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## LES simulation of a devolatilization experiment on the IPFR facility

*F. Donato, G. Rossi, B. Favini, E. Giacomazzi, D. Cecere  
F.R. Picchia, N.M.S. Arcidiacono*



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## LES SIMULATION OF A DEVOLATILIZATION EXPERIMENT ON THE IPFR FACILITY

F. Donato, E. Giacomazzi, D. Cecere, F.R. Picchia, N.M.S. Arcidiacono (ENEA)  
G. Rossi, B. Favini (Università di Roma, Sapienza – DIMA)

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Responsabile del Progetto: Stefano Giammartini, ENEA

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## Abstract

Oxy-combustion of pulverized coal has raised some interest from industrial players in the energy production field, as a promising technique to meet future emission requirements. The present work is part of a larger activity aimed at developing and validating a Large Eddy Simulation (LES) solver applicable to the study of this kind of burners, even in MILD conditions.

In the present work, after briefly recalling the models implemented in the HeaRT code, the Isothermal Plug Flow Reactor (IPFR) facility is described. Finally the results of the validation of the HeaRT code against the data from a devolatilization test performed on this facility are presented.

## Introduction

The present work reports the results of part of a wider research activity aimed at the development of a coal powder fired combustion system, with low emissions of pollutants and  $CO_2$ , to be employed in power production applications. The technology to be investigated relies on the coal oxidation in presence of oxygen enriched air under MILD conditions, already tested on pilot-scale facilities.

The activity reported in this work is mainly focused on the Large Eddy Simulation (LES) modeling of multiphase flows of interest for the applications above described. In the past years, the research performed at ENEA within the agreement between ENEA and MSE (Italian Ministry for Economical Development), brought to the development of different modules implemented in the HeaRT code. This modules can deal with multiphase flows, coal thermal degradation, heat transfer by radiation, etc., that are physical phenomena that have a deep influence in the evolution of the flow and of the relevant physical variables in a coal powder combustion system. The present report describes the validation activity performed on the such modified version of the HeaRT code within PAR2011 of the ENEA/MSE agreement.

The planned activity comprised a validation of the implemented devolatilization module on an experimental test case considered simple under the flow structure point of view. The data from the Isothermal Plug Flow Reactor (IPFR) facility owned by the International Flame Research Foundation (IFRF) were chosen for this objective. The simulation should have been performed on a 1D domain and the complete model would have then been validated on a more complex configuration to be chosen. However, during the simulation of the IPFR devolatilization experiment, it appeared clear how the real conditions of the burner did not allow a validation on such a simplified configuration. The mixing between the cold nitrogen jet carrying the coal particles and the surrounding hot flow is not instantaneous and the mixing time is not negligible with respect to the devolatilization time. This has an influence on the rate of temperature increase for the coal particles and, as a consequence, on the released mass flow rate. In addition, it was noted how the radiative heat transfer played an important role on the rate of particle temperature increase. A strategy for the coupling of the radiation and of the dispersed phase field was thus developed and implemented in the HeaRT code.

The IPFR devolatilization experiment was therefore simulated on a complete three-dimensional domain and for particles of initial diameter  $d_p = 70\mu\text{m}$ , making use of complete and global devolatilization mechanisms. The complexity and the computational cost of such simulations did not allow to complete the activity with a second simulation on a different burner. Nevertheless, it should be noted that the objective of obtaining a validation of the HeaRT code on a configuration of interest is to be considered reached. The good agreement obtained between the experimental data on coal conversion and the numerical results, given the described complexities, is a proof of the capability of the code in predicting both the rate of coal particles temperature increase and the rate of volatile matter release.

In the following sections the models implemented in the HeaRT code will be briefly recalled. Then the simulation setup and the numerical results will be described.

## Mathematical and numerical model

The version of the HeaRT code used in the present work solves both the continuous and the dispersed phase in an Eulerian frame. The model thus belongs to the Eulerian-Eulerian class of solvers for multiphase flows. The adopted mathematical model for the continuous and the dispersed phase as well as the equations adopted to treat the advected condensed scalars have been described in previous publications [1, 2]. In the present work the only, but crucial, improvement on the model implementation in the HeaRT code has been the coupling of the M1-model for the prediction of the radiative field and the dispersed phase. It was in fact noted during the simulations of the IPFR devolatilization experiment that neglecting the radiation influence on the rise of the coal particle temperature would have induced a large spatial delay in the volatile matter release. The coupling of the radiative and dispersed phase fields was thus necessary in order to compare computed and experimental data, which are only collected at certain sections at given distances in the axial direction from the inlet.

