



Project no.: AST5-CT-2006-030828

TIMECOP-AE

Toward Innovative Methods for Combustion Prediction in Aero-Engines

Instrument: Specific Targeted Research Project (STREP)

Thematic Priority: Aeronautics and Space

Final Activity Report

Final Version

Period covered: M01-M54 (01/06/06-30/11/2010)

Date of preparation: 09/05/2011

Start date of project: 01/06/2006

Duration: 54 months

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Revision: V9

Project coordinator organisation name: **Turbomeca**

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1. GLOBAL INFORMATION

1.1. Acronym table

ACRONYM	MEANING
AFR	Air Fuel Ratio
BC	Boundary Condition
CFD	Computational Fluid Dynamics
CFM	Coherent Flamelet Model
CMC	Conditional Moment Closure
CPU	Central Processing Unit
CSP	Computational Singular Perturbation
DNS	Direct Numerical Simulation
DOW	Description of work: annex I of the contract with the European Community
FGM	Flamelet-Generated Manifold
FID	Flame Ionisation Detector
FM	Fractal Model
FTC-PCM	Flame Tabulated Chemistry with Presumed Conditional Moment
GFM	Ghost-Fluid Method
GT	Gas Turbine
ILDm	Intrinsic Low-Dimensional Manifold
IPCC	Intergovernmental Panel on Climate Change
IPR	Intellectual property rights
LBO	Lean Blow Out
LDA	Laser Doppler Anemometry
LDV	Laser Doppler Velocimetry
LES	Large Eddy Simulation
LIF	Laser Induced Fluorescence
PCM	Presumed Conditional Moment
PLIF	Planar Laser Induced Fluorescence
MPI	Message Passing Interface
NS	Navier-Stokes
PDA	Phase Doppler Anemometry
PDF	Probability Density Function
PDPA	Phase Doppler Particle Analyser
PIV	Particle Imaging Velocimetry
RANS	Reynolds Averaged Navier-Stokes
SHp	Shaft Horse Power
SMEs	Small and Medium Enterprises
SGS	Sub-Grid Scale
STREP	Specific Targeted Research Project
UDF	User Defined Function
VoF	Volume-Of-Fluid

1.2. Co-ordinator Contact Details

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1.3. Contractors involved in the project

Industry

1. Turbomeca SA (TM)
2. Rolls-Royce Deutschland Ltd & Co (RRD)
3. Rolls-Royce plc (RR)
4. MTU Aero Engines GmbH (MTU)
5. SNECMA SA (SN)
6. AVIO S.p.A. (AVIO)

Institutions

7. Centre Européen pour la Recherche et la Formation Avancée en Calculs Scientifiques (CERFACS)
8. Office National d'Etudes et de Recherches Aérospatiales (ONERA)
9. Deutsches Zentrum fuer Luft- und Raumfahrt e.V. (DLR)
10. Institut National Polytechnique de Toulouse (INPT)
11. Centre National de la Recherche Scientifique (CNRS)
12. Centrale Recherche SA (CRSA)
13. Foundation for Research and Technology (ICEHT)
14. Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT)
15. Institut Français du Pétrole (IFP)

Universities

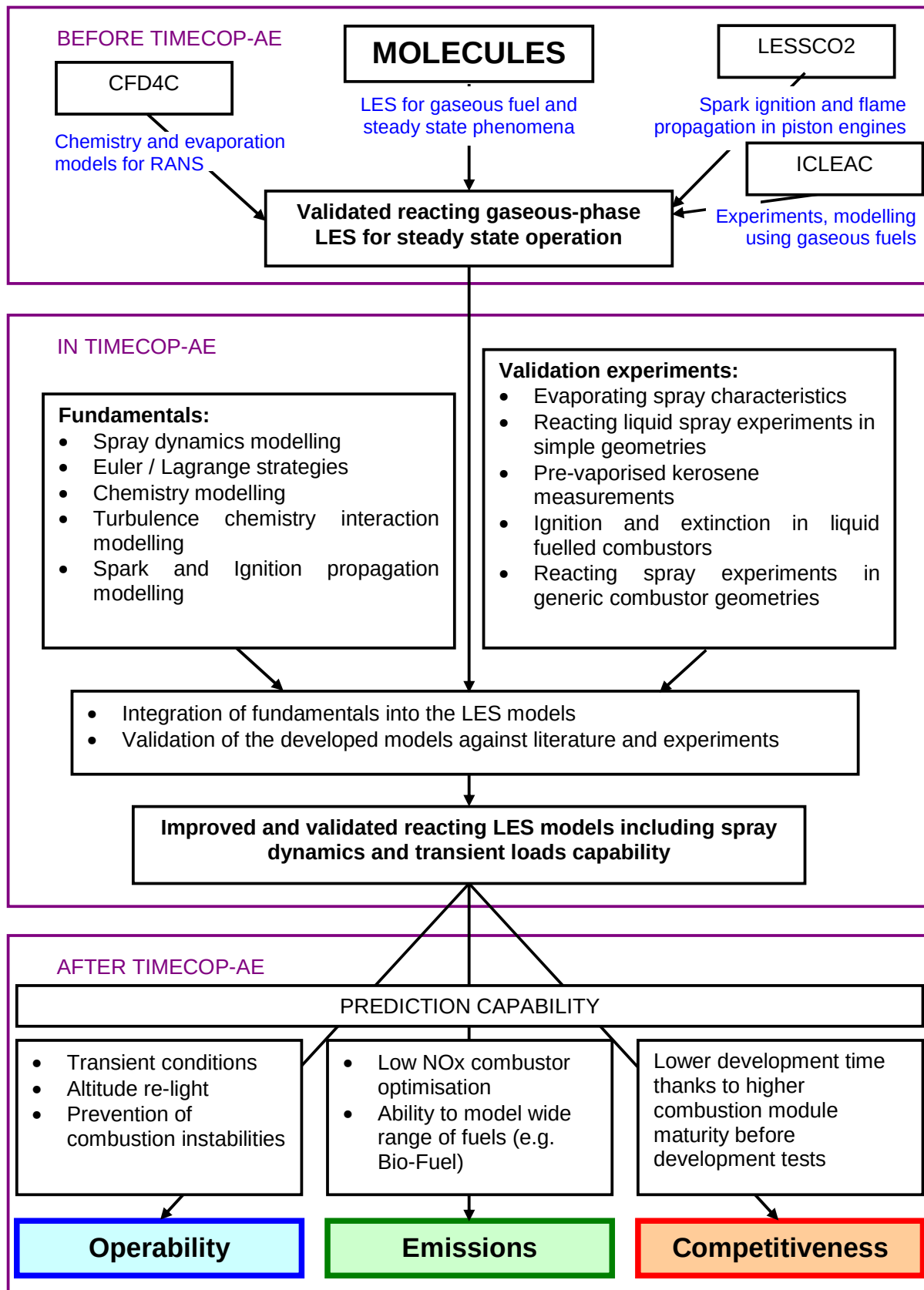
16. The Chancellor, Masters and Scholars of The University of Cambridge (UCAM)
17. Technische Universität Darmstadt (TUD)
18. University of Karlsruhe, Institut für Thermische Strömungsmaschinen (ITS)
19. Technische Universiteit Eindhoven (TUE)
20. Imperial College of Science, Technology and Medicine (IC)
21. Loughborough University (LU)
22. Czestochowa University of Technology, Institute of Thermal Machinery (UC)
23. Department of Mechanics and Aeronautics, University of Rome "La Sapienza" (DMA)

2. PROJECT EXECUTION

2.1. Overview of general project objectives and current relation to the state-of-the-art

The aim of the TIMECOP-AE project is to provide the necessary combustion prediction methods that enable the development of practical advanced combustion systems for future engines that will reduce emission levels and fuel consumption. Predictive tools are required to be able to reduce NOx emissions, to decrease the development time and costs of new combustion systems and to improve the operability of lean-burn combustion systems. All promising approaches to satisfy future emission levels regulations are based on lean combustion technology. However, lean combustion compromises combustor operability, including ignition, altitude re-light, pull-away, weak extinction performance and thermo-acoustic instability behaviour. It is of prime importance to evaluate this transient behaviour in the design stage to ensure good operability. Without these tools the development of these advanced combustion systems will depend on many rig tests. These are costly and time consuming and will reduce our competitiveness.

During the last five years big advances have been made in the field of reactive Large Eddy Simulation (LES) with gaseous fuels. This approach gives promising results with respect to turbulence modelling and can be used to model unsteady processes. Within the framework of TIMECOP-AE, the LES tools have gained the capability for modelling the combustion process within conventional and Low Emission combustors over a wide range of operating conditions on liquid fuels. The operating conditions include mentioned transient phenomena. To be able to model these phenomena improvements are required in the models of turbulence, chemistry, turbulence-chemistry interactions, and liquid spray models. The methods and models have been evaluated against high quality validation data which have been obtained by several validation experiments. Some are designed to validate specific models, one is a generic combustor, representative of an aero-engine combustor, and permits to assess the full range of models.



2.2. Project objectives and achievements per work package

The main objective of the TIMECOP-AE European FP6 project (2006-2010) is to advance LES methods into two-phase flows for gas turbine applications. Therefore it is necessary to:

- develop and study fundamental issues, handled by work package 1
- implement 2-phase capability and perform validation calculations, handled by work package 3
- obtain experimental data for validation, handled by work package 2

Once these 2-phase LES codes are available it is important that the industrial partners can exploit them, and this is the goal of work package 4. Of course there are other means of exploitation, that will be summarised in the Plan for Use and Dissemination of Knowledge.

2.2.1. WP1 - Fundamentals

Within this work package numerical models are developed, improved evaluated and tested. Several models to model two-phase flow, chemistry and ignition have been developed. Both Eulerian and Lagrangian two-phase models have been considered, and the performances of the two approaches have been compared. Chemistry models have been developed for application to LES. Approaches are based on the Flamelet Generated Manifold method, the Conditional Closure Model, the Field PDF method, and the Computational Singular Perturbation method. Furthermore, a specific spark ignition model has been developed. The models have been exploited to industrial partners.

2.2.2. WP2 - Validation experiments

Use of Large Eddy Simulation (LES) techniques to support design of combustors directly has been a long held aim of aero-engine manufacturers. Significant advances have been made in the last couple of decades in the development of enhanced LES-based predictive techniques. However, there are a number of factors that still prevent full utilisation of such sophisticated simulation methods, especially for spray flames, by industry. The need to improve the reactive LES capability is closely dependent on availability of accurate, comprehensive diagnostic measurement data to be used for validation. WP2 focused on development and application of advanced diagnostic techniques on geometries and flow problems ranging from very well defined, easy-to-characterise, academic test cases to industrial test cases. The former tests were used to support model development, the latter to validate models in presence of complex geometries and ambiguity in boundary conditions.

A wide range of advanced diagnostic techniques (e.g. PIV, PTV, PDA, LDA, IMI, PLIF, OH* chemiluminescence, Mie scattering) have been used and often tested to the limit of their capabilities. Attention has been paid to analyse a range of operating conditions, going from altitude relight up to cruise. Both reactive and inert experiments have been carried out. A good combination of single- and two-phase flow experiments has been conducted. The data collected has been then used to both define boundary conditions and validate LES predictions. Important aspects of evaporation, turbulence-chemistry interaction, droplet transport and droplet combustion have been investigated. Notwithstanding the obvious challenges posed by application of these advanced techniques, which often have gone through their own development process within TIMECOP-AE, the objectives of producing a comprehensive matrix of test cases for validation of LES methods has been achieved as per plan.

In summary, the significant achievement of WP2 has been to stretch the capability of existing diagnostic techniques and so provide valuable LES validation data used elsewhere in TIMECOP-AE. In particular, demonstration has been provided that advanced laser diagnostic methods can be directly used on industrial geometries and can produce a wealth of information on the aerothermal behaviour of aero-engine combustors.

2.2.3. WP3 - Numerical validation and implementation of fundamentals

The aim of this work package was to have the fundamental models integrated into the advanced CFD methods, in order to obtain the 2-phase reactive CFD capability to resolve the unsteady behaviour that is natural to turbulent flow. To ensure the proper implementation of these new models, validations were first performed on academic experiments. Once validated, the advanced CFD methods were ready to be tested on complex 3D geometry experiments.

All the tasks defined in the Description of Work of the Timecop project have produced state-of-the-art scientific results and contributions in multiple scientific publications in international conferences and journals. Such a prolific production is the result of the developments and validations of multiple LES strategies to handle two-phase reacting flows not only from a theoretical point of view but also for industry-like configurations. Despite minor adjustments all the tasks with strong links with WP4 (Exploitation) have provided new industrial tools with great potential as illustrated by the industrial partners.

2.2.4. WP4 - Exploitation

Reactive two phase flow, LES is the next evolution in CFD methodologies applied to the conception of aeronautical engines. It should complement/replace actual RANS conception techniques. The justification of this evolution resides in the fact that some engine performances are not predictable with the only use of RANS. Some examples are in flight relight, combustion instabilities, Lean Blow-off prediction, etc. Also RANS is very depending on turbulence modelling and there is no general turbulence model adapted to any geometry/engine operation circumstance. The turbulence modelling in the LES context happens at a more fundamental level and seems today well adapted to capture all kinds of flow features.

