stiff and nonstiff detonation capturing

Author(s): Jian-Hang Wang, Shucheng Pan, Xiangyu Y. Hu, Nikolaus A. Adams
Published in: Combustion and Flame, Issue 204, 2019, Page(s) 397-413, ISSN 0010-2180
Publisher: Elsevier BV
DOI: 10.1016/j.combustflame.2019.03.034

Simulation of supercritical diesel jets using the PC-SAFT EoS

Author(s): C. Rodriguez, P. Koukouvinis, M. Gavaises
Published in: The Journal of Supercritical Fluids, Issue 145, 2019, Page(s) 48-65, ISSN 0896-8446
Publisher: Elsevier BV
DOI: 10.1016/j.supflu.2018.11.003

Investigation of Soot Formation in a Novel Diesel Fuel Burner

Author(s): Natascia Palazzo, Matthias Kögl, Philipp Bauer, Manu Naduvil Mannazhi, Lars Zigan, Franz Johann Thomas Huber, Stefan Will
Published in: Energies, Issue 12/10, 2019, Page(s) 1993, ISSN 1996-1073
Publisher: Multidisciplinary Digital Publishing Institute (MDPI)
DOI: 10.3390/en12101993

A multicomponent real-fluid fully compressible four-equation model for two-phase flow with phase change

Author(s): Ping Yi, Songzhi Yang, Chaouki Habchi, Rafael Lugo
Published in: Physics of Fluids, Issue 31/2, 2019, Page(s) 026102, ISSN 1070-6631
Publisher: American Institute of Physics
DOI: 10.1063/1.5065781

A species-clustered splitting scheme for the integration of large-scale chemical kinetics using detailed mechanisms

Author(s): Jian-Hang Wang, Shucheng Pan, Xiangyu Y. Hu, Nikolaus A. Adams
Published in: Combustion and Flame, Issue 205, 2019, Page(s) 41-54, ISSN 0010-2180
Publisher: Elsevier BV
DOI: 10.1016/j.combustflame.2019.03.036

Simulation of transcritical fluid jets using the PC-SAFT EoS

Author(s): C. Rodriguez, A. Vidal, P. Koukouvinis, M. Gavaises, M.A. McHugh
Published in: Journal of Computational Physics, Issue 374, 2018, Page(s) 444-468, ISSN 0021-9991
Publisher: Academic Press
DOI: 10.1016/j.jcp.2018.07.030

In-situ soot characterization of propane flames and influence of additives in a 100 kW oxy-fuel furnace using two-dimensional laser-induced incandescence

Author(s): J. Simonsson, A. Gunnarsson, M. Naduvil Mannazhi, D. Bäckström, K. Andersson, P.-E. Bengtsson
Published in: Proceedings of the Combustion Institute, Issue 37/1, 2019, Page(s) 833-840, ISSN 1540-7489
Publisher: Combustion Institute
DOI: 10.1016/j.proci.2018.05.035

Modelling of Diesel fuel properties through its surrogates using Perturbed-Chain, Statistical Associating Fluid Theory

Author(s): Alvaro Vidal, Carlos Rodriguez, Phoevos Koukouvinis, Manolis Gavaises, Mark A McHugh
Published in: International Journal of Engine Research, 2018, Page(s) 146808741880171, ISSN 1468-0874
Publisher: Professional Enjineering Publishing Ltd.
DOI: 10.1177/1468087418801712

A Theoretical Multiscale Approach to Study the Initial Steps Involved in the Chemical Reactivity of Soot Precursors

Author(s): Michel Keller, Theodorus de Bruin, Mickaël Matrat, André Nicolle, Laurent Catoire
Published in: Energy & Fuels, Issue 33/10, 2019, Page(s) 10255-10266, ISSN 0887-0624
Publisher: American Chemical Society
DOI: 10.1021/acs.energyfuels.9b02284

Thesis and dissertations (3)

Modeling of Diesel injection in subcritical and supercritical conditions
Author(s): Songzhi Yang
Published in: 2019
Publisher: IFPEN

Thermo-physical property models for well-characterized hydrocarbon mixtures and fuels and effect of composition on fluid properties up to 4,500 bar
Author(s): Babazadehrokni, H. B
Published in: 2019
Publisher: City, University of London

Supercritical, transcritical and subcritical real-fluid mixing at high-pressure conditions using the PC-SAFT EoS
Author(s): Carlos Rodriguez
Published in: 2019
Publisher: CITY, University of London

Book chapters (1)

Cavitation Modelling Using Real-Fluid Equation of State
Author(s): Songzhi Yang Chaouki Habchi Ping Yi Rafael Lugo
Published in: Proceedings of the 10th International Symposium on Cavitation (CAV2018), 2018, Page(s) 227-232, ISBN 9780-791861851
Publisher: ASME Press
DOI: 10.1115/1.861851_ch44

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Permalink: https://cordis.europa.eu/project/id/675528/results

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