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Multidisciplinary approach for assessing the atmospheric impact of launchers

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Abstract

Exhausts from rockets influence the atmospheric chemistry and the atmospheric radiative transfer. Assessing these effects requires a multidisciplinary approach. It ranges from combustion calculations in the rocket engines to plume simulations on different scales. The plume is first analysed with computational fluid dynamic models and engineering methods. Then a diffusion model is applied and lastly a chemical transport model is used for simulations on a global scale. This approach is currently being implemented in the Atmospheric Impact of Launchers project, which is funded by ESA as part of its CleanSpace Initiative. Therefore, the focus of this study lies on rockets launching from Kourou, which are Ariane 5, Vega and Soyuz.

1 Introduction

During ascent a launcher flies through all layers of the atmosphere. Throughout its flight, the rocket's propulsion systems emit chemical products, which can influence the atmospheric chemistry. In addition, the particles coming from the solid rocket motors can affect the atmospheric radiative transfer processes. Especially the potential impact on stratospheric ozone is important. Research in this field serves as a basis for ecologically sensitive design of launch vehicles. This research falls into three main categories: measurement campaigns, computer simulations, and laboratory experiments.

Early studies on the atmospheric impact of launchers were conducted by NASA as part of the Space Shuttle program. Recently, Stevens et al. [21] observed the Space Shuttle's water vapour plume during the Shuttle's last flight.

Two important measurement campaigns were conducted in the US, the Rocket Impacts on Stratospheric Ozone (RISO) campaign and the Atmospheric Chemistry of Combustion Emissions Near the Tropopause (ACCENT) campaign. A WB-57F aircraft was flown through the exhaust plumes of rockets shortly after launch and in-situ measurements were taken. The RISO campaign ran from 1996–1998. Plumes from the Space Shuttle as well as Titan, Delta, Atlas and Athena rockets were investigated [2], [12], [13], [16], [17], [20]. For the ACCENT campaign measurements were made during the years 1999–2000. Plumes from Atlas IIAS, Athena II, Delta II and the Space Shuttle were studied [1], [3], [5], [11], [15], [18].

Simulations have allowed the study of further launch vehicles and scenarios. Denison et al. [4] studied the relevance of NO_x in comparison to Cl_x emissions. Brady, Martin and Lang [1] compared the effects of different propellant combinations including solid rocket propellant, NTO/Aerozine-50, LOX/RP-1 and LOX/LH2. Karol, Ozolin and Rozanov [7] studied the Russian Energia rocket, which utilises both LOX/kerosene and LOX/LH2. Lately, two modelling studies were conducted on the role of NTO/UDMH by investigating the Proton rocket [14], [26]. The impact of Ariane 5 was studied by Jones, Bekki and Pyle [6].

Laboratory experiments have played an important role in studying isolated reactions under controlled circumstances. Especially heterogeneous reactions were studied in the laboratory. Molina et al. [9] determined the reaction rate of the chlorine activation reaction on alumina particles. These particles make up a significant part of the exhaust products of solid rocket motors. Thus, heterogeneous reactions on such particles need to be taken into account.

The objective of this paper is to present a multidisciplinary approach for assessing the atmospheric impact of launchers. This work is part of the Atmospheric Impact of Launchers (ATILA) project, which belongs to the ESA CleanSpace Initiative. The project started in May 2012 for a duration of 18 months. Its aims are twofold. The first objective is to increase the knowledge about the European launchers. The second objective is to conduct a joint study with experts from all relevant disciplines and use higher-order numerical methods where reasonably possible. Engineering models are used to assess the phenomena between the computational points calculated with the higher-order methods. To our knowledge such an approach has not been applied in the past. Murray et al. provide an overview of the uncertainties that need to be addressed [10]. This paper presents a multidisciplinary approach that includes

- the formation of hot gas and the nozzle-exit conditions,
- the early and intermediate evolution of the rocket plume,
- and the impact on the Earth's atmosphere.