TIMECOP-AE has greatly helped to introduce the LES tools into the industrial environment for aeroengine design. Previous to TIMECOP-AE project, the LES was mostly absent from industry and mainly used by researchers without or with a weak link with the aeronautical industry. Some previous research projects (PRECCINSTA, ICLEAC, MOLECULES) have helped the industrials to evaluate and to understand the interest to adopt such LES tools to improve the conception process. TIMECOP-AE has effectively introduced LES in the aeronautical industry, not yet to the conception level, but most industrials in this project have:

- adapted owned CFD tools to perform LES,
- or choose to adopt research tools that have being modified to fit the industrial needs
- or have adopted available commercial tools

2.3. Main project results

2.3.1. Summary Tables of Timecop Achievements

Before and After Timecop-AE

	Situation Before Timecop-AE	Situation After Timecop-AE
2-phase flows	<u>Experimental level:</u> 1 - Lack of accurate measurements of droplet size and velocity in industrial swirling flows 2 - No knowledge if the IMI technique is useful for recording simultaneously droplet size and velocity of technical fuel spray nozzles <u>Numerical level:</u> 1 - Lagrangian and monodisperse Eulerian methods available but not tested on industrial configurations 2 - Stochastic secondary break-up models available but not tested on industrial configurations 3 - No comprehensive accurate methods for specifying unsteady inlet boundary conditions for both gas and dispersed phase 4 - No clear validation of single- and multi-component effects on two-phase LES models 5 - No validation of two-phase reacting LES models on industry-like experimental configurations 6 - Unclear if SGS turbulence has to be accounted for particle dispersion	<u>Experimental level:</u> 1 - Detailed gaseous and liquid phase measurements in industrial burner flows 2 - IMI technique is presently limited to academic test cases with low droplet density. Accuracy with respect to droplet size is not up to par (e.g. PDA) <u>Numerical level:</u> 1 - Polydisperse Eulerian and Lagrangian methods tested on industrial configurations. Assessment of the advantages and drawbacks of each method 2 - A secondary break-up model tested on industrial configurations 3 - An efficient, accurate method has been developed for the gas phase inlet conditions. Similarly, a good methodology for the inlet conditions of the dispersed phase has been developed 4 - Validation of the two-phase LES models for realistic evaporating configurations 5 - First evaluations of the two-phase LES reacting flow models on realistic stationary configurations 6 - Evidence from experiment that SGS turbulence affects droplet trajectories

	Situation Before Timecop-AE	Situation After Timecop-AE
Combustion	<u>Experimental level:</u> 1 - Lack of measurements on industrial configurations of reacting swirling flows 2 - Lack of validation data on reacting two-phase flows at elevated pressure, particularly on spray characteristics like dispersion and evaporation 3 - Lack of spray boundary conditions as starting point for CFD in technical environments at elevated pressure especially with respect to spray concentration and liquid volume flux <u>Numerical level:</u> 1 - Lack of validation on simplified chemical kinetics schemes 2 - Lack of validation of tabulated detailed chemistry for predicting intermediate species in unsteady simulations of real burners 3 - Validation of the LES turbulent combustion models for pollutant predictions	<u>Experimental level:</u> 1 - Detailed flame visualizations and measurements in industrial configurations 2 - Data on fuel placement and fuel/flame interaction at conditions comparable to low to intermediate engine load with respect to temperature and pressure, i.e. droplet size and spray density 3 - Spray characterization: Droplet velocities, sizes, size distributions and volume fluxes in a generic configuration at engine operating conditions <u>Numerical level:</u> 1 - Assessment of detailed chemistry schemes, application of pdf methods on industrial configurations 2 - New progress variable definitions for NOx prediction in unsteady simulations 3 - Validation of tabulated detailed chemistry for unsteady simulations 4 - Extensive comparisons between the reduced chemical kinetic modelling approach and the tabulated chemistry model

	Situation Before Timecop-AE	Situation After Timecop-AE
Ignition	<u>Experimental level:</u> 1 - Lack of experimental evidence to describe the ignition phenomenon 2 - No knowledge on stochasticity of ignition 3 - No detailed validation data <u>Numerical level:</u> 1 - Only semi-empirical ignition models 2 - No model combining spark modelling with turbulent flame spreading for predicting ignition success/failure 3 - No demonstration of the LES unsteady application to the ignition phase 4 - Only simple evaluation of the ignition probability of a burner 5 - Very few understanding of the leading mechanisms resulting in a probabilistic description of the ignition map 6 - No LES simulations 7 - No sub-models	<u>Experimental level:</u> 1 - Visualization of the different phases in the ignition process. Ignition probability maps 2 - Ignition probability maps 3 - Detailed characterization of burners that can be used for validation of codes <u>Numerical level:</u> 1 - Real unsteady multi-factor ignition models tested 2 - Multi-physics models developed 3 - Complex sub-models developed for LES that treat ignition 4 - World-leading capabilities (experimental and numerical)

Summary of Tasks

EXPERIMENT CODE	UCAM 2.1.1	ITS 2.1.2	UC 2.1.3	ONERA 2.2.1	TUD 2.2.2	DLR-VT 2.2.3	DLR-AT 2.3	Other experiment
Chem1D					TUD 3.2.3		RRD 4.1.2 RR 4.1.8	TUE 1.4.1
CMC	UCAM 1.4.2					RR 4.1.7	RR 4.1.5 RR 4.1.8	
LADROP		ITS 3.1.3					RRD 4.1.3	
THETA/SPRAYSIM						DLR-VT 3.2.6 DLR-VT 3.2.6		
SITCOM								CORIA 1.2.1 CRSA 1.3.1a CORIA 3.2.5
DNS-FGM								TUE 1.4.1
FASTEST					TUD 1.2.2 TUD 3.2.3			
HEART	DMA 3.1.4 DMA 3.1.4 DMA 3.1.4			DMA 1.2.3				DMA 3.1.4 DMA 1.4.5 DMA 3.1.4
InPetto								CORIA 1.3.1b
JADIM								INPT 1.3.2
LULES		LU 1.2.5					RR 4.1.8	
SAILOR	UC 1.2.4 UC 3.1.1 UC 3.1.1		UC 1.2.4 UC 3.1.1 UC 3.1.1					
AVBP				CERFACS 3.2.7 TM 4.1.1 SN 4.1.10 CIEMAT 4.2 CERFACS 3.2.7 CIEMAT 4.2 IFP 1.5 TM 4.1.1 CERFACS 3.2.7 TM 4.1.1	CERFACS 3.2.2			INPT 1.3.2
Boffin		IC 3.1.2		IC 3.2.1 IC 1.4.3 IC 1.4.3c		UC 3.2.8 UC 3.2.8	IC 3.2.4 RR 4.1.8	
CFX		ITS 3.1.3				DLR-VT 3.2.6 DLR-VT 3.2.6	MTU 4.1.11 MTU 4.1.11	
N3S				SN 4.1.10 CIEMAT 4.2 SN 4.1.10 CIEMAT 4.2				
OPENFOAM	AVIO 4.1.9 AVIO 4.1.9 AVIO 4.1.9			AVIO 4.1.9 AVIO 4.1.9 AVIO 4.1.9				
PRECISE	UCAM 1.4.2					RRD 4.1.4 RR 4.1.7	RRD 4.1.3 RR 4.1.6 RR 4.1.8	TUE 1.4.1 ICEHT 1.4.4

How to read the table:

The left column contains all the codes that are used in TIMECOP. The upper line contains all the test benches that are used in TIMECOP.

Inside the table are all the TIMECOP tasks with a color code indicating which physical phenomenon they concern:

2-phase flows	Combustion	Ignition
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Code Legend:	Module	Research code	Industrial code
Experiment legend:	Validation of fundamental works	Complex geometries	Two-phase flow Generic Sector Combustor

Deliverables Table

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D0.1.1a	1st Interim Activity Report	0.1.1	TM	M06	Nov-06	Delivered	Nov-06
D0.1.1b	1st Activity & Management Report	0.1.1	TM	M12	May-07	Delivered	May-07
D0.1.1c	2nd Interim Activity Report	0.1.1	TM	M18	Nov-07	Delivered	Nov-07
D0.1.1d	2nd Activity & Management Report	0.1.1	TM	M24	May-08	Delivered	Sep-08
D0.1.1e	3rd Interim Activity Report	0.1.1	TM	M30	Nov-08	Delivered	Dec-08
D0.1.1f	3rd Activity & Management Report	0.1.1	TM	M36	May-09	Delivered	Sep-09
D0.1.1g	Final Interim Activity Report	0.1.1	TM	M42	Nov-09	Delivered	Feb-10
D0.1.1h	Final Reports	0.1.1	TM	M48	May-10	Delivered	Mar-11
D0.1.2a	Cost Statements 1st Period	0.1.2	TM	M12	May-07	Delivered	May-07
D0.1.2b	Cost Statements 2nd Period	0.1.2	TM	M24	May-08	Delivered	Oct-08
D0.1.2c	Cost Statements 3rd Period	0.1.2	TM	M36	May-09	Delivered	Nov-09
D0.1.2d	Cost Statements Final Period	0.1.2	TM	M48	May-10	Delivered	Mar-11
D1.1	Report on programming rules and interfaces	1.1	RRD	M08	Jan-07	Delivered	May-07
D1.2.1	Report on SGS modelling of the transport equation for the mixture fraction variance in the presence of spray and combustion	1.2.1	CNRS	M24	May-08	Delivered	May-08
D1.2.2	Documentation of model to account for turbulence modulation	1.2.2	TUD	M15	Aug-07	Delivered	Nov-07
D1.2.3	SGS Fractal Model of droplet vaporisation and combustion	1.2.3	DMA	M18	Nov-07	Delivered	Nov-07
D1.2.4a	Report and software package – Implementation of liquid fuel spray model into SAILOR-LES code	1.2.4	UC	M12	May-07	Delivered	May-07
D1.2.4b	Report and software package – Implementation of liquid fuel spray model into SAILOR-LES code	1.2.4	UC	M24	May-08	Delivered	Jul-08
D1.2.4c	Report and software package – Implementation of flamelet, CMC and pdf combustion models into SAILOR-LES code	1.2.4	UC	M36	May-09	Delivered	Oct-09
D1.2.5a	Report on implementation of droplet/spray initialisation methods in LES code	1.2.5	LU	M12	May-07	Delivered	May-07
D1.2.5b	Report on optimum droplet tracking method/dispersion model	1.2.5	LU	M18	Nov-07	Delivered	Nov-07
D1.2.5c	Report on model evaluation against experimental data	1.2.5	LU	M24	May-08	Delivered	Dec-08

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D1.3.1a	A report "LES multi-fluid formulation and applied math issues" and "access to the two-phase DNS databases to any interested TIMECOP-AE partners" (CRSA/CNRS)	1.3.1	CRSA	M12	May-07	Delivered	May-07
D1.3.1b	"Complete report with comparisons of Lagrangian and Eulerian formulation from both the physical and the numerical point of view" (CRSA-EM2C / CNRS)	1.3.1	CRSA	M24	May-08	Delivered	Oct-08
D1.3.2a	Database for thermal and evaporating slab	1.3.2	INPT	M24	May-08	Delivered	Oct-08
D1.3.2b	Model for LES Euler-Euler evaporating dispersed phase	1.3.2	INPT	M30	Nov-08	Delivered	Apr-09
D1.4.1a	Reduced chemical model for kerosene (FGM database with interface subroutines)	1.4.1	TUE	M20	Jan-08	Delivered	Jan-08
D1.4.1b	Report on CFM/FGM subgrid scale model	1.4.1	TUE	M30	Nov-08	Delivered	Mar-09
D1.4.1c	CFM/FGM subgrid scale model for LES simulations	1.4.1	TUE	M42	Nov-09	Delivered	Nov-10
D1.4.2a	Predictions of autoignition in turbulent flows with air/fuel ratio inhomogeneities	1.4.2	UCAM	M24	May-08	Delivered	Mar-09
D1.4.2b	Predictions of flame establishment in turbulent flows with air/fuel ratio inhomogeneities	1.4.2	UCAM	M36	May-09	Delivered	Apr-10
D1.4.3a	A stochastic field method for solving the sub-grid joint pdf equation for species mass fraction and temperature: the code Boffin-LES will be supplied to industrial partners	1.4.3	IC	M18	Nov-07	Delivered	Jul-08
D1.4.3b	Final model including combined stochastic field method and reduced chemical scheme for kerosene: the code Boffin-LES will be supplied to industrial partners	1.4.3	IC	M30	Nov-08	Delivered	Oct-09
D1.4.3c	Predictions of auto-ignition with the sub-grid pdf method	1.4.3	IC	M36	May-09	Delivered	Dec-09
D1.4.4a	Construction of final version of the reduced mechanism valid for steady operating conditions (high pressure and high inlet temperature)	1.4.4	ICEHT	M24	May-08	Delivered	Sep-10
D1.4.4b	Construction of final version of the reduced mechanism valid for relight conditions (low pressure and low inlet temperature)	1.4.4	ICEHT	M30	Nov-08	Delivered	Jun-09

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D1.4.5	Ignition and Auto-Ignition Model in Two-Phase Flows	1.4.5	DMA	M24	May-08	Delivered	Dec-08
D1.5a	Report on a first version of the AKTIM-LES spark ignition model and its implementation into AVBP	1.5	IFP	M12	May-07	Delivered	May-07
D1.5b	Report on a version of the AKTIM-LES spark ignition model adapted to gas turbine applications	1.5	IFP	M24	May-08	Delivered	Sep-09
D1.5c	Report on coupling the AKTIM-LES spark ignition model with other turbulent combustion models	1.5	IFP	M30	Nov-08	Delivered	Jul-08
D1.5d†	Report on the application of the AKTIM-LES model for gas turbine engine to the LES of the MERCATO configuration	1.5	IFP	M48	May-10	Delivered	Jun-10
D2.1.1	Experimental data for ignition and flame establishment in turbulent inhomogeneous flows with gaseous and liquid fuels	2.1.1	UCAM	M36	May-09	Delivered	Jun-09
D2.1.2a1	Results on gas flow and two phase flow with non evaporating mono- and polydisperse droplets (monodisperse report)	2.1.2	ITS	M18	Nov-07	Delivered	Sep-09
D2.1.2a2	Results on gas flow and two phase flow with non evaporating mono- and polydisperse droplets (polydisperse report)	2.1.2	ITS	M18	Nov-07	Delivered	Sep-10
D2.1.2b	Results on gas flow and two phase flow with evaporating mono-disperse droplets for single component fuel (report)	2.1.2	ITS	M37	Jun-09	Delivered	Nov-10
D2.1.3a	Report on velocity and temperature fields in cold/hot jets and flame	2.1.3	UC	M12	May-07	Delivered	Jul-08
D2.1.3b	Report on the experimental investigations of the atomisation process in cold/hot jets	2.1.3	UC	M18	Nov-07	Delivered	Dec-08
D2.1.3c	Report on the experimental investigations of fuel spray dynamics in hot jets	2.1.3	UC	M24	May-08	Delivered	Sep-09
D2.1.3d	Report on the measurements of spray characteristics in jet flame	2.1.3	UC	M36	May-09	Delivered	May-10
D2.2.1a	Report on ignition and extinction results at ambient conditions	2.2.1	ONERA	M24	May-08	Delivered	Nov-08

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D2.2.1b	Report on ignition and extinction results at altitude conditions	2.2.1	ONERA	M30	Nov-08	Delivered	Mar-10
D2.2.1c	Report on injection system two-phase flow characterisation (LDA-PDA) at tested injection conditions	2.2.1	ONERA	M36	May-09	Delivered	Nov-08
D2.2.1d †	Report on Statistic investigation of ignition and additional characterisation of the two-phase flow	2.2.1	ONERA	M38	Jul-09	Delivered	Jul-09
D2.2.2a	Report on characterisation of flame structure	2.2.2	TUD	M24	May-08	Delivered	Oct-08
D2.2.2b	Report on characterisation of flow field	2.2.2	TUD	M36	May-09	Delivered	Oct-08
D2.2.3a	Report on the results of measurement campaigns at RR-rig	2.2.3	DLR-VT	M24	May-08	Delivered	Apr-09
D2.2.3b	Report on the experiments at the lab scale combustor	2.2.3	DLR-VT	M42	Nov-09	Delivered	Jul-10
D2.3a	Report on initial conditions for spray	2.3	DLR-AT	M24	May-08	Delivered	Oct-09
D2.3b	Report on results of planar measurement techniques	2.3	DLR-AT	M30	Nov-08	Delivered	Apr-09
D2.3c	Report on results of point measurement techniques	2.3	DLR-AT	M36	May-09	Delivered	Oct-09
D3.1.1a	Report on LES modelling of fuel atomisation in counter current jets - validation against experimental data of PDA measurements in task 2.1.3	3.1.1	UC	M24	May-08	Delivered	Nov-08
D3.1.1b	Report on LES modelling of fuel spray dynamics - validation against experimental data of PDA measurements in task 2.1.3	3.1.1	UC	M36	May-09	Delivered	Oct-09
D3.1.1c	Report on LES combustion modelling -validation against measurements in task 2.1.3	3.1.1	UC	M42	Nov-09	Delivered	Jul-10
D3.1.1d	Report on recommendations and guidelines of LES modelling of two-phase combustion	3.1.1	UC	M48	May-10	Delivered	Nov-10
D3.1.2a	Report on LES results of two phase flow with non-evaporating mono and poly-dispersed droplets	3.1.2	IC	M30	Nov-08	Delivered	Oct-09
D3.1.2b	Report on LES results of two phase flow with evaporating mono and poly-dispersed droplets	3.1.2	IC	M48	May-10	Delivered	Feb-11
D3.1.3a	Demonstration of functionality of sub-grid turbulence model coupling (report)	3.1.3	ITS	M30	Nov-08	Delivered	Jan-09

