Flash-evaporation of oxidizer spray during start-up of an upper-stage rocket engine

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Abstract
The low-pressure oxidizer preflow during start-up of an upper-stage rocket engine is analyzed computationally. An iterative Euler-Lagrange approach is used to describe the three-dimensional two-phase flow of oxidizer vapor and spray which is characterized by intense phase transfer. Multipoint injection and flash-atomization of liquid oxidizer is modelled by stochastic droplet injection according to injector locations and spray characteristics. Based on the framework of classical $D^2$-theory, a flash-evaporation model is developed to describe heat and mass transfer between superheated liquid droplets and vapour flow. The computed transsonic flow field agrees well with experimental characteristics such as pressure level and temperature decrease and further provides detailed local information on vapour flow homogeneity and liquid wall deposit.

Introduction
During start-up of an storable propellant upper-stage rocket engine, a steady flow of vaporizing liquid oxidizer is maintained in the combustion chamber to ensure well-defined conditions prior to injection of liquid fuel and hypergolic ignition. Due to the absence of combustion, this flow regime is characterized by thermodynamic conditions far from nominal operation of the engine. The pressure and temperature levels in the chamber are predominantly controlled by the evaporation rate of the oxidizer. Due to the extreme pressure drop from oxidizer dome to combustion chamber (see figure 1) the injected liquid is superheated. Rapid vapour formation and expansion within the liquid leads to flash-atomization, a mechanism which is characterized by extended spray cones and significantly reduced droplet sizes. Accordingly, heat and mass transfer between spray and vapour flow is governed by flash-evaporation. In contrast to conventional droplet evaporation, this mechanism is controlled by heat transfer within the droplet.

However, only a fraction of the injected oxidizer is evaporated in the combustion chamber during preflow. Aside of a finite-rate phase-change and the short residence time in the chamber flow, this is mainly due to the limited superheat energy content and the absence of other energy sources. A considerable part of the flashing spray deposits on the chamber walls. Evaporation and transport of this wall film depend on the thermal state of the wall, the shear stress on the vapour-film interface and body forces such as gravity or thrust. The remaining spray fraction is accelerated in the expanding nozzle flow and exposed to a steep drop of pressure and temperature. In this region, the two-phase mixture exhibits considerable non-equilibrium behaviour. This is indicated in figure 1 by phase-trajectories of metastable vapour (neglecting homogeneous condensation) and a flash-evaporating 50 $\mu$m-droplet.

The objective of the present study is a detailed 3D-CFD analysis of the preflow regime in a generic configuration of combustion chamber and expansion nozzle. Particularly emphasized are modelling issues associated with the low-pressure conditions, i.e. flash-atomization, flash-evaporation of spray and wall deposit as well as the intense phase interaction. In general, these physical processes are out of the scope of state-of-the-art CFD tools. Secondary breakup of droplets and spray-wall interaction are accounted for by a detailed modelling framework, which has been published previously. Not considered are vapour dissociation, droplet-droplet interaction, transport...
and build-up of liquid wall film, homogeneous condensation and ice formation. The CFD-package METIS developed at the Institute for Thermal Turbomachinery (ITS), University of Karlsruhe, is used as a computational platform for model implementation and flow analysis.

**Computational methodology**

The general approach involves a finite volume method (METIS) for discretization of the continuous vapour flow and a Lagrangian droplet tracking method (Ladrop2) to describe spray transport, dispersion and evaporation. Since the vapour flow is driven exclusively by evaporation of liquid oxidizer, two-way coupling between continuous and disperse phase is of essential importance. As illustrated in figure 2, this is realized by exchanging flow field data and spray source data data within an iterative procedure. To account for the transonic character of the flow, a compressible formulation of the SIMPLEC pressure correction scheme is used to describe the coupled pressure-velocity field. The standard high- Reynolds number \( k-e \) model is included by considering transport equations for the turbulent kinetic energy \( k \) and its dissipation rate \( e \). Applying a contour-fitted finite-volume discretization, the final set of equations is cast into a general form

\[
\sum_{nb} a_{nb}^{\phi} \phi_{nb} = c_{nb}^{\phi} \phi_{nb} + S_{\phi,0} + S_{\phi,d}, \quad \phi = p', u, v, w, h, k, e \tag{1}
\]

where the index \( nb \) comprises all neighbouring volumes of volume \( P \). The constant part of the general single-phase source term is given by \( S_{\phi,0} \) whereas \( S_{\phi,d} \) represents the spray source term. This term is evaluated during droplet tracking in Ladrop2 by averaging trajectory data on the finite volume mesh

\[
S_{m,d} = S_{p',d} = \sum_{k=1}^{N} f_{k} \left( m_{d}^{n} - m_{d}^{n+1} \right) \tag{2}
\]

\[
S_{\phi,d} = \sum_{k=1}^{N} f_{k} \left( m_{d}^{n} \phi_{d}^{n} - m_{d}^{n+1} \phi_{d}^{n+1} \right), \quad \phi = u, v, w, h \tag{3}
\]