2 Launchers under study

The ATILA project investigates two types of scenarios. First, a flight from the ACCENT measurement campaign was selected to validate the applied methods. It corresponds to the measurement performed on 24 September 1999 when the WB-57F aircraft flew six times through the exhaust plume of an Athena II rocket at an altitude of 18.7 km. Second, launchers operating from Kourou in French Guiana are studied. These launchers are Ariane 5, Soyuz and Vega. In addition to 18.7 km, the altitudes 30 km, 42 km and 50 km were selected as reference altitudes where higher-order methods are used.

3 Methods

Studying the impact of launchers on the atmosphere requires several disciplines. Therefore, the study is conducted in a number of steps, which are shown in Fig. 1. The overall approach is to use higher-order methods where it is reasonably possible and lower-order methods and tailored engineering models in all other cases. The higher-order methods applied are computational fluid dynamics (CFD) and a chemical transport model (CTM). Lower-order methods are used for calculating the nozzle-exit

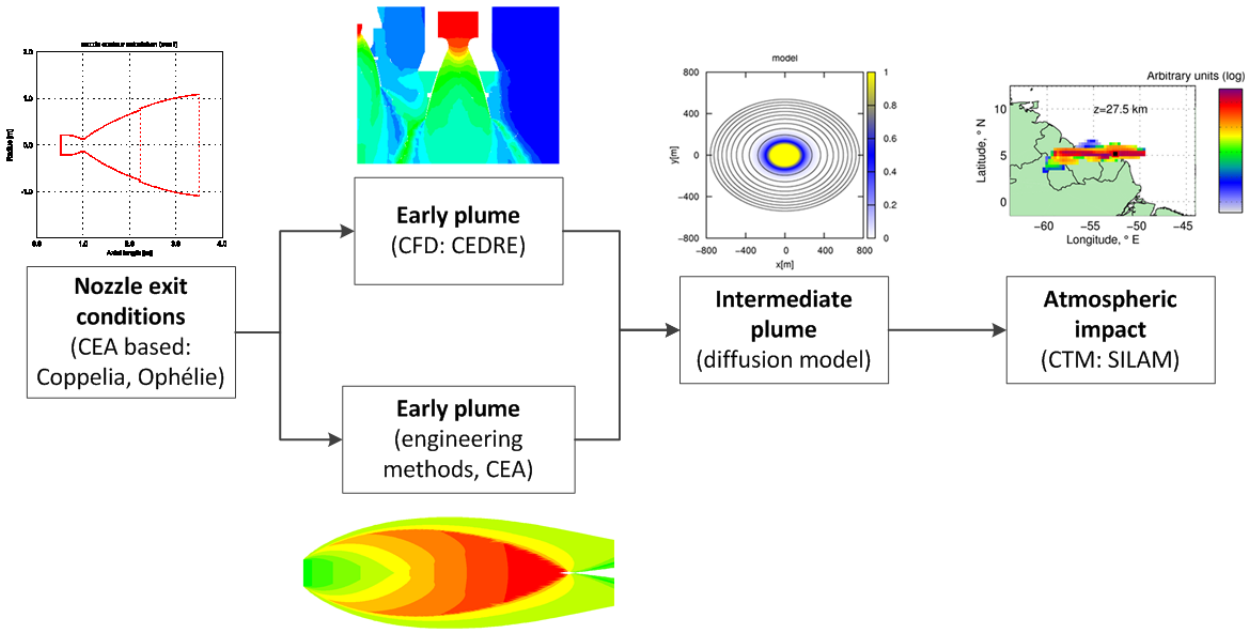

Fig. 1 Simulation tool chain

conditions and partly the evolution of the plume behind the nozzle. Nose-to-tail CFD computations are computationally expensive. Therefore, this method was only used for a few selected cases. The results of these computations serve as reference points for the engineering methods.

3.1 Nozzle-exit conditions

The first step is to calculate the thermodynamic conditions and chemical products in the nozzle exhaust plane. The launchers under study have liquid and solid propulsion systems. For both systems tools were used that are based on NASA's CEA code (Chemical Equilibrium with Applications). The results at the nozzle-exit are then fed into the early plume model. Nose-to-tail CFD computations were performed for selected points using ONERA's CEDRE code. These computations included the gas expansion in the nozzle. The conditions in the chamber were used as input to the CFD computations. The chemical reactions in the nozzle and the afterburning reactions in the rocket plume were considered as part of the CFD computations. The CFD meshes were generated on the basis of CATIA V5 models.