As far as the continuous phase is considered, the equations solved are the conservation of mass, momentum, energy, species mass fraction and conservation of mass for the advected scalars. The advected scalars are here used to take into account the evolution of condensed chemical species released from the coal (TAR). They are assumed in mechanical and thermal equilibrium with the gas phase, which means that they share the same velocity and temperature of the continuous phase. This assumption is justified by the small dimension of the TAR droplet released from the coal. Gas phase kinetics has been neglected. The chemical species released from the coal may thus react with the coal particle through heterogeneous reactions modeled after [3] or may simply be advected by the flow. When the dispersed phase is considered, equations for the particle number density, mass and momentum conservation and particle enthalpy are solved. Additional equations for the evolution of the functional groups representative of the chemical composition of the coal have been introduced. The coal thermal decomposition has been modeled after [4] (Full mechanism) and after [5] (Simplified mechanism). All the equations solved for the continuous and the dispersed phase are written in conservative form.

The radiative field is associated to the multiphase mixture. The equations considered are solved for the radiative flux and the radiative energy. The adopted model has been taken from [6]. The coupling strategy has been developed taking advantage from what has been reported in [7]. Due to the very low characteristic time of the radiative field evolution compared to the acoustic time, quasi steady state has been assumed for the radiative field and time dependence has been neglected. The steady

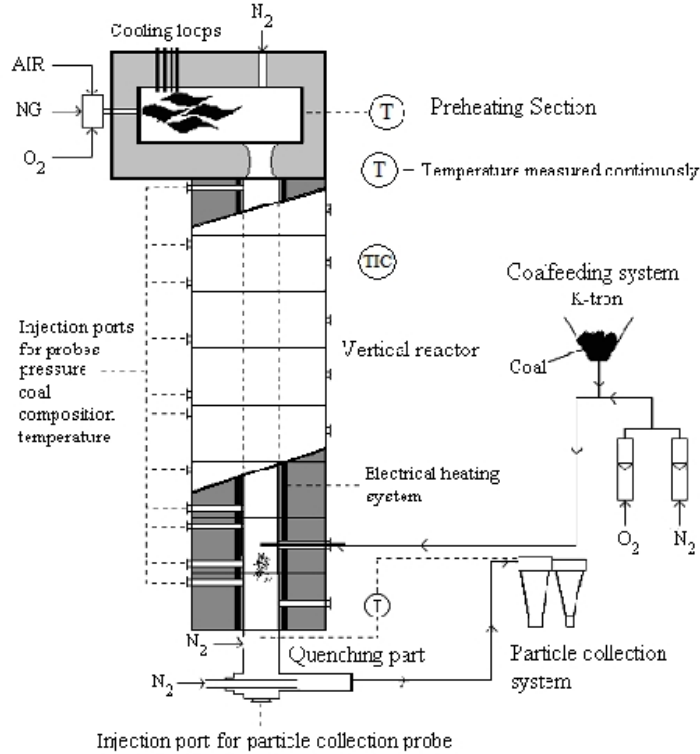


Figure 1: Scheme and characteristics of the IPFR facility (Taken from ref. [8])

state solution is searched for every time step iteratively.

The cited analytical models have been implemented in the HeaRT code owned by ENEA. The gas phase solver is based on a finite difference central 2nd order staggered scheme. The dispersed phase solver is based on a finite volume 2nd order upwind scheme with ENO reconstruction at the cell interface. Further details on the HeaRT code and on the implemented models can be found in [1, 2].