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D3.1.3b	Validation calculations of premixing nozzle (report)	3.1.3	ITS	M36	May-09	Delivered	Jun-10
D3.1.3c	Source code and documentation made available to partners	3.1.3	ITS	M36	May-09	Delivered	Dec-09
D3.1.4	Porting DMA Models and Validating them using the HeART Code	3.1.4	DMA	M36	May-09	Delivered	Nov-10
D3.2.1a	LES version of Boffin with droplet pdf method incorporated	3.2.1	IC	M09	Feb-07	Delivered	Jan-08
D3.2.1b	Report on the droplet pdf method for liquid fuel sprays	3.2.1	IC	M24	May-08	Delivered	Jul-08
D3.2.1c	Validated LES Boffin code for spray combustion(to industrial partners and UC only)	3.2.1	IC	M46	Mar-10	Delivered	Apr-10
D3.2.2-3.2.3+*	LES of advanced pre-vaporized burner-TUD configuration-Comparisons of LES predictions and approaches	3.2.2/ 3.2.3	CERFACS/TUD	M54	Nov-10	Delivered	Dec-10
D3.2.2a	A report will be provided on the prediction capabilities of the LES version of the subgrid scale closure FTC-PCM	3.2.2	CNRS	M30	Nov-08	Delivered	Oct-08
D3.2.2b	Assessment of the implemented reduced scheme for laminar and turbulent academic cases	3.2.2	CERFACS	M30	Nov-08	Delivered	May-09
D3.2.2c	LES results of the reacting Darmstadt rig using the standard approach	3.2.2	CERFACS	M36	May-09	Delivered	Mar-10
D3.2.2d	LES results of the reacting Darmstadt rig using the new approach	3.2.2	CERFACS	M42	Nov-09	Delivered	Oct-10
D3.2.3a	Validated LES code for simulating single-phase reactive flows with realistic pre-vaporised fuel, taking advantage of FGM chemistry model	3.2.3	TUD	M36	May-09	Delivered	Apr-10
D3.2.3b	Validated LES code for simulating two-phase flows in realistic geometries	3.2.3	TUD	M36	May-09	Delivered	Nov-09
D3.2.4*	Report on LES results of the DLR experiment of task 2.3	3.2.4	IC	M46	Mar-10	Delivered	Dec-10
D3.2.5a	Report on the FTC-PCM method for SGS modelling of turbulent spray combustion	3.2.5	CNRS	M32	Jan-09	Delivered	Mar-09
D3.2.5b	Report on the validation against laboratory experiment of the FTC-PCM SGS modelling	3.2.5	CNRS	M36	May-09	Delivered	Jul-09

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D3.2.6a	Report on issues of numerical modelling of altitude relight	3.2.6	DLR-VT	M24	May-08	Delivered	Jul-09
D3.2.6b*	Report on numerical simulation of the lab scale experiments of subtask 2.2.4	3.2.6	DLR-VT	M48	May-10	Delivered	Dec-10
D3.2.7a	Report on the validation of the AVBP two-phase flow LES modules implemented within TIMECOP-AE (academic cases: cf. Task 1.3.2)	3.2.7	CERFACS	M18	Nov-07	Delivered	Nov-07
D3.2.7b	LES of two-phase flow: FAUGA experiment – Impact of the mono and poly – disperse approaches	3.2.7	CERFACS	M30	Nov-08	Delivered	Jan-09
D3.2.7c	Assessment of the Ignition/extinction modeling process for two-phase flows: FAUGA experiment	3.2.7	CERFACS	M36	May-09	Delivered	May-10
D3.2.7d	LES of two-phase reacting flow: FAUGA rig, ignition/extinction capabilities and predictions	3.2.7	CERFACS	M42	Nov-09	Delivered	Nov-10
D3.2.8*	LES altitude relight simulations of two-phase combustion	3.2.8	UC	M48	May-10	Delivered	Nov-10
D4.1.1	Report on LES calculation by TM	4.1.1	TM	M48	May-10	Delivered	Jun-10
D4.1.10a	Report on 2-phase flow non reactive RANS calculation and comparisons	4.1.10	SN	M12	May-07	Delivered	Sep-08
D4.1.10b	Report on 2-phase flow reactive RANS calculation and comparisons	4.1.10	SN	M24	May-08	Delivered	Dec-10
D4.1.10c	Report on 2-phase flow reactive LES calculation and comparisons	4.1.10	SN	M36	May-09	Delivered	Dec-10
D4.1.10d	Report on extinction RANS prediction and comparisons	4.1.10	SN	M48	May-10	Delivered	Mar-11
D4.1.11	Report on “commercial” LES results of the DLR experiment of task 2.3	4.1.11	MTU	M46	Mar-10	Delivered	Jul-10
D4.1.2a	Report on application of FGM model in RANS code	4.1.2	RRD	M24	May-08	Delivered	Sep-08
D4.1.2b	Report on application of FGM model in LES code	4.1.2	RRD	M36	May-09	Delivered	Apr-10
D4.1.3	Report on application of two-phase model of ITS	4.1.3	RRD	M42	Nov-09	Delivered	Nov-10
D4.1.4	Report on assessment of altitude relight modelling	4.1.4	RRD	M48	May-10	Delivered	Nov-10
D4.1.7*	Report on altitude relight calculation	4.1.7	RR	M42	Nov-09	Delivered	Nov-10
D4.1.8	Report on 2-phase flow generic combustor calculation	4.1.8	RR	M48	May-10	Delivered	Nov-10

Del. N°	Deliverable Name	Task N°	Lead Participant	Due Date from Annex I	Due Date	Delivered Yes/No	Actual / Forecast Delivery Date
D4.1.9a	Evaluation of auto-ignition in premixing duct geometries	4.1.9	AVIO	M40	Sep-09	Delivered	Mar-11
D4.1.9b	Results of application on a real combustor geometry of LES models for spray combustion in commercial codes	4.1.9	AVIO	M48	May-10	Delivered	Mar-11
D4.2	Report, and routines, to construct a LES initial condition from a RANS solution	4.2	CIEMAT	M36	May-09	Delivered	Jun-09

* These deliverables include direct comparisons of Timecop results

† These deliverables are additional reports beyond the work originally described in the DoW

2.3.2. Experimental Tools and Results

Experimental facilities aimed at the validation of fundamental works

Task 2.1.1 Experimental measurements of flame propagation speed (UCAM)

This task aimed to provide the physical behaviour and quantitative results of the flame following spark ignition in gaseous and spray inhomogeneous mixtures. The experimental results have been presented in Deliverable 2.1.1. "Experimental data for ignition and flame establishment in turbulent inhomogeneous flows with gaseous and liquid fuels". These experiments have been used to provide validation data for various partners who performed numerical simulations (Imperial College, CNRS-INRIA) and have been requested widely from laboratories across the world, providing therefore a leadership position to the TIMECOP-AE project.

Task 2.1.2 Experimental validation of evaporating fuel sprays in premixing zones (ITS)

A new test rig has been developed at ITS which is dedicated to the investigation of the unsteady droplet dispersion phenomenon. The setup features an acoustically excited flow configuration where large-scale vortices evolve periodically and interact with the injected droplets. It is possible to generate either a chain of mono-sized drops, or a "quasi" poly-disperse spray based on the control of the droplet generator developed in-house. The gas- and dispersed-phase, as well as the two-phase flow were characterized experimentally by means of LDA, PIV, IMI and back-light visualisation measurements and can serve as validation data for any CFD calculations.

Task 2.1.3 Experimental investigations of droplet / turbulence and combustion chemistry / turbulence interaction in simple geometry (UC)

With the framework of the D.2.3.1.a deliverable, UC performed 3 series of experiments. The first two series of experiments were performed on cold and hot jets, the third series of experiments was performed on flames. Measurements were carried out with CTA, CCA and LDA techniques.

The results of the research confirmed that the counter-current jet proved to be capable to provide the well controlled environment to perform evaporation studies. In particular it was proved that by changing the suction rate the mean velocity, turbulence intensity and scales of turbulence can be controlled in every point. The data base obtained during this study for each measuring points provides the information about: velocity, its gradient, turbulence intensity, turbulence kinetic energy, temperature, micro and macro scales.

With the framework of the D2.1.3.b deliverable, UC performed experimental investigations of the atomisation process in cold/hot jets. This experiment was performed for three types of injectors, the first two were based on the Rayleigh instability phenomenon and the third one was based on the GÖdde principle. A measurement technique based on phase-locked image recording was used.

For the selected injector based on Rayleigh phenomenon the jet length before disintegration into droplets and PDF distribution of droplets was investigated for two test cases without and with excitation. Experimental investigations for injectors based on the GÖdde principle showed that with this type of injector it is possible to produce droplets with sizes 25% smaller than the ones obtained with Rayleigh instability for the same exit diameter of the injector.

Within the framework of the D2.1.3.c deliverable, UC performed experimental investigations of fuel spray dynamics in hot jets. This experiment was performed for the injector based on the GÖdde principle. The experimental work was done for two types of liquid: water and kerosene for different temperature conditions.

The experimental investigations on the influence of the frequency excitation showed that an increase in the frequency of excitation caused a decrease in the distance between consecutive

droplets and caused generation of smaller and more uniform droplets. Experimental work concerning evaporation in isothermal and non-isothermal conditions showed that overheat caused faster change in initial droplets diameter for both the investigated liquids.

Within the framework of the D2.1.3.d deliverable, UC performed experimental investigations of fuel droplets dynamics in flame. This experiment was performed for the injector based on the Gdde principle for kinetic and diffusive type of flames. Due to limitations of the measurement techniques droplets were introduced in the outer flow and the influence of flame radiation on droplets evaporation was investigated.

The result obtained revealed that the droplets are evaporating faster in diffusive flames in comparison with kinetic ones and this due to influence of differences in spectral contents of radiation, although it may also result partly from the difference of the extent of the region of higher flow temperature in flames investigated

Experimental facilities aimed at the validation in complex geometries

Task 2.2.1 Two-phase flow FAUGA experiment (ONERA)

In this task, ONERA provided an extensive and detailed experimental data base on ignition and extinction downstream of an actual single sector injection system of a turbojet engine under altitude conditions. This data base is composed of an accurate description of the set-up and of the operating points, of the ignition and extinction domains vs. the operating conditions (D221a & D221b) and finally of the detailed air-kerosene flow characterisation, obtained with optical diagnostics, for several operating points investigated in ignition (D221c & D221d).

Task 2.2.2 EKT experiment – Pre-vaporised kerosene (TM injector) (TUD)

The aim of this work was to replace the natural gas that was used in the former EU project MOLECULES with pre-vaporized liquid fuel. For this purpose an appropriate method of pre-vaporization was worked out which took advantage of recent experience at DLR Cologne. A mixture of carrier gas and pre-vaporized fuel needed to be avoided.

To achieve comparable conditions with previous methane based studies for mixing and combustion a primary-pressure of at least 4 bar was necessary to supply sufficient momentum for the fuel-jet in this specific configuration. A set-up designed by DLR was used, where liquid kerosene was vaporized at a minimum temperature of 673 K in a flowing system.

The lay-out of the generic Turbomeca (TM) injector was kept identical to those used in the MOLECULES project, whereas the operating points were changed in order to achieve stable operating points for the measurements of the turbulent kerosene flame.

Flow fields and flame stabilization were investigated using state-of-the-art Laser Doppler velocimetry (LDV) (Subtask 2.2.2.a) and planar laser-induced fluorescence (PLIF) methods (Subtask 2.2.2.b).

As a result, a comprehensive database containing datasets of the velocity fields of the flow as well as the characteristic parameters of the flame derived from the spectroscopic measurements has been built. This database has been successfully used for model validation and numerical simulation. The results of the experiments were shared with the partners for LES-validation within subtasks 3.2.2 (CERFACS) and 3.2.3 (TUD).

The flame stability and structure of a turbulent, vaporized kerosene flame under high pressure conditions was investigated using laser measurement techniques such as OH-LIF and kerosene LIF as well as chemiluminescence recordings (Subtask 2.2.2.a:). For comparability, test rig conditions, such as combustion air temperature, pressure loss over the nozzle and similar test rig pressures, were chosen similar to those used in the MOLECULES project.

In all investigated test cases the flame burned attached to the nozzle and no dominant fuel jet was detected, as in the MOLECULES experiments, as the vaporized kerosene concentrated in the vicinity of the nozzle. Further on, no significant pressure influence on the apex angle of the flame and on flame structure itself could be found. Detailed information about the set up, measurement techniques and results are given in Deliverable D2.2.2a ("Report on characterization of flame structure").

A turbulent vaporized kerosene flame under high pressure conditions was investigated for velocity components, including RMS and autocorrelations in Subtask 2.2.2.b. This study showed typical phenomena for turbulent swirled flow fields, such as coherent structures, recirculation zones, and stagnation points. In all investigated test cases symmetrical and consistent distributions were found. The streamline plot and also the velocity distributions have shown the existence of a recirculation zone responsible for stabilization of the flame and a stagnation point near the nozzle, causing the lift off height of the flame.

Task 2.2.3 Validation experiments for altitude relight (DLR-VT)

Various optical and laser-based measurements were performed at a generic lab-scale model combustor at DLR-VT in Stuttgart (FRG) and at the high-altitude industrial test-rig at RR in Derby (UK). In the newly built model combustor one-, two- and three-dimensional mono-disperse fuel droplet loads were generated and ignited with focused laser radiation. At the RR test-rig the spray from a lean-burn fuel injector, installed in a twin-sector combustor, was ignited with a standard spark igniter. The transient phenomena during ignition and flame establishing were investigated.

From the measurements at the RR altitude test facility new information and data about the ignition and combustion process under realistic altitude relight conditions were obtained, as reported within the Deliverable D2.2.3a. From the measurements at the DLR-VT test-rig at atmospheric conditions validation data for the numerical simulation of spray ignition and of altitude relight were generated and provided to the TIMECOP-AE consortium – see Deliverable D2.2.3b.