Calculations for the liquid propulsion engines were performed by ONERA. Their in-house code Coppelia (Calcul et Optimisation des Performances Energétiques des Systèmes Liés à l'Autopropulsion), which is derived from CEA, was used. The engines under study are Vulcain 2 for Ariane 5 and the RD-107/108 engines with their main and steering chambers for Soyuz.

In the case of the solid rocket motors Herakles used their thermodynamic code Ophélie, which is based on CEA. Nozzle-exit conditions for the motors Castor 120 for Athena II, P80 for Vega and EAP for Ariane 5 were calculated.

3.2 Early plume

In the frame of the ATILA project the early plume describes the region of the plume that is still affected by shocks and afterburning reactions. The CFD computations performed at chosen altitudes include that entire area. For all other points an engineering model is being developed at the DLR. Afterburning reactions are foreseen to be calculated with CEA.

3.2.1 CFD

3D models are used for Ariane 5 and Soyuz while Athena II and Vega are represented with a 2D axisymmetric mesh each. Meshes are about 200,000 cells for the Vega cases, generated with the GMSH open source mesh generator, and about 3 million cells for the 3D cases of Soyuz

and Ariane 5, created with the CENTAUR™ mesh generator. The models include refinements near the nozzle exit and in the mixing layer between plume and outer flow. The model domains extend 700 m (Vega, Soyuz), 750 m (Athena II) and 1500 m (Ariane 5) downstream from the nozzle exit. The outer radius of the meshes varies between 40 and 300 m. A single mesh was used for the Vega calculations at 18.7 km, 30 km and 42 km. In case of Ariane 5 the outer radius had to be increased for the 50 km case when compared to the 30 km case. Soyuz was computed at 30 km only.

Turbulence is modelled through a k-ω shear-stress transport model. However, these Reynolds-averaged Navier-Stokes models are not fully adapted to axisymmetric flows. Therefore, some constants of the original model by Menter [8] were modified following a strategy already used for a k-ε model by Turpin and Troyes [23]. The modified values of these constants are $\sigma_{\omega 2}$=0.714, β_2=0.0783 and γ_2=0.47.

The chemistry is modelled using a semi-detailed kinetic scheme shown in Table 1. More details and reaction rates are provided in [22]. The chemical scheme consists of three main paths of reactions: H_2 and O_2 reactions 1 to 8, CO and CO_2 reactions 9 to 11 and chlorine species reactions 12 to 17. In the Soyuz case only the first 11 reactions of the chemical kinetic scheme are used as no chlorine species are present in the exhaust gas.

Alumina particles are modelled in two ways depending on their size. The smallest particles, estimated to represent about 5% of the total particle mass, are treated as an equivalent gas phase within the gas solver. The large particles, estimated to have a diameter of 8 µm and representing 95% of the total mass, are treated by a dedicated Eulerian dispersed phase solver.

Table 1 Chemical reactions taken into account in the CFD simulations

Number	Reaction
1	$H + O_2 \Leftrightarrow OH + O$
2	$O + H_2 \Leftrightarrow H + OH$
3	$OH + H_2 \Leftrightarrow H + H_2O$
4	$OH + OH \Leftrightarrow O + H_2O$
5	$H + H + M \Leftrightarrow H_2 + M$
6	$H + OH + M \Leftrightarrow H_2O + M$
7	$H + O + M \Leftrightarrow OH + M$
8	$O + O + M \Leftrightarrow O_2 + M$
9	$CO + OH \Leftrightarrow CO_2 + H$
10	$CO + O2 \Leftrightarrow CO_2 + O$
11	$CO + O + M \Leftrightarrow CO_2 + M$
12	$H + HCl \Leftrightarrow H_2 + Cl$
13	$H + Cl_2 \Leftrightarrow HCl + Cl$
14	$HCl + OH \Leftrightarrow H_2O + Cl$
15	$HCl + O \Leftrightarrow OH + Cl$
16	$Cl + Cl + M \Leftrightarrow Cl_2 + M$
17	$H + Cl + M \Leftrightarrow HCl + M$

A comparison of the Mach number distribution at different altitudes is shown in Fig. 2. The general plume structure is also visible in this plot. In addition, the boundaries of the mixing layers were extracted, s. Fig. 3. The plots show that the plume structure is similar across all three altitudes but that with increasing altitude and thus decreasing atmospheric pressure the plume becomes wider and more elongated.