## Simulation of a devolatilization experiment on the IPFR facility

In the present section the results obtained by simulating a devolatilization experiment performed on the IPFR facility at IFRF in Livorno (Italy) are described. With reference to Figure 1 The combustion chamber is composed by a modular drop tube with inner diameter  $D_1 = 0.15$  m and total length  $L_1 = 4.5$  m. The tube is equipped with probe accesses at several sections for both coal feeding and sampling. A natural gas fired combustor is present at the top of the facility and the exhaust gases coming from this burner are used to set up the desired experimental condition inside the drop tube. The possibility to dilute such exhaust gases with Nitrogen is also considered in order to have greater flexibility. At the bottom of the combustion

chamber a quenching system and a system for coal residuals and ashes collection are present. The residence time can be varied by changing the access for the coal feeding probe. Further information about the facility or the experimental procedure can be found in [8].

In the configuration adopted for the simulated test the coal injection is located at the tube axis through a hole with diameter  $D_{inj} = 0.0085$  m. The proximate and ultimate analysis for the tested coal are reported in Table 1.

Proximate analysis (as fired- %w/w)				Ultimate analysis (as fired- %w/w)			
Moisture	Volatiles	Ash	Fixed carbon	C	H	N	S
3.39	25.26	15.32	56.04	69.56	4.54	1.64	0.57

Table 1: Proximate and ultimate analysis for the tested coal

The simulated domain extends to  $Z_{max} = 3.05$  m. A detail of the adopted grid for the first 0.2 m in axial direction is reported in Figure 2. The cells with the smallest dimensions are at the top center of the domain, where the coal injection takes place. The smallest cell size in the axial direction is  $\Delta z_{min} = 0.001$  m while in radial direction is  $\Delta r_{min} = 0.000425$  m. The radial discretization is independent from the axial position while the grid is stretch in the axial direction and the maximum cell dimension reaches  $\Delta z_{max} = 0.019$  m at the outlet section. The azimuthal direction has been discretized using 16 planes with constant distribution, while 48 cells have been used in the radial direction and 500 in the axial direction. The grid is therefore composed by 384000 cells.

The imposed boundary conditions for the gas phase are adiabatic viscous walls at  $r = R_{max} = 0.075$  m while at the outlet section ( $z = Z_{max}$ ) a characteristic equations treatment [9] is imposed, with asymptotic pressure equal to 1 atm. For the dispersed phase an upwind outlet is imposed at both walls and at the outlet section. The reason for the treatment chosen for the walls is due to the nature of the Eulerian-Eulerian two-fluid formulation. Only by taking into account the uncorrelated energy [1] in the model it could be possible to describe the dispersed phase rebounding process at walls. The "outlet" solution has been selected in alternative to letting the dispersed phase to accumulate at walls. This allows the conversion data to be numerically measurable, through the advected dispersed phase mass, only up to the third sampling section located at 0.89 m from the inlet. The inlet section at  $z = Z_{min}$  is divided into 3 regions: the coal injection, the injector wall and the exhaust gas inlet. The coal injection is positioned for  $0 \text{ m} < r < 0.00425$  m. Here coal and  $N_2$  as carrier gas enter the domain with mass flow rates  $W_{coal} = 3.05556 \cdot 10^{-5}$  kg/s and  $W_{N_2}^{inj} = 5.80093 \cdot 10^{-4}$  kg/s and imposed temperatures  $T_{coal} = 298.15$  K and  $T_{N_2}^{inj} = 293$  K. In order to simulate the expansion cone at the injection, a radial mean component has been added to the carrier gas velocity which present a linear dependence from the radial coordinate. This component is 0 at the axis and equal to the axial component for  $r = 0.00425$  m. The dispersed phase is here injected with volumetric fraction  $\alpha^{inj} = 4.316 \cdot 10^{-4}$  and axial velocity  $u_{p,z} = 1$  m/s. The