Two-phase flow generic sector combustor experiment

Task 2.3 Two-phase flow Generic Sector Combustor experiment - droplet characterisation (DLR-AT)

The Generic Single Sector Combustor (SSC) with optical access was operated with a burner designed for operation on Jet A-1 kerosene fuel for partially premixing or diffusion flames under realistic gas turbine combustor conditions. Flame, fuel spray and flow field were investigated by planar optical methods like Mie scattering, PLIF, and chemiluminescence, as well as PDA and LDA. Data on fuel spray placement and flame structure were published in Deliverable D2.3b; measurements of fuel droplet velocities and sizes, along with air velocity distributions, are reported in Deliverables D2.3a and c (one document).

2.3.3. Numerical Tools

Industrial codes

AVBP: developed by CERFACS and IFP. Used by CERFACS, IFP, TM, SNM, CIEMAT.

- ▶ Unstructured flow solver
- ▶ Developed by CERFACS and IFP,
- ▶ External/internal flows,
- ▶ Fully compressible turbulent reacting flows,

- DNS/LES approaches,
- Unstructured hexaedral, tetraedral, prisms & hybrid meshes,
- Massively parallel,
- C/Fortran languages,
- SPMD approach.
- Numerics:
 - Finite-Volume, cell-vertex formulation (Crumpton et al., 1993; Rudgyard, 1995; Giraud et al., 1995; Schonfeld & Rudgyard, 1999)
 - Explicit temporal integration
 - Spatially centered schemes
 - Lax-Wendroff (Lax & Wendroff, 1960),
 - Two-step Taylor-Galerkin (Quartapelle, 1988; Donea, 1984; Colin & Rudgyard, 2000)
 - Stabilization by use of artificial viscosity (Jameson, 1989) : 2ème et 4ème order
- Turbulent combustion
 - Compressible reacting Navier-Stokes
 - Realistic thermo-chemistry (JANAF)
 - Physical models
 - Turbulence: Smagorinsky (Smagorinsky, 1963), WALE (Nicoud & Ducros, 1999)
 - Kinetics: Arrhenius & reduced chemical scheme, Tabulated chemistry
 - Combustion: Thickened Flame (O'Rourke & Bracco, 1979; Colin et al. 2000), CFM, PCM
 - NSCBC boundary conditions (Poinsot & Veynante, 2005)
- Two phase flow
 - Euler/Euler solver:
 - Euler continuous representation model (benefit from the gas phase parallelisation and algorithmic)
 - Locally mono-dispersed
 - Modeling needed (IMFT model)
 - D2 evaporation model
 - Euler/Lagrange solver
 - Particle tracking solver
 - Multi-dispersed
 - D2 evaporation model

BOFFIN: developed by IC and used by IC and UC.

- Block-structured boundary conforming coordinates
- Language: Fortran with Fortran 90 front end for dynamic memory allocation
- Parallelisation via MPI – efficiencies in excess of 90%
- Numerics:
 - Finite-Volume, pressure based method.
 - Energy conserving convection term discretisation with approximate factorisation method for pressure
- LES modeling
 - Eddy viscosity Sub-grid scale models
 - Smagorinsky model
 - Dynamic model
- Combustion modeling
 - Non-Premixed turbulent combustion model: conserved scalar + Beta pdf + flamelet
 - Premixed and partially premixed combustion: two-variable model (Y_f & Z) + Beta and delta pdf's + flamelet
 - Full SGS PDF evolution equation method (LMSE/IEM model) + Eulerian field stoch. Solver + reduced chemical mechanisms
- Two phase flow
 - Probabilistic treatment of spray => representation of the Spray pdf by SDEs.
 - Stochastic particles each with a velocity, temperature, radius and number values.
 - Lagrangian description.

- Fully coupled to gas phase.

CFX: Commercial CFD package developed by ANSYS and used by ITS, DLR-VT, MTU within TIMECOP

- ▶ Commercial CFD package with all the needed support and development environment of the ANSYS comp.
- ▶ Solution of the steady and unsteady Euler, laminar N-S, RANS and LES/DES incompressible fluid mechanics equations on 2D and 3D unstructured meshes
 - Supported elements :
 - 3D : hexahedral, pyramids, prisms & tetrahedral
 - 2D : quadrilaterals & triangles
- ▶ Numerical keywords :
 - Cell-vertex finite element approach, MUSCL
 - Coupled Algebraic multigrid (incompressible solver)
 - Available precision : $O(2)$ in space
- ▶ Multi-platform & fully parallel solver (MPI & PVM)
- ▶ Turbulence modeling and wall modeling
 - One, Two equations turbulence models :k- ϵ model & variants. K-w model
 - Full Reynolds stress closures
 - Smagorinsky type of LES models
 - Wall law & Low Reynolds approaches available
 - SAS approaches: Scale Adaptive Simulations
- ▶ Two phase flow
 - Lagrangian approach: Tracking of droplets trajectories
- ▶ Combustion modeling
 - Multi-step Eddy Break-up, finite rate chemistry, Nox and soot models as well as state-of-the-art flamelet and Simont models

N3S: developed by SAFRAN and used by SAFRAN and CIEMAT

- ▶ Solution of the steady and unsteady Euler, laminar N-S & RANS compressible fluid mechanics equations on 2D and 3D unstructured meshes
 - Supported elements :
 - 3D : hexahedral, pyramids, prisms & tetrahedral
 - 2D : quadrilaterals & triangles
- ▶ Numerical keywords :
 - Cell-vertex approach, MUSCL
 - ROE-TOUMI multi-species solver $\diamond$ JANAF thermodynamics database for kerosene
 - Gauss-Seidel, Jacobi and Parallel Multi-Grid matrix inversion techniques
 - Low Mach number matrix pre-conditioning
 - Precision for standard steady calculations $\diamond$ $O(2)$ in space (Van Albada) & $O(1)$ in time
 - Available precision : $O(3)$ in space, b-g scheme & $O(4)$ in time, RK4
- ▶ Multi-platform & fully parallel solver (MPI & PVM)
- ▶ Turbulence modelling and wall modelling
 - Two equations turbulence models :k- ϵ model & variants. K-w model
 - Wall law & Low Reynolds approaches available
- ▶ Boundary conditions
 - Ease to introduce profiles at the boundaries
 - For the combustion calculations most boundary conditions are flux based. Better global conservation
 - Translational & rotational periodicity
 - Different adiabatic/non adiabatic wall laws :1 & 2 scales, LTM (self adapting law to take into account compressibility/incompressibility near wall)
 - Special boundary conditions for Snecma combustors applications like effusion cooling/porosity (partially developed inside INTELLECT) , and all the standard boundary conditions that can be found in any commercial CFD software

- ▶ Two phase flow
 - Lagrangian approach : Tracking of droplets trajectoires
 - Kerosene as liquid fuel.
 - D2 model, infinity, limited and effective conductivity models available
 - Account for stochastic contribution to the trajectories
- ▶ Combustion modelling
 - Several combustion models : CLE, PCM-FPI, Cramer, Arrhenius, etc
 - Pollutants computed with PCM-FPI model. Used in Sia-Team, TLC & TECC
 - Soot modelling : CFD4C Lund model & Sia-team model
- ▶ Other additional features
 - Rotating frame de reference (source terms)
 - EDF peripheral version allows meridian rotor/stator calculation
 - Automatic partitioning of the mesh (only the number of processors should be indicated)

OPENFOAM: open-source code developed by DMA and used by AVIO within TIMECOP

- ▶ Discretization by finite volume method
- ▶ Opportunity to study, both in steady and transient conditions, complex and coupled physical phenomena (e.g. fluid-structure interaction, heat/mass transfer, internal combustion engine, etc.) and multi-phase phenomena (Lagrangian tracking of the dispersed phase)
- ▶ Use of the equations for the physical continuum mechanics (P.D.E.)
- ▶ Simplicity in the programming language used (C + +) for writing the equations of motion
- ▶ Decomposition of the computational domain for the parallelization of the calculations
- ▶ User friendly libraries and editing capabilities
- ▶ Combustion models
 - Premixed (or partially premixed) combustion
 - Flamelet approach
 - Turbulence modeling
 - Chemistry describe by a one-step reaction mechanism
- ▶ Two-phase flows
 - The fuel droplets were divided into three classes of particles characterized by different initial diameters
 - These conditions had to be compatible with the total number of particles and the total volume fraction
 - The fuel injection was linked with the geometry through the additional inlets for fuel
 - Coupling physics of the problem by modifying the OpenFOAM tutorial (ReactingFoamMPH Multiphase)
 - Suitable models for the atomization and evaporation of fuel were chosen

PRECISE: developed and used by RR and RRD

- ▶ PRECISE -MB
 - Multiblock / structured code
 - Parallised using block-structure
 - ADI solver
- ▶ PRECISE-UNS
 - Unstructured code (Hexa, Tetra, Prism, Pyramid, polyhedra mixed meshes)
 - Parallised using ParMETIS
 - BCGSTAB / HYPRE multigrid solver
- ▶ Cell-centred, low Mach number, incompressible formulation using pressure correction method
- ▶ 2nd order discretisation schemes, in space and time, TVD for scalars
- ▶ Several combustion models (global mechanism/Flamelets/FGM)
- ▶ Chemistry-turbulence interaction using: EBU/Presumed PDF/Transported PDF/CMC (MB)
- ▶ Several turbulence models: k-epsilon/Reynolds Stress/Large Eddy Simulation

- ▶ LES: standard and dynamic Smagorinsky models
- ▶ NOx and soot models
- ▶ Lagrangian spray model (steady / transient), including atomisation (LU-secondary break-up model (MB)) / evaporation (in-house / LADROP-coupling (UNS))

Research codes

DNS-FGM: developed by TUE, used by RR and RRD

BEFORE TIMECOP-AE

- ▶ Single phase DNS/LES finite volume code.
- ▶ Incomp/low M variable r , reacting flows.
- ▶ Block-structured, staggered Cartesian grid.
- ▶ Explicit, hybrid time stepping scheme for mom. equ. (3rd order Adams-Bashforth for convective fluxes, Euler forward for viscous fluxes)
- ▶ 2nd order CD for spatial discretization.
- ▶ Van Leers 3rd order MUSCL for scalars (TVD)
- ▶ Multi-grid solver for a Poisson equation of pressure.
- ▶ Models:
 - SGS stresses: Smagorinsky; dynamic Smagorinsky; Germano and Vreman model.
 - SGS scalar fluxes: gradient-diffusion model.
 - Combustion: Flamelet Generated Manifold (FGM).
 - SGS combustion: Presumed (beta) PDF model

AFTER TIMECOP-AE

- ▶ Parallelization: both domain decomposition (MPI), as well as parallel processing using OpenMPI library.
- ▶ Combined FGM for partially-premixed combustion: online determination of local “premixedness” and applying the suitable FGM type (premixed, non-premixed or a continuous combination).
- ▶ Applications/Validations
 - Sandia Flames (Barlow&Frank, Schneider et al.)
 - Turbulent planar Bunsen flame (Vreman et al.) with stratification in span-wise direction.

FASTEST: developed by TUD, used by RRD

BEFORE TIMECOP-AE

- ▶ Single phase LES finite volume code (hexahedral CV)
- ▶ Incomp/low M variable r , non-reacting/reacting flows.
- ▶ Boundary-fitted non-orthogonal block-structured grid (matching interfaces and collocated grid)
- ▶ Implicit and Semi-implicit temporal, 1st and 2nd order spatial discretisation schemes (TVD for scalar)
- ▶ Multi-grid solver for convergence acceleration
- ▶ Parallelisation based on domain decomposition (MPI)
- ▶ Models:
 - SGS stresses: Smagorinsky with Germano procedure; anisotropic model (Horiuti model); one-equ. model
 - SGS scalar flux: Eddy diffusivity with dynamic procedure; anisotropic model (Sadiki model)
 - Combustion: Flamelet; Thickened Flame Model; Flame surface Density
- ▶ Multiphase LES
 - Lagrangian particle tracking with two-way coupling

- Divers evaporation models

AFTER TIMECOP-AE

- ▶ Single phase combustion
 - Explicit Runge-Kutta 2nd order schemes
 - Flamelet Generated Manifolds(Task 3.2.2)
- ▶ Multiphase flow simulation capability
 - Turbulence modulation models (Task 1.2.2)
 - Spray module including turbulence modulation and Evaporation process (Task 3.2.2b)
- ▶ Applications/Validations
 - EKT Combustion chamber (MOLECULES)
 - Pre-vaporized kerosene combustion chamber (EKT Experiment)
 - Particle laden vertical channel flow (Geiss et al., 2005)
 - Solide particle laden swirling two-phase flow in a combustor configuration (Sommerfeld & Qiu, 1991)
 - Evaporating Spray in a combustion chamber configuration (Sommerfeld & Qiu, 1994)

HEART: developed by DMA, used by AVIO

BEFORE TIMECOP-AE

- ▶ Single phase LES finite difference code
- ▶ Fully compressible non-reacting/reacting flows.
- ▶ Block-structured, polar/cartesian, staggered grid
- ▶ Explicit, 3rd order Runge-Kutta for time stepping and 2nd order CD for spatial discretisation
- ▶ Parallelisation based on domain decomposition (MPI)
- ▶ Models:
 - SGS stresses: Fractal Model(FM)
 - SGS scalar fluxes: gradient-diffusion model
 - Combustion: EDC model based on FM

AFTER TIMECOP-AE

- ▶ Implementation within HeaRT
 - Multiphase flow simulation capabilities:
 - Eulerian/Eulerian approach (Task 1.2.3)
 - SGS particle/turbulence interaction (1.4.5)
- ▶ Applications/Validations
 - Swirling particulate two-phase flow (Sommerfeld & Qiu)
 - Heptane spray ignition (UCAM)
 - LPP duct (AVIO) - Autoignition

ASPHODELE (formerly InPetto): developed by CNRS-CORIA

BEFORE TIMECOP-AE.

- ▶ two-phase DNS finite difference code
 - Incomp/low M, variable r , non-reacting/reacting flows.
 - Explicit, 3rd order Runge-Kutta temporal, and 6th order Padé for spatial discretisation
 - Direct solver for a Poisson equation of pressure
- ▶ Models:
 - Dispersed phase : Lagrangian solver, two-way coupling (momentum – mass – energy), elastic collisions
 - Combustion: fast chemistry; POPE; Chemkin coupling (VODE solver)

AFTER TIMECOP-AE

- Spectral solver capability
- FFTW3
- Cold flame single chemistry
- Development of a specific mass two-way coupling procedure
- Coupling with MUSE solver (Dispersed Eulerian) from EM2C – Marc Massot.
- Applications
 - Preferential segregation analysis
 - Impact of the preferential segregation on the vapour/air mixing
 - Impact of the preferential segregation on the flame propagation

NTMIX: developed by INPT

BEFORE TIMECOP-AE

- DNS code for variable density flows
- Limited to simple geometries with structured Cartesian meshes
- 6th order compact scheme
- 3rd order Runge-Kutta time discretization
- Parallelisation based on domain decomposition
- Lagrangian tracking of particles or/and droplets including heat transfer and evaporation.