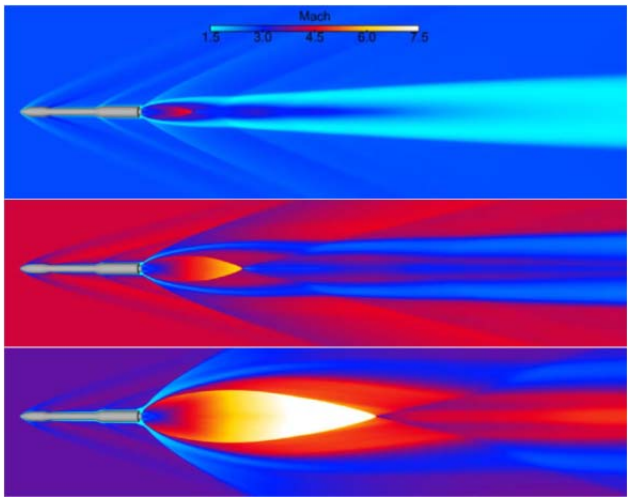

Fig. 2 Mach number evolution with altitude for the Vega rocket: 18.7 km (top), 30 km (middle) and 42 km (bottom).

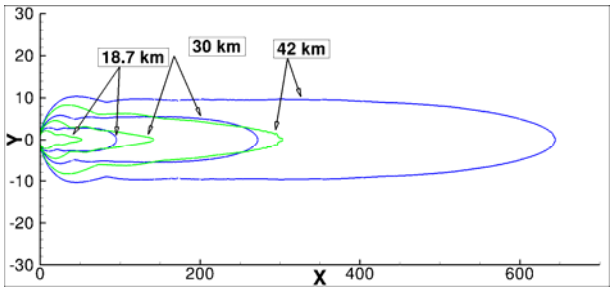

Fig. 3 Self-similar behaviour of the plume of Vega at different altitudes: internal (green) and external (blue) boundaries of the mixing layer.

3.2.2 Engineering methods

The CFD simulations are computationally intensive. Therefore, alternative approaches need to be implemented for calculating approximate solutions for the early plume at altitudes which are not considered by the CFD. Rocket exhaust plumes exhibit a characteristic structure [19] that can be divided into a near- and a far-field. In the near-field directly behind the nozzle exit the plume consists of an approximately inviscid core that is surrounded by a viscous mantle. In the viscous mantle surrounding air mixes with the exhaust gases and afterburning reactions occur. The inviscid core is separated from the viscous region by a shock wave. The pressure from the external flow turns this shock wave towards the centreline where it is ultimately reflected. This process repeats and so a periodic structure forms. Further downstream in the far-field this structure erodes due to dissipative effects.

The geometrical structure and thermodynamic properties of the exhaust flow in the near-field can be modelled with the method of characteristics [24]. The main input parameter to this model is the static pressure ratio, which is the pressure at the nozzle exit divided by the external pressure.

Woodroffe [25] developed a one-dimensional model for the far-field. It targets low-altitudes up to about 50 km and also takes chemical reactions into account.

3.3 Intermediate plume

The intermediate plume region begins when shocks and afterburning reactions have subsided. During this phase the strong concentration gradients in the radial direction are the main driver in the evolution of the plume. Fast chemical reactions and mixing with ambient air occur. These effects are described by a tailored plume model, which was developed at the IUP. The simulated domain is the cross section of the plume; a typical timescale is about an hour. The model consists of a chemical module and a short-range transport module. The chemistry module simulates gas phase and heterogeneous reactions in the plume. The transport module calculates the mixing with ambient air by solving the axisymmetric diffusion equation

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial C}{\partial r}\right) \qquad (1)$$

where r is the radial coordinate, C is the concentration of a chemical species, and D is the diffusion coefficient.