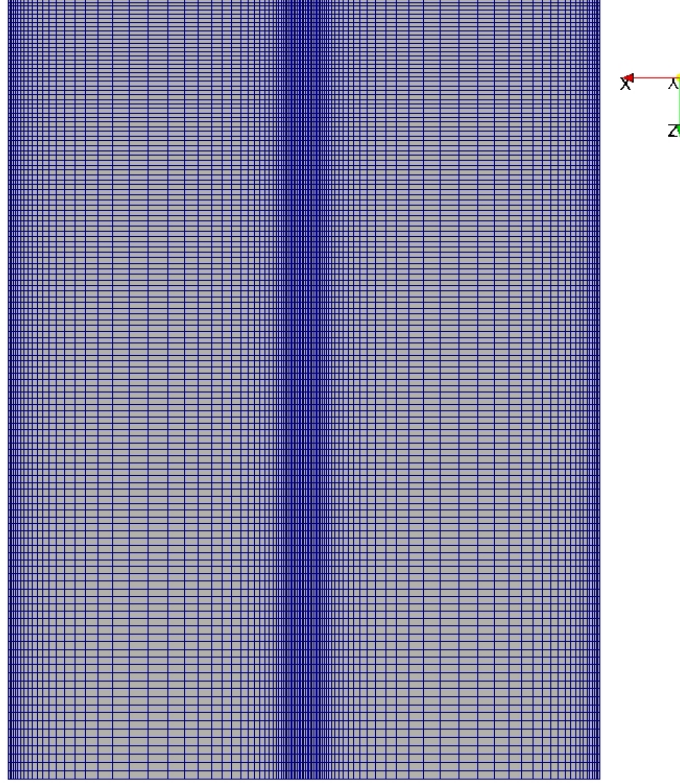


Figure 2: Adopted grid for the first part of the domain (0.2 m in axial direction)

experiment has been run with particle diameter  $d_p$  at the injection in the range  $[38 : 90] \mu\text{m}$ . The adopted model has been chosen to be mono-dispersed for computational time constraints, although the HearT code is able to deal with different classes of particles with different initial dimensions. The particle number density at the inlet  $n_p^{inj}$  has been imposed in order to have a particle dimension of  $d_p^{inj} = 70 \mu\text{m}$ . The radial velocity has been imposed following the law  $u_{p,r} = 12.83 \text{ s}^{-1} \cdot r$ . The exhaust gases enter the inlet with the following composition in terms of mass fraction:  $Y_{CO_2} = 0.104292$ ,  $Y_{H_2O} = 0.0853841$ ,  $Y_{O_2} = 0.00824372$  and  $Y_{N_2} = 0.80208018$ . The temperature is given by the nominal set point  $T_{eg}^{ann} = 1373 \text{ K}$  while the total mass flow rate is  $W_{eg}^{ann} = 1.26103 \cdot 10^{-2} \text{ kg/s}$ . The dispersed phase enters from this section with a volumetric fraction  $\alpha_{eg}^{ann} = 1 \cdot 10^{-12}$  which is just a numerical approximation to zero. The injector wall ranges from  $r = 0.00425 \text{ m}$  to  $r = 0.0063561 \text{ m}$ . In this interval the temperature and chemical species values are linearly interpolated between the values imposed at the coal injection and at the exhaust gas inlet in order to enhance the stability of the radiative solver. Null pressure gradient is imposed on the entire inlet where synthetic turbulence is injected following the procedure described in [10]. Finally, null gradient is also imposed on all the radiative variables on the entire domain boundary.