AFTER TIMECOP-AE

- No specific development
- NTMIX was used to create numerical databases.

LULES: developed by LU, used by RR and RRD

BEFORE TIMECOP-AE

- Single phase LES finite volume code
- Incomp/low M variable ρ , non-reacting/reacting flows.
- Block-structured, curvilinear orthogonal, staggered grid
- Explicit, 2nd order Adams-Bashforth temporal, and 2nd order CD for spatial discretisation (TVD for scalar)
- Multi-grid solver for a Poisson equation of pressure
- Parallelisation based on domain decomposition (MPI)
- Models:
 - SGS stresses: Smagorinsky model and a dynamic version (Germano procedure)
 - SGS scalar fluxes: gradient-diffusion model
 - Combustion: fast chemistry; steady laminar flamelet model; flame surface density

AFTER TIMECOP-AE

- Two-phase flow simulation capabilities (1.2.5)
- Lagrangian particle tracking
- Secondary breakup model
- Hybrid parcel/droplet approach to improve computational efficiency
- Linear stochastic model for droplet SGS dispersion
- Applications/Validations
 - Swirling particulate two-phase flow (Sommerfeld & Qiu)
 - Break-up of a water jet in a turbulent stream (Lasheras et al.)

- Particle dispersion in free shear layer (Lazaro & Lasheras)

SAILOR: developed by UC

BEFORE TIMECOP-AE

- LES code for low M variable density flows
- Limited to simple geometries with structured cartesian mesh
- 6th order compact/Fourier pseudo-spectral approximation
- 3rd order Runge-Kutta time discretization
- Projection method for pressure/velocity coupling
- Parallelisation based on domain decomposition
- Models
 - SGS models: Smagorinsky; dynamic Smagorinsky; structure function models

AFTER TIMECOP-AE

- Spectral LES treatment of multi-phase combustion of liquid fuel (Task 1.2.4)
- Fully compact difference discretization with an additional time intergration by pre –corr scheme
- Applicable to non-cartesian meshes
- Atomisation model (Level-Set, VoF, coupled Level-Set and VoF, ghost fluid method)
- A stochastic model for droplets SGS dispersion; a secondary breakup model (Reitz-Diwakar) and a droplet vaporization model (D2 model)
- Combustion models: flamelet; Conditional Moment Closure and Eulerian PDF
- Applications/Validations
 - Atomisation model: Plateau-Rayleigh break-up and liquid jet break-up;
 - Secondary break-up in cross flow air flow, wall bounded periodic channel ;
 - Combustion models: Sandia D, E, F flames and bluff-body flames.

Modules

Chem1D: developed by TUE, used by RRD

- One-dimensional reacting flow solver
 - 1D Finite Volume code using an adaptive meshing procedure.
 - Multiple flame configurations (free-flow, counterflow, radially/spherically expanding flames etc.)
 - Capable of steady (modified damped Newton solver1) and unsteady (2nd order implicit in time) simulations.
 - 2nd order exponential scheme for spatial discretization.
 - Combustion Approximation for decoupling of acoustics.
 - Detailed chemistry (ChemKin format).
 - Diffusion models:
 - Constant Lewis numbers.
 - Mixture averaged diffusion coefficient.
 - Detailed multicomponent diffusion model.
- Applications in TIMECOP-AE:
 - Generate flamelets to construct Flamelet Generated Manifolds2 for kerosene/air combustion.
 - 1D validation of new FGM approach for partially-premixed flames.

CMC: developed by UCAM, used by RR and RRD

BEFORE TIMECOP-AE

- Module for RANS that solves the Conditional Moment Closure equations for gaseous combustion
- No CMC theory for sprays yet

AFTER TIMECOP-AE

- Governing equations
 - Derivation and modelling of CMC equations with spray terms added
- Applications/Validations
 - Validation of CMC equations with spray for autoignition against Direct Numerical Simulation data (Deliverable D.1.4.2a)
 - Validation of RANS/CMC package for swirling spray spark ignition (simulated experiment of Task 2.1.1) (Deliverable D.1.4.2b)
 - Preliminary tests with LES/CMC for jet spray flame (Deliverable D 1.4.2b).
 - Code delivered to RR UK

SPRAYSIM: developed by DLR-VT, used by RR and RRD

BEFORE TIMECOP-AE

- Lagrangian solver for spray simulation on unstructured grids
 - 8 ODEs solved with the Adams Predictor-Corrector scheme (for non-stiff problems, internal variable timestep)
 - No droplet/wall interaction model
 - No droplet/droplet collision or droplet deformation models.
- Primary atomization (jet-in-cross-flow) & secondary atomization (TAB, ETAB, Reitz-Diwakar, Schmell)
- Generic spray boundary conditions (droplet size and velocity distribution as input)
- Droplet evaporation: infinite conductivity, limited conductivity, and effective conductivity
- Droplet turbulent dispersion: Gosman-Ioannides and Blümcke (spectral)
- Steady two-way coupling with different CFD Eulerian solver: ANSYS-CFX, Fluent, THETA

AFTER TIMECOP-AE

- Implementation of Real fuel droplet evaporation model
- Multicomponent-fuel effect taken into account using the continuous thermodynamics theory in the evaporation model as well as for thermophysical properties
- Extension to unsteady spray Lagrangian computations on two platforms: SPRAYSIM-CFX & SPRAYSIM-THETA (DLR in-house code for turbulent combustion)

SiTCOM: developed by CORIA

- Finite volume solver, structured mesh
- Fully compressible formulation
- 4th order in space and 3rd order in time
- Tabulated detailed chemistry using PCM-FPI (developed within TIMECOP)
- Run over 4096 processors with 95% efficiency (developed within TIMECOP)
- Lagrangian dynamic SGS; WALE and Structure function SGS modeling (developed within TIMECOP)
- Two papers published within TIMECOP (simulation of the Cabra flame and of the Cambridge spark ignition burner)

2.3.4. Two-Phase flows

Different approaches to model two-phase flows are developed and evaluated by several partners. Both Eulerian and Lagrangian approaches are considered.

Task 1.2.1 LES modelling of evaporation, micro-mixing for combusting two-phase flows (CNRS)

During the first year, a DNS database has been developed in order to test the models allowing to close the transport equation of the subgrid mixture fraction variance.

Multiple interactions may be defined between turbulent flow, spray dispersion, vapor micro-mixing and combustion. To reduce the number of varying parameters, a forced isotropic homogeneous turbulence, with statistically stationary properties, is used as carrier phase. A forcing scheme allowing mean stable properties of the turbulence (energy, dissipation, integral length scale) has been introduced in a spectral formulation describing the evolution of an incompressible gas phase. The dispersed spray evolution is modelled thanks to a Lagrangian formulation describing the position, the velocity and the mass of any droplet embedded in the gas phase.

During the second year, both equations of filtered mixture fraction and mixture fraction variance have been developed and analyzed. It appeared that models for the partially premixed flames propagating in the domain also need information about the progress variable evolution. Although it was not in the initial Description of Work, it was decided to develop the two-phase specific transport equations for the large scale progress variable and its corresponding subgrid variance evolution. All the terms of these transport equations have been evaluated. Then, several subgrid models have been tested in the framework of reacting two-phase flows. Scale similarity models for the mixture fraction variance and the progress variable were first selected. However, these models do not provide satisfactory results. Thus, choice has been made to test the models that are necessary to close the transport equations of the mixture fraction and the progress variable variances. Both these data are necessary to use combustion models that take into account the presence of the liquid phase. Closures have been evaluated for the various mass and chemical source terms but also for the dissipation rate of both mixture fraction and progress variable variances. It appears that closures are satisfactory concerning the progress variable evolution but some difficulties appear as far as the mixture fraction source terms are involved (see D1.2.1: "Report on SGS modelling of the transport equation for the mixture fraction and progress variable variances in the presence of spray and combustion").

Task 1.2.2 Turbulence / droplet interaction modelling for LES (TUD)

A physically consistent SGS-model describing the influence of droplet diameter and interface transport on the gas phase turbulence as well as the effect of the droplet evaporation on the mass and heat transfer processes (turbulent modulation) has been improved and implemented into the FASTEST-3D LES code. Using this model the interface transport processes observed in poly-dispersed liquid gas two-phase flows can be simulated properly as documented in deliverable 1.2.2.

Task 1.2.3 Fractal Model of Turbulent combustion in two-phase flows (DMA)

In task 1.2.3 DMA analysed the dispersed phase equations in the Euler/Euler approach. After performing similitude theory analysis, the results indicate that the models present in the literature (at that time) have neglected 2nd order effects in the Knudsen number, and they are relevant for inertial particle dispersion in turbulent flows.

DMA has proposed a modified Euler/Euler approach that, although partially, still takes into account 2nd order effects. This approach takes advantage from the analogy of drop transport theory with the theory of rarefied gases. A model for such applications has in fact been adapted for dispersed two-phase flows of inertial particles.

Task 1.2.4 Development of spectral LES treatment of multi-phase combustion of liquid fuel (UC)

Within task 1.2.4 two-phase flow and combustion models were implemented into the in-house LES SAILOR high order code. For two-phase flows both Euler-Lagrange and Euler-Euler approaches were applied. Within the Euler-Lagrange methodology the stochastic model was implemented while for the Euler-Euler Level-Set, Volume-of-Fluid and coupled VoF Level-set method were applied complemented with the ghost-fluid approach. As to combustion models unsteady flamelet, Eulerian stochastic fields and CMC models were applied. The details of the implementation were described in three deliverables D.1.2.4a, b and c.

Task 1.2.5 Assessment and Development of Eulerian/Lagrangian approach (LU)

A Eulerian/Lagrangian approach has been developed/validated for multiphase flow simulation and the main work performed are in the following areas: a) the Eulerian/Lagrangian approach has been validated for several test cases; b) development/validation of a stochastic secondary break-up model; c) droplet tracking computational efficiency study has been carried out; d) a linear stochastic Sub-Grid Scale (SGS) model has been developed/validated for droplet SGS dispersion modelling.

A hybrid droplet-parcel model developed to improve computational efficiency has been assessed in several test cases and the speedup is significant and the results look plausible (D.1.2.5b). A linear stochastic model for droplet SGS dispersion has been developed/validated and the predicted results with the SGS model agrees better with the experimental data (D1.2.5b). A swirling flow and a mixing layer flow cases have been used to validate the Eulerian/Lagrangian approach and a good agreement with experimental data has been obtained (D1.2.5c).

Task 1.3.1 Operational evaluation of Euler versus Lagrange formulations for polydisperse evaporating sprays (CRSA/CNRS)

The derivation of the Eulerian multi-fluid model, with associated set of assumptions, mathematical structure and dedicated numerical methods has been completed (**D1.3.1a**). The key issues are the ability to resolve the polydispersity of the spray and the ability to capture the dynamics of droplets of various sizes. Three configurations have been delineated and a DNS database of polydisperse sprays in three configurations has been obtained (**D1.3.1a**).

Then, Eulerian computations of sprays with the multi-fluid model previously derived were performed on these three configurations and were compared to the Lagrangian DNS database from both the physical and numerical points of view, and the computational efficiency of both methods are evaluated (**D1.3.1b** is a complete report on operational evaluation of both methods).

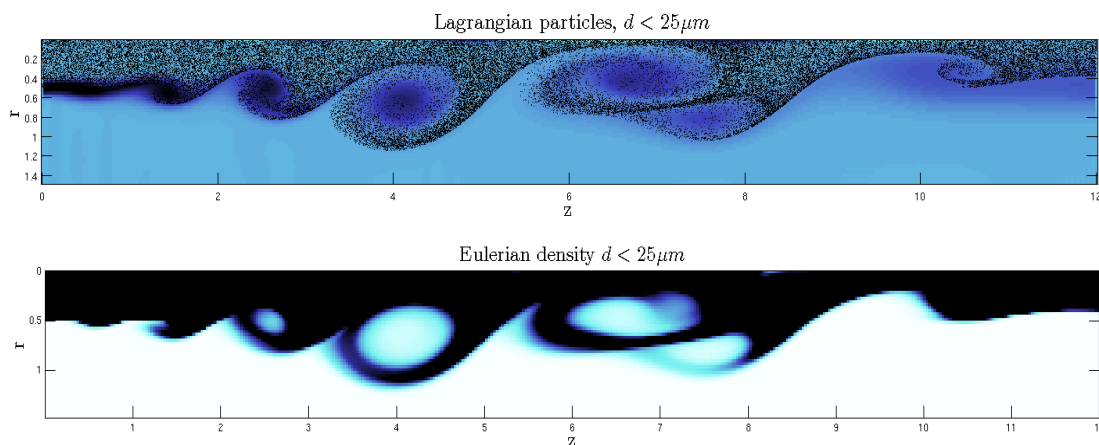


Figure 1.3.1.A : top : 2D vorticity field of the gaseous phase in an axisymmetrical jet with Lagrangian droplets in a non-evaporating case, bottom : droplet number density for a droplet size range with relatively small Stokes number obtained with the Eulerian model.

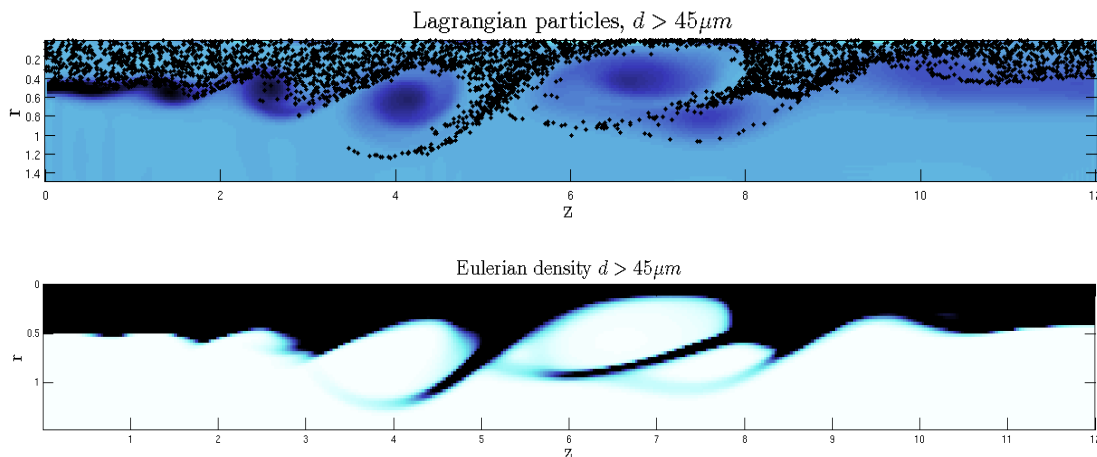


Figure 1.3.1.B : top : 2D vorticity field of the gaseous phase in a axisymmetrical jet with Lagrangian droplets in a non-evaporating case, bottom : droplet number density for a droplet size range with relatively large Stokes number obtained with the Eulerian model.