Denison et al. [4] have related diffusion coefficients to observed plume expansion rates. They have introduced a radius dependent diffusion coefficient $D(r)$ with an empirical parameter b.

$$D(r) = br \qquad (2)$$

As the mean radius of the plume increases with time, also the mean $D(r)$ acting on the plume increases. Therefore, $D(r)$ qualitatively resembles the effect of a diffusion coefficient increasing with time as predicted by Taylor's turbulent diffusion theory. For $D(r)$ as defined in Eq. (2) an analytic solution of the axisymmetric diffusion equation exists. It can be fitted to the experimental data, and the parameter b can be determined.

For Athena II a comparison between model runs and measurement data was performed. Fig. 4 shows the observed plume diameter as a function of time in comparison with the modelled plume size. Four model runs were performed with different radius dependent diffusion coefficients $D(r)$.

The diameter of the plume was measured by Danilin et al. [3] at six aircraft intercepts between 3.7 min and 36.2 min after launch. Additionally, from the data of Popp et al. [11] the plume size at five of these intercepts can be calculated. Popp et al. use the full-width at half-maximum (FWHM) volume mixing ratio of ClO to determine the plume size. In order to convert the FWHM to diameter it has been assumed here that the distribution of species in the plume is a Gaussian, and that the diameter is given by four standard deviations. Note, however, that in particular the ClO measurements of Popp et al. show scatter and the distributions deviate from a Gaussian.

The diffusion model was initialised with data from the Athena II CFD simulations 700 m behind the launcher. At this distance from the rocket, the gas temperature has decreased below 400 K, and the chemical scheme of the model can be used without missing any high-temperature reactions.

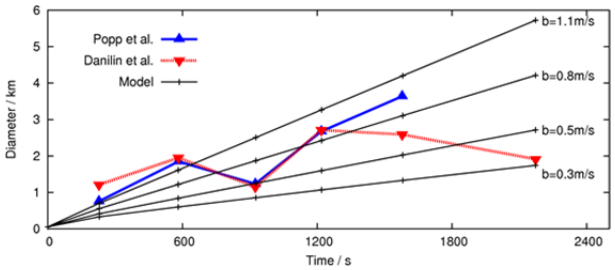

Fig. 4 Observed Athena II plume diameter [3], [11] as a function of time in comparison with model results.

3.4 Atmospheric impact

Finally, the output of the intermediate plume model is inserted into a CTM as point sources along the vertical dimension. The data is linearly interpolated to give a smooth vertical profile as a source term. At the FMI the in-house code SILAM (System for Integrated Modeling of Atmospheric Composition) is used. With SILAM it will be possible to calculate the effect of the exhaust gases on the atmosphere and the spread of the particles in the stratosphere over many years. SILAM has been adapted to the special case of simulating rocket plumes. In particular, (i) the model transport modules were extended to handle dispersion in both the free troposphere and the stratosphere, (ii) the chemistry transformation scheme was adjusted and extended, and (iii) an interface to the intermediate plume model, s. section 3.3, was created. Extension (i) is necessary because SILAM has been developed for the troposphere, but here we wish to also consider stratospheric impacts, e.g. in the ozone layer. This poses the challenge to configure optimal grid and numerical procedures for the horizontal and the vertical dimensions at such great altitudes. In case of (ii) one important family of reactions is chlorine chemistry. It plays a significant role for solid rocket motors.

4 Conclusion and outlook

Assessing the effect that rocket exhausts have on the atmosphere requires a multidisciplinary effort. The simulations within the ATILA project span several time and size scales ranging from combustion in rocket engines to simulations on a global scale. By bringing together partners from several European institutions ATILA will allow to assess the global effects and in particular increase the current knowledge about European launchers. Especially by applying higher-order methods, in this case CFD and CTM simulations, we intend to deepen the knowledge about the effects of rocket exhausts. In addition, we learn more about the modelling aspects of this integrated effort, which can then benefit other research teams.

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