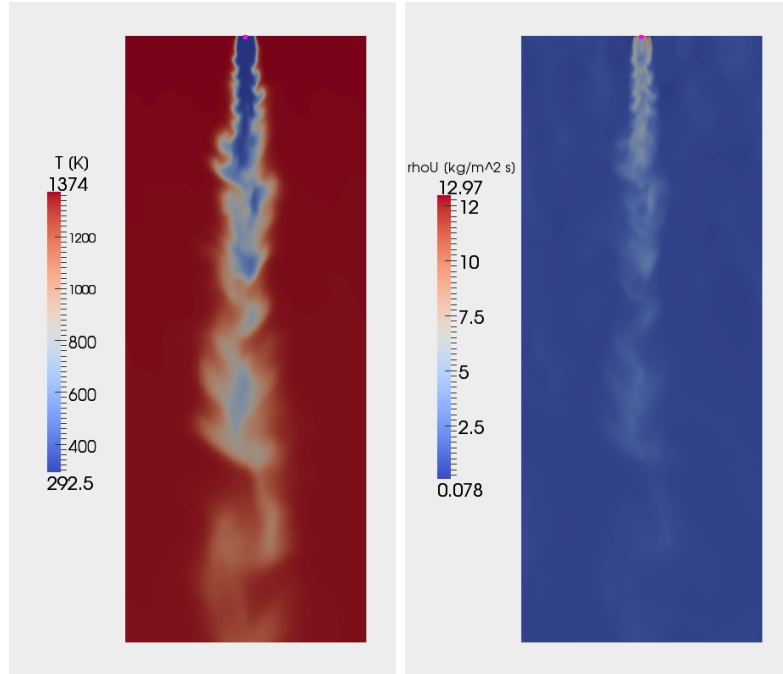


Figure 3: Gas phase temperature (left) and momentum module (right) instantaneous distribution.

The initial conditions are set equal to the variable values at the exhaust gas inlet with the exception of the velocity of both phases which is set to zero.

## Results

In Figure 3 an instantaneous field of the gas temperature  $T$  and of the momentum module  $\rho u$  are presented for the first 0.4 m of the domain in axial direction. The reported figure has been obtained for the full devolatilization mechanism computation but similar distributions have been obtained making use of the simplified scheme. It can be seen how the cold jet enters the chamber till  $z = 0.3$  m and even further. This feature of the flow has a strong influence on the coal conversion since the gas temperature influences the particle heating up. The jet momentum reaches the equilibrium with the outer flow approximately at the same distance from the inlet.

In Figure 4 instantaneous distributions of the  $CO$  mass fraction and of the dispersed phase volume fraction are reported. Again, no major differences between the full and the reduced mechanism computations were observed. It can be seen how the released  $CO$  concentrates around the zones with the higher particle concentration.

Finally, in Figure 5 the numerical and experimental data on coal conversion are compared, at least for two sampling points. The numerical data are obtained by taking the averaged values of the dispersed phase mass flow rate on the planes where measures are available. Data are sampled with a frequency of  $\nu = 10000$  Hz on four radial directions for an integrated interval  $\Delta t = 0.1$  s. The averaged values are

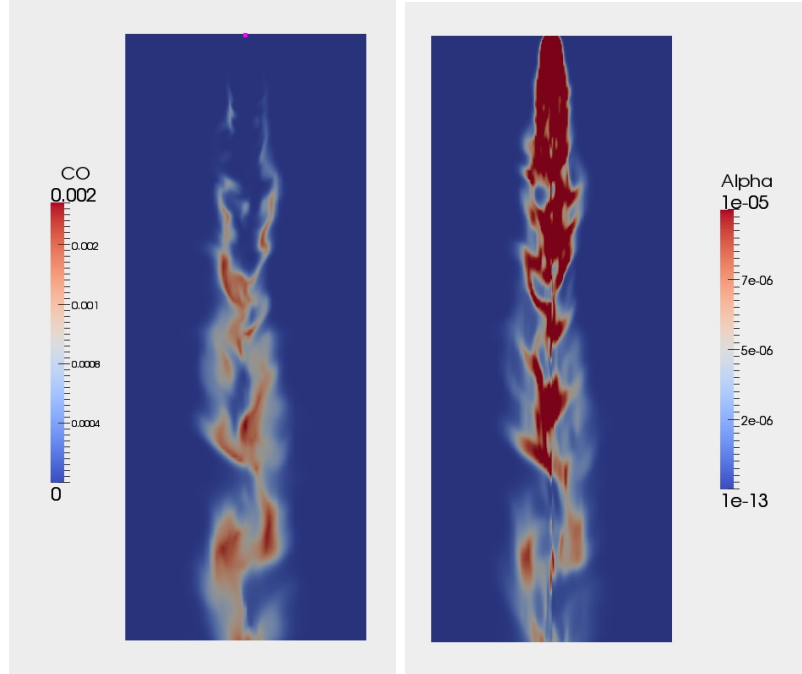


Figure 4:  $CO$  mass fraction (left) and dispersed phase volume fraction (right) instantaneous distribution - Full mechanism.

then numerically integrated on the surface to obtain the mass flow rate  $W_{int}$  passing through it. By assuming the ashes mass flow rate constant through the combustor, the coal conversion  $C$  can be evaluated by

$$C = 100 \left( 1 - \frac{W_{int}}{W_{coal}} \right) \quad (1)$$

It can be seen how the numerical data are well within the uncertainty range of the measures for both the complete and the reduced devolatilization mechanisms. It should be here remarked how the first sampling section is positioned at  $z = 0.29$  m, which is approximately the extension of the cold jet in axial direction. The fact that numerical data well reproduce the experimental ones at this section is a proof of the good performance of the code in terms of prediction of the mixing and of the interaction among phases.