Task 1.3.2 DNS of two-phase flows: Numerical experiments for the development and validation of Euler-Euler LES approach in gas turbine (IMFT)

The numerical database, (D1.3.2a) representing the continuous dispersed phase, was obtained by Lagrangian data carried out by using the Direct Numerical Simulation (DNS) of the turbulent carrier flow coupled with a Discrete Particle Simulation (DPS) of the particle phase. The application of the statistical approach (the Mesoscopic Eulerian Formalism) led to define local instantaneous Eulerian fields which were computed by means of a projection algorithm. The database containing the Eulerian fields of dispersed phase is now available to be used by all partners of TIMECOP-AE consortium. Moreover, the period M25-M36 was spent to provide the Euler-Euler Large Eddy Simulation approach for evaporating two-phase flows. The Eulerian equations derived in the task 1.3.2a were spatially filtered and the period was dedicated to the physical analysis and modelling of the unclosed terms. In order to model the sub-grid correlations, a classical “low Mach” sub-grid fluid model extended to the evaporating dispersed phase was tested. An extensive study was done to model the mesoscopic particle velocity and temperature moments as, for instance, the quasi-Brownian motion tensor, the quasi-Brownian heat flux as well as the dispersion velocity. In addition, the mass transfer terms appearing in the filtered Eulerian equations were analyzed and tested. Validations were performed by *a priori* testing using the database supplied with the deliverable D1.3.2a. The outcome of the study is described in D1.3.2b.

Task 3.1.2 LES validation stochastic modelling of kerosene injection modelling (IC)

The LES Lagrangian spray pdf method incorporated Boffin-LES for droplet breakup, dispersion evaporation has been developed and validated by comparison with measurements obtained in non-evaporating and evaporating fuel sprays. It has been demonstrated to be capable of representing secondary droplet breakup [4], droplet dispersion [3] and droplet evaporation [1, 2, 5]

References

1. D3.1.2a: Report on LES results of two phase flow with evaporating poly-dispersed droplets
2. D3.1.2b: Report on LES results of two phase flow with evaporating mono and poly-dispersed droplets
3. Jones, W.P., S Lyra and A J Marquis, Large Eddy Simulation of a droplet laden turbulent mixing layer, Int. J. Heat Fluid Flow, 31, 93-100 (2010).
4. Jones, W. P. and Lettieri, C., Large Eddy Simulation of Spray Atomisation with Stochastic Modelling of Breakup, Physics of Fluids, to appear, (2010)

5. Jones, W.P., S Lyra and A J Marquis, Large Eddy Simulation of Evaporating Kerosene and Acetone Sprays, Int. J. Heat Mass Trans., 53, 2491-2505 (2010).

Task 3.1.3 Numerical prediction of evaporating fuel sprays in turbulent flows based on full LES models (ITS)

The goal of task 3.1.3 is to investigate the droplet motion and evaporation in turbulent flows with periodic vortex structures. As a test case, the results from task 2.1.2 were used. The numerical predictions within task were performed using the LES solver of ANSYS CFX in combination with the ITS Lagrangian droplet code LADROP. The results revealed that for small droplets, i.e. a Stokes number of 1-10 the turbulence contained within SGS model cannot be neglected and that appropriate SGS models must be used within the droplet tracking code for a correct prediction of the droplet dispersion.

Task 3.2.1 Euler / Lagrange LES of the two-phase FAUGA experiment (IC)

The performance of Boffin-LES has been evaluated, [1-2] in complex geometries representative of aero-engine combustors by application to FAUGA, Task 3.2.1. The simulated velocity fields for both the continuous and dispersed phases have been demonstrated to be in good agreement with measurements. Ignition simulations have been completed and the results compared with measurements.

References

1. D3.2.1b: Report on the droplet pdf method for liquid fuel sprays
2. D3.2.1c: Validated LES Boffin code for Spray Combustion.

Task 3.2.4 Euler / Lagrange LES of the two-phase flow genrig experiment (IC)

Boffin-LES, incorporating the sgs pdf equation/stochastic field solution method and the LES spray pdf, has been applied, [1] to the Generic Combustion chamber studied experimentally at DLR-AT (Task 2.3). The results have been compared with measurements and with the results of the simulations carried out in Tasks 4.1.2 and 4.1.8 but using different approaches. The isothermal LES flow field simulations compared very well with the measured LDA data. For the combustion case a global 4-step kerosene-air reaction mechanism was incorporated and the results show that the observed V-shape of the flame was captured quite well. However the simulated temperature field was considerably over predicted in the centre region. As similar discrepancies were also evident in the PRECISE LES results using other combustion models it is likely that uncertainties in the estimated droplet velocity and size distributions at the injector are responsible for the differences in the measure and simulated temperatures.

References

1. D3.2.4: Report on LES results of the DLR experiment of task 2.3

Task 4.1.3 Implementation and application of the two phase model of ITS (RRD)

The ITS LADROP code has been coupled with the Rolls-Royce in-house combustion CFD code PRECISE-UNS. The interface is established using files written out in CGNS format. The coupling of the codes has been tested out on the TIMECOP generic rig of DLR-AT, for which experimental data are available. The results look similar to those obtained with the in-house spray model, however, when using the LADROP spray code evaporation starts earlier due to the more advanced multi-component evaporation model.

Task 4.1.6 Implementation of Eulerian/Lagrangian Spray Model (RR)

The objective of this task was to implement into the RR in-house combustion CFD code PRECISE a secondary break up model for spray developed by LU within TIMECOP-AE. The secondary

break up model developed by LU in a Lagrangian framework is based on an analytical solution of a Fokker-Planck equation and allows breaking up of a droplet in a continuous range of droplet diameters when break up conditions are met. The break up model was initially developed by LU in their own in-house code to allow proper validation based on a range of representative test cases, for which accurate experimental data was available. The work done within task 4.1.6 focused on the implementation of such break up model into the PRECISE code and a comparison with a pre-existing break up model was performed. During the implementation, attention was paid to clip the probability density function to avoid generating too large droplets. A comparison between bounded and unbounded break up model implementation was carried out on a simple test case that was representative of the flow field found in aero-engine combustors. The model was found to behave as expected and the corresponding milestone was achieved on time. The work carried out within this task allowed transferring an alternative, advanced secondary break up model to the in-house code PRECISE. The model was later tested on a ranged of different geometries of industrial relevance within this research programme.

2.3.5. Combustion

Several approaches are assessed to reduce the computation effort of detailed reaction mechanisms for LES simulations.

Task 1.4.1 FGM & CFM methods for reacting kerosene in LES (TUE)

In task 1.4.1 the combustion chemistry mechanism for a kerosene model fuel has been reduced using the Flamelet Generated Manifold (FGM) method. Replacement of detailed chemistry by FGM chemistry enables accurate predictions of combustion in industrial applications (including pollutant emissions), which are impossible using detailed chemistry due to the enormous computational costs.

FGM chemistry tables for kerosene-air combustion have been created and provided to partners (RRD, TUD and CERFACS) for take-off, cruise and altitude relight conditions (D1.4.1A); an example is shown in figure 1. For the application of FGM in LES of turbulent flames, the turbulent fluctuations have to be accounted for. A detailed analysis of the accuracy of FGM tables in turbulent flames has been performed (D1.4.1B). The FGM method has been extended to deal with the full range of stratification levels, from fully premixed to non-premixed. The coupling of FGM chemistry tables with LES subgrid models for partially premixed combustion has been investigated. The CFM (Coherent Flamelet Model) subgrid model is assessed for modelling globally lean, partially-premixed combustion. Direct numerical simulations of a representative stratified burner set-up, of which snapshots are shown in figure 2, are performed to validate the applicability of a CFM subgrid model (D1.4.1C).

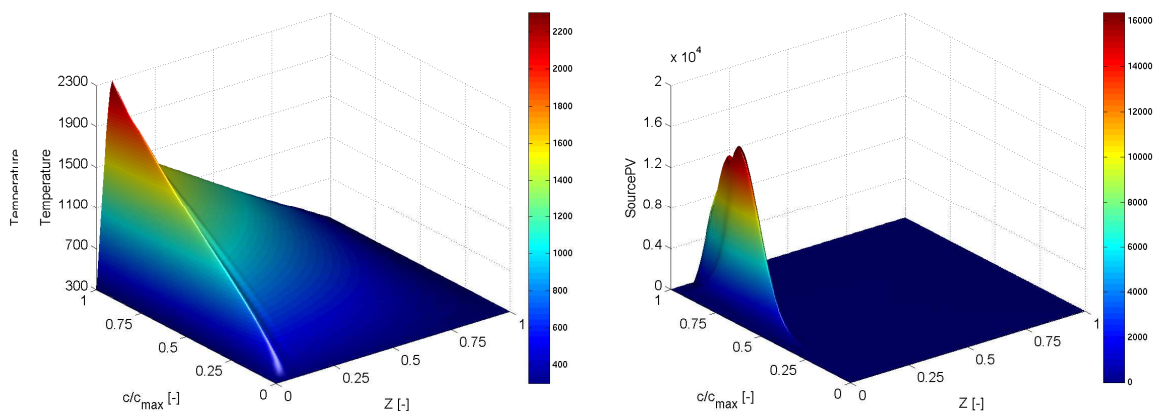


Figure 1: FGM chemistry table for ambient conditions ($p = 1$ bar, $T_{ox} = 300$ K, $T_{fu} = 300$ K). Gas mixture temperature is shown left and the source term of the reaction progress variable is shown right.

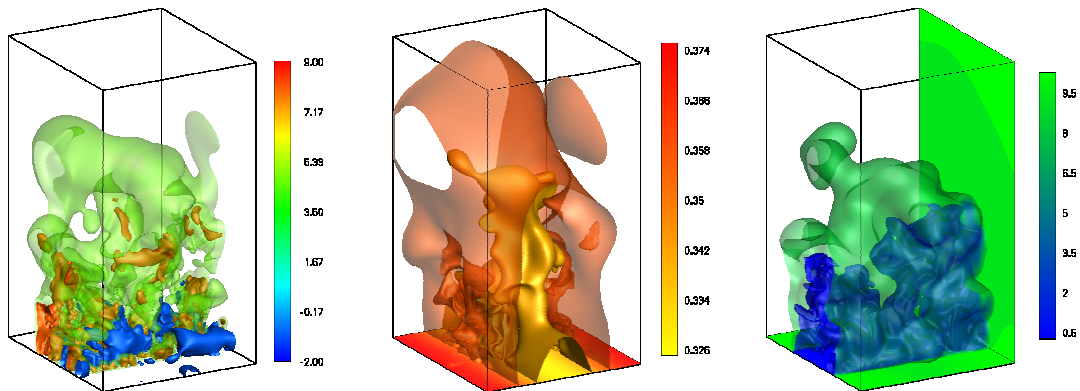


Figure 2: snapshots of instantaneous axial velocity (left), mixture fraction (middle) and reaction progress variable (right) field in a stratified planar Bunsen flame. The Reynolds number, based on slot width, is approximately 400.

Task 1.4.4 Reduced kinetic mechanisms and time scale analysis for steady and unsteady combustion of CFD4C model fuel (ICEHT)

Reduced chemical kinetics models for the CFD4C fuel (n-decane and n-propylbenzene) were constructed within the task 1.4.4. Two reduced models were constructed, one for steady operating conditions (high pressure and high inlet temperature) and one for relight operating conditions (low pressure and low inlet temperature). The results are described in D1.4.4a for the steady conditions and D1.4.4b for relight conditions.

Both reduced models were constructed so that they successfully simulate the full kinetics CFD4CC model in a wide range of operating conditions. For the steady conditions, the 20-steps reduced model constructed is valid for initial temperatures in the range 500-900oK, pressure in the range 10-35bar, stoichiometry in the range 0.6-1.8 and 70-90% n-decane in the initial fuel mixture (see D1.4.4a). For the relight conditions, the 20-steps reduced model constructed is valid for initial temperatures in the range 200-300oK, pressure in the range 0.1-1bar, stoichiometry in the range 0.6-1.8 and 70-90% n-decane in the initial fuel mixture (see D1.4.4b).

The two reduced models exhibit a number of differences in the variables retained in the stoichiometry of the model and in the variables considered at steady state.

Both reduced models were shown to provide significant accuracy (in comparison to the full CFD4C model), not only for the variables in the reduced model (temperature and major species mass fraction) but on the variables considered at steady state (minor species mass fraction) as well.

Task 3.1.1 LES calculations, of spray formation, evaporation of droplets and combustion / turbulence interaction in high turbulence intensity environment (UC)

The main objective of the task 3.1.1 was to validate the models implemented in the LES-SAILOR code within task 1.2.4. The Euler-Lagrange stochastic approach was validated against DNS literature data for particle laden channel flow. The coupled VoF-Level-set approach was validated on the primary jet atomization. Combustion models were validated against Sandia D.E and F flames. Variety of models and numerical schemes allowed producing a set of guidelines for LES combustion predictions. The details of the validation process are described in four deliverables D.3.1.1 a, b, c and d.

Task 3.2.2 LES of “advanced” pre-vaporised reacting experiment (CERFACS/CNRS)

In this task, a tabulated chemistry approach was implemented and validated (D3.2.2a). For comparison of the LES combustion model against the TUD experiment, a new chemical scheme for kerosene was implemented (D3.2.2b) and assessed in the context of the standard LES modelling available at CERFACS. A more advanced approach is then exploited for all three operating condition of the TUD facility (D3.2.2c) which is of interest for a direct comparison with the TUD numerical predictions of task 3.2.3. All of these developments are explored and validate in WP4 by Turbomeca and Snecma in their respective LES computations.

Task 3.2.3 LES of the EKT experiment (TUD)

A LES based complete model for a reliable description of combustion processes in a gas turbine combustion chamber was designed taking the advantage of FGM for solving combustion and implemented in FASTEST-3D code. Use of a look up table generation for kerosene using data from TU-Eindhoven allows carrying out simulations for Single Sector EKT-configuration for both 4 and 6 bar cases. Good agreement with experimental data was achieved as documented in deliverables 3.2.3a.

The FASTEST-3D code has been extended for simulating evaporating sprays in complex geometries using LES. For this purpose, a complete spray module, that accurately describes all essential fuel preparation processes, has been designed using the inputs from D1.2.2 and validated successfully in two different Sommerfeld & Qui configurations. All the achievements have been documented in deliverables 3.2.3b. Spray combustion has not been addressed here.

Task 3.2.5 Pollutant prediction using FTC-PCM (CNRS)

The objective of this task was to develop and test sub-grid scale flame closures that account for detailed chemistry. Oversimplified chemistry cannot be used to predict, with accuracy, pollution or flame response to dilution by burnt gases; the precise description of flame ignition also imposes to include sufficiently detailed chemistry in the modelling. The methods developed in this task were grounded on flamelet-tabulated chemistry.