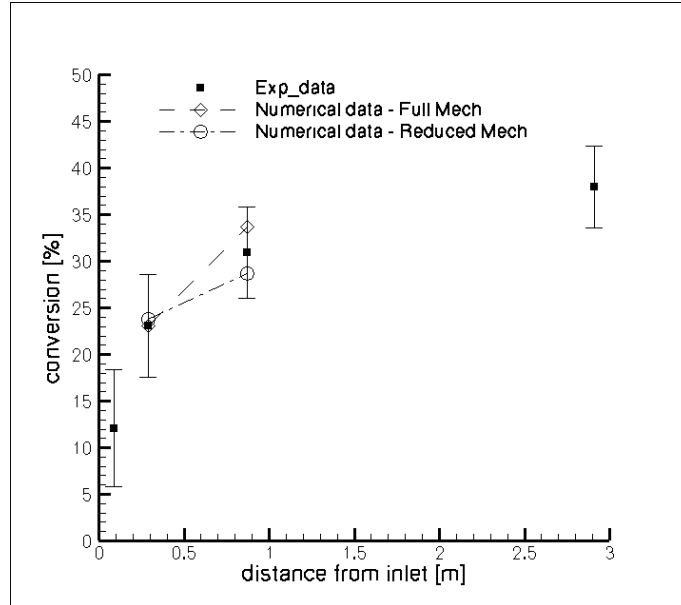


Figure 5: Comparison between experimental and numerical data on coal conversion

## Conclusion

In the present work the validation of the HeaRT code against a IPFR devolatilization experiment is presented. The implementation of the POLIMI devolatilization model in the HeaRT code has proved its capability in well reproducing the coal conversion experimental data for both the full mechanism [4] and the reduced mechanism [5].

It should also be noted that in order for the validation to be successful, the coupling of a radiative solver with the dispersed phase model was necessary. The very good agreement between the numerical and experimental coal conversion data at short distance from the injector ( $z = 0.29$  m), where the influence of the cold Nitrogen jet is clearly present, can be considered a good test for the entire model, including turbulence mixing, phase interaction models and radiation field solver.

Further validation activities should be performed to complete the code assessment. This may include an oxidation test on the same IPFR configuration and a pilot-scale oxy-combustion burner.

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**Prof. Bernardo Favini**  
**Univ. Di Roma "Sapienza"**

**Curriculum vitae**

**1954** nato a Roma il 14 novembre.

**1980** laureato in Ingegneria Meccanica con 110/110 e lode, Facoltà di Ingegneria , Università di Roma *la Sapienza*.

**1983** ricercatore in Fluidodinamica, ING-IND/06, presso il Dipartimento di Meccanica e Aeronautica della Facoltà di Ingegneria, Università di Roma *la Sapienza*.

**1992** professore associato in Fluidodinamica, ING-IND/06, presso il Dipartimento di Meccanica e Aeronautica della Facoltà di Ingegneria, Università di Roma *la Sapienza*.

**1998-2001** responsabile settore Applicazioni per il Consorzio Interuniversitario per le Applicazioni del Super Calcolo per l'Università e la Ricerca, CASPUR.

**1998-2005** Membro del Collegio dei Docenti del Dottorato in Ingegneria Aerospaziale, Università di Roma *la Sapienza*.

**2006** Membro del Collegio dei Docenti del Dottorato in Tecnologia e Scienza Aerospaziale, Università di Roma *la Sapienza*.

**2012** Membro del Collegio dei Docenti del Dottorato in Matematica, Università di Roma *la Sapienza*.

**Attività didattica**

Docente di diversi corsi del raggruppamento di Fluidodinamica, in particolare: Gasdinamica, Fluidodinamica, Ipersonica, Magnetofluidodinamica, Gas Rarefatti, Aerotermochimica, Modellistica per la Propulsione a Solido, Metodi Numerici per le Equazioni alle Derivate Parziali Non-Lineari.