Two test cases have been considered to estimate the prediction capabilities of combustion LES with tabulated detailed chemistry. The first concerned flame stabilization by burnt gases. The second dealt with the ignition process in a swirling flow. Improvements to the modelling were proposed to better reproduce experimental observations, specifically concerning NO_x emission and strain-rate induced effects controlling success or failure of transient burner ignition. The mesh-structured code SITCom (Simulating Turbulent Combustion) was used for this task.

Task 4.1.2 Implementation and application of FGM combustion models (RRD)

The FGM model developed by the Technical university of Eindhoven has been implemented into the unstructured Rolls-Royce in-house CFD code PRECISE-UNS. The model can be used for RANS as well as for LES applications. The model has been validated by comparing CFD results against experimental data of generic combustors: the MOLECULES generic combustor of DLR-AT, where methane has been used as fuel, and the TIMECOP-AE generic rig of DLR-AT, where liquid kerosene has been used as fuel have been used to validate the FGM model. The results show that the FGM is able to represent the flame structure well for both gaseous as well as for liquid spray flames.

Task 4.1.5 Implementation of CMC-CSP combustion modelling (RR)

The objective of this task was to implement into the RR in-house combustion CFD code PRECISE the Conditional Moment Closure (CMC) model for non-premixed flames developed by UCAM within the framework of TIMECOP-AE. The implementation was then to be tested and validated on laboratory scale experiments for which plenty of high quality measurement data is available. The implementation had to allow direct utilisation of the kerosene CSP-reduced reaction mechanisms

obtained by ICEHT within this programme. The PRECISE CFD solver was interfaced with the CMC module to allow parallel computations. The CFD solver provides the CMC module with space and time resolved predictions of velocity, turbulent quantities, mixture fraction and its variance. The CMC module, relying on the DVODPK solver, returns density, temperature and reactive species to the CFD solver. The coupling works for both RANS and LES applications. The implementation was tested and validated through a Sandia flame D flame simulation based on a 19 species reaction mechanism. The CMC PRECISE model was able to predict temperature and CO mass fraction accurately at a number of planes downstream of the burner. Both time-averaged and fluctuation profiles were well predicted. The work was completed by M34 as planned, which allowed claiming the milestone in time. The work carried out in this task allowed transferring to the industrial code PRECISE the advanced CMC chemistry-turbulence interaction model that was later further tested and validated on geometries and conditions of industrial relevance.

Task 4.1.8 Calculation of 2-Phase Flow in the Generic Combustor (RR)

The objective of this task was to simulate the isothermal and reactive experiments carried out by DLR-AT within TIMECOP-AE using a range of different LES modelling approaches. Initially, focus was put on simulation of the cold flow aerodynamics, for which detailed time-resolved measurements were available. A standard $k-\epsilon$ RANS simulation based on a hybrid grid was run and comparison of the results against measurements showed that although the time-averaged velocity profiles could be predicted quite accurately, the unsteady components were severely underpredicted. An isothermal simulation based on a purposely built multi-block structured grid produced a better tie up with measurements in terms of both time-averaged and unsteady velocity components. The upshot of the isothermal simulation campaign was that, as expected, LES was found to produce more accurate predictions of the flow field than RANS, especially as far as the unsteady components were concerned. The second phase of the task was focused on validation of reactive LES against available intermediate pressure (4 bar) measurements of temperature based on the spray characterisation done by DLR-AT. The detailed profiles of droplet size and velocity provided by DLR-AT were used to derive simplified spray boundary conditions for the LES. Different combustion models were exercised: presumed PDF, EBU and CMC. All combustion models were able to capture the two-lobed nature of the flame front, although some details were not predicted accurately. Utilisation of a LU-developed secondary break up model produced a more diffuse temperature distribution leading to improvements in the prediction in certain regions of the flame front. All the details of the work are contained in D4.1.8. All in all, the activities associated with this task allowed further validation of the CMC model against measurements on a geometry that shows similar features to industrial injectors. Moreover, CMC results were compared against results obtained with other combustion models. The work done within this task also showed that more research is needed in the field of spray modelling in order to enhance the predictive capability of CFD tools.

Task 4.1.10 LES performance in light of RANS and experiments (SN)

RANS and LES have been evaluated against the experimental data obtained by ONERA in the MERCATO facility. To obtain the same degree of accuracy than LES using RANS, it has been necessary to evaluate different numerical parameters and turbulence models. The amount of engineer work needed to obtain good results using RANS (D4.1.10a, D4.1.10b, D4.1.10d) is greater than for LES, where the standard models were used. The RANS parameters retained are not general and certainly should be modified to match the experimental data for any other geometry. The RANS Lean Blow-Off model has permitted to reproduce the behaviour of the MERCATO facility (D4.1.10c), nevertheless, LES seems best fitted for this kind of engine performance evaluation.

Task 4.1.11 Application of commercial LES code for the calculation of the generic combustor (MTU)

Comprehensive CFD calculations have been carried out for the generic single sector combustor that was experimentally investigated in task 2.3 by DLR using the LES feature of the commercially available CFD solver CFX. Calculations have been carried out for two test cases, an isothermal

and a reacting case. For the isothermal test case a nearly perfect agreement could be observed for the predicted mean and also RMS velocities in comparison to the experimental LDA data. For the reacting case, the overall agreement for the temperature field is also very good, in particular if the assumptions are regarded that have been made for the LES. The results are described in details the deliverable report D4.1.11.

Task 4.2 LES calculations initiating from RANS calculations (CIEMAT)

A methodology to initialize a LES calculation from a RANS solution has been developed and tested. The method allows in principle to reach more rapidly a stationary solution for turbulent spray flames in complex geometry, which is of interest for industrial, high cost simulations. The corresponding subroutine and recommendations have been reported in deliverable D4.2.

2.3.6. Ignition

Task 1.4.2 Ignition and Auto-ignition predictions using CMC (UCAM)

This task aimed to develop a method in which spray evaporation effects were explicitly included in the Conditional Moment Closure (CMC) combustion model. In Deliverable 1.4.2a, the governing equations were derived and some validation presented by comparison with Direct Numerical Simulation data, while in Deliverable 1.4.2b the model has been used in RANS to predict spark ignition of the Cambridge spray burner described in Deliverable D2.1.1. In addition, a Large Eddy Simulation effort with CMC has been initiated.

Task 1.4.3 Turbulence/chemistry interactions (IC)

The sub-grid pdf/stochastic field method for representing sub-grid scale turbulence-chemistry interactions has been developed so that it is capable of simulation local extinction effects and auto and spark ignition in gaseous fuelled systems, [1-4]. When combined with the Lagrangian spray pdf method it has also been demonstrated to be capable of reproducing ignition and burning in liquid kerosene fuelled flames. [5-6].

References

1. D1.4.3a: A stochastic field method for solving the sub-grid joint pdf equation for species mass fraction and temperature: the code Boffin-LES will be supplied to industrial partners
2. D1.4.3b: Final model including combined stochastic field method and reduced chemical scheme for kerosene: the code Boffin-LES will be supplied to industrial partners
3. D1.4.3c: Predictions of auto-ignition with the sub-grid *pdf* method.
4. Jones, W P. and Prasad, V N, Large Eddy Simulation of the Sandia Flame Series (D, E and F) using the Eulerian stochastic field method, *Combustion and Flame*, **157**, 1621-1636 (2010).
5. Jones, W P and Prasad, V N, LES-PDF Simulation of a spark ignited turbulent methane jet, *Proceedings of the Combustion Institute*, **33**, 1355-1363 (2011)
6. Jones W. P., Lyra S. & Navarro-Martinez S., *Large Eddy Simulation of a swirl stabilized spray flame*, *Proceedings of the Combustion Institute*, **33**, 2153-2160 (2011)

Task 1.4.5 Ignition and Auto-Ignition Modelling in Two-Phase Flows (DMA)

In task 1.4.5 DMA has made an extensive review of the data on kerosene auto-ignition. Numerical simulations of kerosene droplets auto-ignition in still atmosphere for different initial conditions have been performed in order to assess the importance of the evaporation phase on the overall ignition delay time. In addition, an extension to a former fractal theory for turbulence has been proposed and used in order to produce an SGS model accounting for particle clustering and that can be implemented in LES CFD codes.

(WP1.4.5) DMA has proposed a SGS model based on fractal theory. The main idea is to exploit the information about the volume occupied by the different turbulent scales coming from the fractal theory in order to estimate the volume where particles tend to cluster. This data will then be used in

the SGS model in order to obtain modified source terms for evaporation, heat exchange and chemical reactions.

Task 1.5 Spark model for LES (IFP)

A new spark ignition model called ISSIM-LES (Imposed Stretch Spark Ignition Model) has been developed in AVBP. It includes an electrical circuit model representative of inductive ignition system, a spark model which describes the elongation of the electrical spark, an ignition model that accounts for multi-spark capability and flame deformation by turbulence and convection. Unlike its predecessor model AKTIM-LES, ISSIM-LES is fully based on the flame surface density equation. This allows it to describe multi-spark ignition, the effect of convection and turbulence stretch is a more realistic way. ISSIM-LES is coupled to the ECFM-LES combustion model.

Deliverable D1.3a, reports on a first version of the ISSIM-LES spark ignition model and its implementation into AVBP. The electrical circuit model of ISSIM-LES is coupled to the TFLES combustion model. The ignition system is validated against experiments for various conditions (electrode diameter, spark gap, available energy, flow convection). The coupling with TFLES is checked by performing a 3D simulation of the ignition of propane/air mixture.

Deliverable D1.5c presents the development of a spark ignition model for LES, coupled with the TFLES combustion model. ISSIM-LES is validated against well documented experiments. It is applied to the simulation of the Leeds bomb, consisting of studies of spark ignitions under conditions close to a homogeneous isotropic turbulence. The simulated cases concerned iso-octane/air mixtures under various pressure, equivalence ratios and turbulence conditions. The stretch effect on the laminar flame speed has been taken into account using experimental measurements of the Markstein lengths ISSIM-LES was found to satisfactorily predict the time evolution of the flame radius for the simulated cases.

Deliverable D1.5b is a report on a validated version of the LES spark ignition. An empirical electrical model has been proposed to fulfil the requirement of reproducing the specific behaviour of the MERCATO system

- Preliminary simulations of 3D laminar ignitions have been performed to verify the numerical implementation and to examine the sensitivity of the flame growth to the energy deposited
- The ignition model (electrical circuit+TFLES) is applied to the MERCATO configuration. Both ignitions are successful, but the examination of the flame kernel evolution show that ignition is favoured near the wall, where the amount of fuel is high.

Deliverable D1.5d demonstrates the application of the spark ignition model to the MERCARO aero-engine ignition system.

Task 3.1.4 Porting DMA Models and Validation of HeART Code (DMA)

In WP3.1.4 DMA has proposed a new numerical approach for the Euler/Euler formulation applied to two-phase flows. This approach has been implemented in the HeaRT code, its results validated against Sommerfeld and Qiu test case and then also implemented in the OpenFOAM code for partner's exploitation. The models developed by DMA in WP1 were finally implemented in the two codes.

The validation of the proposed numerical approach against Sommerfeld and Qiu test case with the HeaRT code proved to be successful.

Task 3.2.6 URANS Simulation of altitude relight (DLR-VT)

In the first part of the task, the numerical issues related to the simulation of high altitude relight have been investigated and reported in detail. Then, a URANS approach coupled with a Lagrangian particle tracking code capturing real fuel effects have been validated and employed for the simulation of non-reacting multiphase flow under different pressure-temperature conditions. In the second part of the task, models for the ignition and flame propagation in multiphase flows have been developed. The combustion process is modelled using the turbulent flame speed closure

model (TFC-model). It was combined to an ignition delay sub module that accounts for numerically-unreachable transients between the plasma kernel generated by the laser pulse (or any other ignition device) and simulation initial conditions. Simulations have been carried out using the DLR in house code THETA-SPRAYSIM. The method proved to be very appropriate for modelling the DLR lab scale experiment, as the experimental results have been matched with a very satisfying accuracy. Both the general features of the flame as well as the flame center velocity agree well with the experimental data set.

Task 3.2.7 LES of the two-phase “advanced” experiments (CERFACS)

The main objective of task 3.2.7 was to validate and demonstrate the ability of the LES Euler/Euler modelling strategy for two-phase flow applications with industrial complexity. Such a process was demonstrated in three steps, each of which highlighting the advantages and limitations of the approach. First, dispersion models as devised by IMFT are gauged in D3.2.7a. Use on the Mercato facility is then demonstrated in D3.2.7b where ignition sequences are presented by use of LES. Variability in the prediction in terms of success or failure is shown to be reproduced by the model. Finally, a strategy relying on cold flow Euler/Euler LES predictions is presented in D3.2.7c to predict ignition probability of an industrial system. For this work the method is validated on the Mercato configuration. Turbomeca and Snecma have then evaluated all these developments in WP4 (Exploitation).

Task 3.2.8 LES Simulation of altitude relight (UC)

The main part of the work was to perform LES simulation of altitude relight, which, due to connection with Task 2.2.3, became a numerical reproduction of DLR's experiment. Simulated geometry mirrors the experiment with minor simplifications. Methodology is RANS-LES; RANS (FLUENT) is used for the part of combustion chamber upstream to injection location, with LES (Boffin-LES) applied for injector using profiles generated by RANS. Discrete Lagrangian droplet model is used to trace the droplets, spark is modelled as a source in the enthalpy equation, and the combustion mechanism for kerosene is based on 7- species, four-step mechanism for hydrocarbons. Successful simulations of ignitions have been performed within this methodology. Further calculations aimed at reproducing the ignition probability map, with preliminary results. To complete this goal, series of calculations were performed with varying parameters (air inflow stream, injected fuel stream, spark energy) and the results were compared with experimental data from DLR (see D3.2.8).

Task 4.1.1 Use of AVBP for in house LES calculations (TM)

The objective of Task 4.1.1 was to validate different features of the LES code AVBP for TM's in-house burner simulations. Two configurations have been computed: i) the MERCATO burner of ONERA using AVBP's Eulerian 2-phase module, ii) the EKT burner from TUD for an assessment of the chemistry treatment at elevated pressure (9 bars). These simulations, detailed in D4.1.1, have shown the good performance of LES in combustion simulation and encouraged its use at an industrial level.

Task 4.1.4 Assessment of altitude relight modelling (RRD)

The altitude relight rig (SARS rig at Rolls-Royce UK, Derby), has been modelled using the in-house CFD code PRECISE-UNS. The FGM model, as integrated within Task 4.1.2, has been used to model the combustion process. At the low temperature and pressure conditions at altitude relight, the FGM model had to be extended with the enthalpy equation to enable ignition. This was necessary since at these low temperatures kerosene hardly does evaporate. As a consequence the mixture fraction is far below flammability limits. By putting in additional heat, simulating ignition, the evaporation heat increases, so that self sustained flames can be obtained. The CFD results have been compared with experimental data of OH* and luminosity. Some features of the flame are captured by the CFD, but not all details.

Task 4.1.7 Calculation of Altitude Relight Using CMC (RR)

The objective of this task was to exercise the CMC model implemented into the in-house combustion CFD code PRECISE to simulate the DLR-VT experiment carried out in task 2.2.3. DLR-VT applied a range of diagnostic techniques (OH chemiluminescence, OH PLIF, kerosene PLIF, flame luminosity) in a RR test rig (called SARS), which is able to run at altitude relight conditions. A comprehensive set of measurements were taken on a test run with an RRD lean burn injector and the CMC model was validated against that dataset. An isothermal RANS simulation through the swirlers was carried out to start with, in order to derive velocity and turbulent quantities profiles at planes located downstream of the swirlers' trailing edges for definition of boundary conditions of the subsequent LES. A high quality LES mesh was then built of the two-sector rig, on which an isothermal LES was run. The comparison between RANS and LES predictions showed strong similarities as far as the cold flow field was concerned. After that, a range of reactive RANS simulations were carried out, to be later compared against the LES solution. A 3D CMC LES was then run and results compared against measurements as well as the other predictions. The CMC LES was able to capture the flame front correctly, which was assessed against the DLR-VT measurements. The predicted fuel distribution compared well against kerosene PLIF measurements taken on a plane parallel to the fuel injector, showing some asymmetry spotted by the diagnostics. Eventually, the concentration of hot gases predicted by the CMC was in line with flame luminosity measurements. Sensitivity studies were carried out against secondary break up modelling and reaction mechanisms, showing that the LU secondary break up model produced too diffuse a mixture fraction distribution and the ICEHT 15-step mechanism was too slow for industrial use. Comparison was also carried out against RRD simulations of the same test, which proved the CMC model to provide more accurate prediction of the flame front than the FGM model for this configuration. All the details of the work can be found in deliverable 4.1.7. All in all, the work done within this task allowed validating the CMC model developed by UCAM and ported to the RR code PRECISE on a geometry of industrial relevance at very challenging operating conditions (~0.5 bar). As a result, a claim can be made that the CMC model is able to capture fine details of the flame structure generated at altitude relight conditions by lean burn injectors and as such can be used by RR for supporting direct development of lean burn technology.

Task 4.1.9 Exploitation DMA Models for Spray Combustion and for predicting Auto-ignition (AVIO)

The task of AVIO in TIMECOP-AE was the exploitation of two-phase flow models for LES developed by University of Rome (DMA).

The model developed was incorporated into the CFD code at DMA (HeART).

Different commercial codes used at AVIO were considered for the porting, namely Fluent and CFX. Finally it was decided to use the open source code, OpenFOAM that is at moment more and more used both by Universities and Industries for simulations of flows inside combustion chambers.

DMA provided to AVIO a version of OpenFOAM updated with the new models on liquid fuels.

In the frame of cooperation between AVIO and DMA two different applications were planned: the first one was the simulation of autoignition in a premixing duct of the LPP type (Lean premixed prevaporized). The second one was the simulation of a sector of a full annular combustor of AVIO interest.

3. DISSEMINATION AND USE

3.1. Section 1 - Exploitable knowledge and its Use

In TIMECOP-AE, Work Package 4 is devoted to the exploitation of the knowledge developed within the project. Section 2.2.4 explains in details how this exploitation has been carried out. The results of this exploitation are the numerical codes presented in section 2.3.3.

TIMECOP-AE has helped consolidate the requirements that LES tools should satisfy to be integrated in the aeroengine industry conception process. Models required by industry needs have

been developed by the research partners of this project, integrated in the industrial tools and then evaluated in by the industrials against academic and real combustor engine geometries. The industrial LES related methodologies have started to be developed by each company. The research effort in this field should be continued; noticeably to obtain faster solvers to fit the conception timeline of aeronautical engines and to improve the models developed in TIMECOP.

3.2. Section 2 - Dissemination of knowledge

3.2.1. Overview table – External Dissemination

Planned/ Actual Dates	Type	Type of Audience	Countries Addressed	Size of Audi ence	Partner Respon sible / Involved	Internal Ref. N°
2007	Publication: Spark ignition of turbulent non-premixed bluff-body flames	Combustion and Flame 151			UCAM	KP#0a
9-13 September 2007	Presentation: Ignition behaviour of recirculating spray flames using multiple sparks	5th Mediterranean Combustion Symposium	Monastir, Tunisia		UCAM	KP#0b
July 2007	Presentation: Effectiveness of localised spark ignition in recirculating n-heptane spray flames	21st ICDEERS	Poitiers, France		UCAM	KP#0c
14 November 2007	Publication: Large-eddy simulation of a lifted methane jet flame in a vitiated coflow	Combustion and Flame 152 (2008)			CNRS	KP#1
16 January 2008	Publication: Ignition of turbulent swirling n-heptane spray flames using single and multiple sparks	Elsevier			UCAM	KP#2
	Publication: Direct Numerical Simulations of Autoignition in Turbulent Two-phase Flows	Colloquium SPRAY AND DROPLET COMBUSTION			UCAM	KP#3
10-14 August 2008	Presentation: Euler-Euler Large-Eddy Simulation Approach for Non-Isothermal Partial-Laden Turbulent Jet	ASME Fluids Engineering Division Summer Conference	Jacksonville, Florida, USA		INPT	KP#4
4-6 June 2008	Presentation: Modeling of Liquid Jet Break-up with Level Set and ghost fluid method	7th International ERCOFTAC Symposium on Engineering Turbulence Modelling and Measurements (ETMM7)	Limassol, Cyprus		CU	KP#5
3-8 August 2008	Presentation: Statistics of Relative and Absolute Velocities of Turbulent Non-premixed Edge Flames Following Spark Ignition	32nd International Symposium on Combustion	McGill University, Montréal, Canada		TUD, UCAM, DLR	KP#6

Planned/ Actual Dates	Type	Type of Audience	Countries Addressed	Size of Audi ence	Partner Responsi ble / Involved	Internal Ref. N°
January 2009	Presentation: Spark Ignition in a Turbulent Shearless Fuel-air Mixing Layer: Average Flame Growth Rates	47th AIAA Aerospace Sciences Meeting			UCAM	KP#7
21-25 September 2008	Presentation & Publication: Experimental Analysis of Velocity Field Structure in Isothermal Countercurrent Jets	XVIII National Conference on Fluid Mechanics & Journal of Theoretical and Applied Mechanics	Gdansk, Poland		UC	KP#8
21-25 September 2008	Presentation & publication: Experimental Analysis of Droplet Generation	XVIII National Conference on Fluid Mechanics & Archives of Thermodynamic s	Gdansk, Poland		UC	KP#9
August 2008	Presentation: Large-Eddy Simulations of the polydisperse gas-particle flow in an academic combustor	AIAA conference			CERFAC S	KP#10
8-10 September 2008	Publication: Large Eddy Simulation of a two-phase reacting flow in an experimental burner	DLES7 conference			CERFAC S	KP#11
23-24 October 2008	Presentation & publication: Evaluation of numerical strategies for two-phase reacting flows	2nd INCA Workshop	Rouen, France		CERFAC S	KP#12
2009	Publication: A Novel Application of Barycentric Coordinates for Lagrange Two-Way Coupled Spray Calculations	International Journal of Multiphase Flow			ITS	KP#13
2009	Publication: Large Eddy Simulation of a Turbulent Droplet Laden Mixing Layer	DLES7 conference proceedings			IC	KP#14
5-8 January 2009	Publication: Validation of a Multicomponent Fuel Model for Spray Computations	AIAA 47 th Aerospace Science Meeting	Orlando, Florida, USA		DLR	KP#15
30 March - 1 April 2009	Publication: Two Stage Ignition of n-heptane: Identifying the Chemistry Setting the Explosive Time Scales	Model Reduction for Reacting Flows meeting	Notre Dame, Indiana, USA		ICEHT	KP#16
7-11 September 2009	Publication: Experimental Investigation of Ignition of an Air-kerosene Spray in Altitude Conditions	ISABE 2009 conference	Montréal, Canada		ONERA	KP#17
7-10 September 2009	Publication: Large-Eddy Simulation of a Two-Phase Plane Mixing-Layer	12th EUROMECH European Turbulence	Marburg, Germany		LU	KP#18

Planned/ Actual Dates	Type	Type of Audience	Countries Addressed	Size of Audi ence	Partner Resposi ble / Involved	Internal Ref. N°
		Conference (ETC 12)				
	Publication: SGS analysis of the evolution equations of the mixture fraction and the progress variable variances in the presence of spray combustion	The International Journal of Spray and Combustion Dynamics (published by Multi-Science Publishing Co.)	United Kingdom		CNRS	KP#19
14-18 September 2009	Publication: 'Measurement' of mesoscopic Eulerian particle velocity and temperature moments from DNS-DPS of a cold droplet-laden planar jet crossing a homogenous isotropic decaying turbulent gas flow	6th International Symposium on Turbulence, Heat and Mass Transfer	Rome, Italy		INPT	KP#20
14-18 September 2009	Publication: Modeling of interaction of single droplet with turbulent flow	6th International Symposium on Turbulence, Heat and Mass Transfer	Rome, Italy		UC	KP#21
4-7 January 2010	Publication: Simulations of spark ignition of a swirling n-heptane spray flame with conditional moment closure	AIAA 48th Aerospace Sciences Meeting	Orlando, Florida, USA		UCAM	KP#22
	Publication: Large-Eddy Simulation of forced ignition of an annular bluff-body burner	Combustion and Flame (ELSEVIER)			CNRS	KP#23
16-17 September 2009	Publication: Droplet Dispersion in an Unsteady Vortex Street	VDI 24. German Flame Day - Combustion and Furnaces conference	Bochum, Germany		ITS	KP#24
14-18 June 2010	Publication: Statistical Evaluation of Ignition Phenomena in Turbojet Engines	ASME Turbo Expo 2010: Power for Land, Sea and Air GT2010	Glasgow, UK		ONERA	KP#25
	Publication: Large Eddy Simulation of a droplet laden turbulent mixture	International Journal of Heat and Fluid Flow			IC	KP#26
	Publication: Large Eddy Simulation of Evaporating Kerosene and Acetone Sprays	International Journal of Heat and Mass Transfer			IC	KP#27
30 May - 4 June, 2010	Publication: Modeling the Random Uncorrelated Velocity Stress Tensor for Unsteady Particle Eulerian Simulation in Turbulent Flows	International Conference on Multiphase Flow 2010 (ICMF-2010)	Tampa, Florida, USA		INPT/CER FACS	KP#28

Planned/ Actual Dates	Type	Type of Audience	Countries Addressed	Size of Audi ence	Partner Respon sible / Involved	Internal Ref. N°
14-18 June 2010	Publication: Experimental Analysis of Altitude Relight Under Realistic Conditions Using Laser and High-speed Video Techniques	ASME TurboExpo 2010 conference	Glasgow, UK		DLR	KP#29
1-6 August 2010	Publication: A Spark Ignition Model for LES based on a FSD Transport Equation	33rd International Symposium on Combustion	Beijing, China		IFP	KP#30
6-8 September 2010	Publication: Measurement of Initial Conditions of a Kerosene Spray from a Generic Aeroengine Injector at Elevated Pressure	ILASS-Europe 2010, 23 rd Annual Conference on Liquid Atomization and Spray Systems	Brno, Czech Republic		DLR	KP#31
	Publication: Large Eddy Simulation of the Sandia Flame Series D-E-F using the Eulerian stochastic field method	Combustion and Flame			IC	KP#32
	Publication: LES-PDF Simulation of a spark ignited turbulent methane jet	Proceedings of the Combustion Institute			IC	KP#33
	Publication: Large Eddy Simulation of a swirl stabilized spray	Proceedings of the Combustion Institute			IC	KP#34
9-11 June 2010	Publication: Large Eddy Simulation of the Two-Phase Flow in an Experimental Swirl-Stabilized Burner	ETMM8: 8th International ERCOFTAC Symposium on Engineering Turbulence Modelling and Measurements	Marseille, France		IC	KP#35
6-10 June 2011	Publication: Detailed Characterization of a Swirled Air-kerosene Spray in Reactive and Non-reactive Conditions Downstream from an Actual Turbojet Injection System	ASME Turbo Expo 2011: Power for Land, Sea and Air GT2011	Vancouver, Canada		ONERA	KP#36
6-10 June 2011	Publication: LES of Pre-vaporised Kerosene Combustion at High Pressures in Single Sector Combustor Taking Advantage of the Flamelet Generated Manifolds Method	ASME Turbo Expo 2011: Power for Land, Sea and Air GT2011	Vancouver, Canada		TUD	KP#37
6-10 June 2011	Publication: Spray and Flame Structure of a Generic Injector at Aero-engine Conditions	ASME Turbo Expo 2011: Power for Land, Sea and Air GT2011	Vancouver, Canada		DLR	KP#38
6-10 June	Publication: Conditional	ASME Turbo	Vancouver,		RR, UCAM	KP#39

Planned/ Actual Dates	Type	Type of Audience	Countries Addressed	Size of Audience	Partner Responsible / Involved	Internal Ref. N°
2011	Moment Closure LES Modelling of an Aero-engine Combustor at Relight Conditions	Expo 2011: Power for Land, Sea and Air GT2011	Canada		and DLR	

3.2.2. Dissemination within the Consortium:

Task 1.2: LES modelling of two-phase flow

- 1.2.2: Turbulence/Droplet interaction (TUD)
FASTEST => RR & RRD in-house CFD code
- 1.2.3: Fractal Model of Turbulent Combustion (DMA)
HeaRT code => Avio
- 1.2.4: Spectral LES of two-phase combustion (UC)
SAILOR code => all partners
- 1.2.5: Development of Eulerian/Lagrangian spray model (LU)
LULES => RR & RRD in-house CFD code

Task 1.3: Theoretical studies for two-phase approach in LES

- 1.3.1: Evaluation of Euler versus Lagrange approach (CRSA/CNRS)
DNS data bases => to all partners
- 1.3.1b: Computational efficiency of E. versus L./DNS (CNRS)
Generation DNS databases => all partners

Task 1.4: Chemistry models for two-phase flow

- 1.4.1: FGM and CFM methods for LES (TUE)
RR and RRD in-house CFD code
Data bases to all partners => TUD
- 1.4.2: CMC-spray model for RANS and LES (delay w.r.g start)
RR and RRD in-house CFD code
- 1.4.3: Turbulence / Chemistry interactions, TPDF (IC)
BOFFIN LES code => all industrial partners
- 1.4.4: Reduced kinetic mechanisms for kerosene (ICEHT)
UCAM (CMC) => RR & RRD in-house CFD code
- 1.4.5: (Auto) Ignition Modelling in Two-Phase Flows (DMA)
Heart code => AVIO

Task 1.5: Ignition model for LES (IFP)

AVBP => CERFACS => SN & TM

- ▶ All of WP2 experiments are computed by WP3 partners for model and code validation:
 - simple academic experiments
 - complex industry-like experiments
 - multiple meetings between WP2 & WP3 partners for cross-validation
- ▶ Most of the developed/investigated models in WP1 are included in WP3
- ▶ Industry: major/advanced/reliable/efficient LES codes are or will be used by the industrial partners.