Docente del Master in Calcolo Scientifico, Università di Roma *la Sapienza*, in: Fluidodinamica Numerica e Fluidodinamica Ambientale.

Docente del Master in Sistemi di Trasporto Spaziale, Università di Roma *la Sapienza*, in: Gasdinamica Numerica.

**Attività Scientifica**

Ricerche svolte nell'ambito della Fluidodinamica con particolare interesse per: Metodi numerici per flussi comprimibili stazionari e non-stazionari in presenza di urti, Flussi ipersonici attorno a corpi di rientro, Flussi turbolenti reattivi, Gasdinamica dei motori a propellente solido.

13 pubblicazioni su riviste internazionali e 49 a congressi internazionali.

Responsabile di finanziamenti Murst, Convenzioni ENEA e AVIO, e partecipante a gruppi di ricerca di Convenzioni ASI, AVIO e ESA-Esrin, ESA-ESTEC.

# Giacomo Rossi

## Curriculum Vitæ

9, Via Girolamo Cocconi  
00171 Roma, Italy

+393408816643

+39062593332

✉ rossigiacomo82@gmail.com

Roma, January 29, 1982



## Education

November  
2009

**PhD Student in Aerospace and Aeronautical Technology**, Department of Mechanical and Aerospace Engineering, Sapienza University, Faculty of Civil and Industrial Engineering, Via Eudossiana 18, Rome, Italy

2006-2009

**Master of Science in Space Engineering**, University "Sapienza", Faculty of Aeronautical and Spatial Engineering, Rome, Italy

Mark 106/110

Thesis Entitled

*Soffocamento Supersonico nel Transitorio degli Endoreattori a Propellente Solido (Supersonic Choking during Solid Rocket Motors Ignition Transient)*

2000-2005

**Bachelor of Science in Aerospace Engineering**, University "Sapienza", Faculty of Engineering, Rome, Italy

Mark 97/110

Thesis Entitled

*La Deportanza nelle Autovetture da Competizione (Downforce in Race Cars)*

1995-2000

**Secondary High School Focusing on Sciences**, Liceo Scientifico Statale "Tullio Levi Civita", class with physics and computer science profile, Rome, Italy

Mark 100/100

## Professional Experiences

2010

**Project Worker**, Dipartimento di Ingegneria Meccanica e Aerospaziale, 18, Via Eudossiana, Rome, Italy, University "Sapienza", Faculty of Aeronautical and Spatial Engineering, Job: Analysis of Gasdynamic Fields in Solid Rocket Motors Combustion Chambers

1998-1999

**Project Worker**, Cartest s.r.l., 912, Via Tiburtina, Rome, Italy., Job: Archive Setting and Electronic Database Management

## Principal Subjects

✓ Aerospace Propulsion, Thermal Control, Fluid Dynamics

✓ Computational Fluid Dynamics

## Languages

Italian **Native Speaker**

English **Very Good**

---

## Computer Skills

Operating Systems	GNU/Linux, Microsoft Windows XP, Microsoft Windows Vista, Microsoft Windows Seven
Office Suites	OpenOffice, Microsoft Office XP, Microsoft Office 2007
Grafical Editing	Inkscape, The Gimp, Photoshop
Scientific Visualization Tools	Paraview, Tecplot
Languages	Fortran 90, Fortran 95, $\LaTeX$ , Matlab

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## Publications

### Conference

**B. Favini, E. Cavallini, G. Rossi, M. Di Giacinto, A. Di Mascio and F. Serraglia,** *On the NDP Onset in Pre-Ignition Transient of High Performance SRMs: VEGA Z9A Experience*, 5th International Conference on Recent Advances in Space Technologies, June 2011, Istanbul, Turkey

### Technical Reports

**A. Di Mascio, R. Broglia, R. Muscari, G. Rossi, S. Zaghi, B. Favini,** *Aerothermal Fluxes of Vega Launcher*, Technical Report VG-ESA-SOW-004-IPT, February 2011, Rome, Italy

*Roma, September 27, 2012*

Giacomo Rossi