The quantities \( \phi_{d}^{n} \) and \( \phi_{d}^{n+1} \) represent droplet trajectory data on entry and exit of each finite volume, \( f_{k} \) denotes the droplet number rate on a trajectory and \( N \) the total number of trajectories. Spray source terms for the \( k-e \) model are not considered at present. The central coefficients in equations (1), are computed as

\[
a_{p}^{dd} = \sum_{nb} a_{nb}^{d} - S_{p',1}, \quad a_{p}^{\phi} = \sum_{nb} a_{nb}^{\phi} - S_{\phi,1} + S_{m,d}, \quad \phi = u, v, w, h, k, e . \tag{4}
\]

where the \( S_{\phi,1} \) represent linear contributions to the general single phase source term. \( S_{m,d} \) is a closing term linked to interphase mass transfer. According to equation (4), this term does not contribute to the central coefficient of the pressure-correction equation.

Due to the relative magnitude of the spray source terms, the following implementation is required to ensure stability of the iterative solution process:

- If \( S_{\phi,d} \) and \( \phi \) are of opposite sign, \( S_{\phi,d} \) is not added to the right hand side of equation (1), but treated implicitly by subtracting \( S_{\phi,d} / \phi \) from \( a_{p}^{\phi} \).
- If \( S_{m,d} \) is negative, \( S_{m,d} \) is not added to \( a_{p}^{\phi} \) as defined by equation (5), but treated explicitly by subtracting \( S_{m,d} \phi \) from the right hand side of equation (1).

In this way, spray source term contributions are consistently treated implicitly, when they enhance the diagonal dominance of the system matrix. A robust numerical solution of the resulting linearized system is achieved by using the Bi-CGSTAB algorithm.

The Lagrangian tracking method is employed because of its inherent suitability for detailed modelling of complex polydisperse sprays. According to Gosman and Ioannides, the effect of turbulence on spray dispersion is simulated by stochastic velocity fluctuations along individual droplet trajectories. Wall impact of droplets is modelled by a detailed set of interaction mechanisms, including deposition, splashing, nucleate boiling, film boiling and reflection. A detailed compilation of the theoretical framework has been published. Modelling of droplet deformation and breakup
by aerodynamic forces is taken into account by empirical correlations describing classification, temporal and spatial evolution as well as secondary fragment size spectra of various mechanisms.3

Flash-atomization

During preflow, the coaxial injector elements operate as plain orifice injectors in a flash-atomization mode. Compared to classical jet breakup, rapid vapour formation within the liquid results in a burst-like expansion upon entering the low-pressure chamber environment. This mechanism is characterized by widely extended spray cones and significantly reduced droplet sizes. Experimental spray visualizations, as shown in figure 3 (left), indicate cone angles of about 100° for typical preflow conditions.

![Figure 3 Flash-atomization from individual injector element](image)

Although the influence of liquid superheat and pressure drop within the injector has been quantified in many experimental studies, most of the data is not compiled in non-dimensional form. This is partly due to the complex dependency on phase change properties of the fluid and the internal injector design. Consequently, experimental data based on test fluids can not be used for more than qualitative assessment of propellant flash-atomization. However, analyses of sprays with superheat, pressure drop and visual appearance similar to preflow situations indicate that maximum droplet diameters do rarely exceed 100 \(\mu m\) and Sauter mean diameters \(D_{32}\) typically range from 10 \(\mu m\) up to 50 \(\mu m\).\(^{8,7}\)

In the present study, droplet sizes are assumed to follow a Rosin-Rammler distribution.\(^{8,10}\) Lacking any specific information on droplet sizes, three different initial sprays will be considered. The parameters \(D_{63}\) and \(n\) of the Rosin-Rammler distribution are summarized in table 1 together with the corresponding value of \(D_{32}\).

<table>
<thead>
<tr>
<th>(D_{63} [\mu m])</th>
<th>(n [-])</th>
<th>(D_{32} [\mu m])</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>2.4</td>
<td>31.3</td>
</tr>
<tr>
<td>100</td>
<td>2.4</td>
<td>62.4</td>
</tr>
<tr>
<td>150</td>
<td>2.4</td>
<td>91.7</td>
</tr>
</tbody>
</table>

Table 1 Initial droplet size spectra

Figure 3 (right) illustrates the stochastic modelling of the remaining droplet initial conditions. To simulate a solid cone spray, the off-axis angle \(\theta\) is generated from a clipped normal distribution \(N(\mu, \sigma)\) with mean value \(\mu = 0^\circ\), variance \(\sigma = 45^\circ\) and maximum \(\theta_{\text{max}} = 50^\circ\). In this way, droplet density is high on the injector axis and decreases towards the outer region of the spray cone. Droplet velocity and temperature are set to constant values \(v_{d,0} = 20 m/s\) and \(T_{d,0} = 300 K\).

Based on this single injector model, a representative number of injector elements is assembled on the baseplate. A specific configuration is illustrated in figure 4 by visualizing droplet initial positions, sizes and velocities.

![Figure 4 Multipoint flash-atomization from injector matrix](image)

Droplet flash-evaporation

An essential component of the present study is an extension of classical \(D^2\)-theory to flash-evaporation of superheated droplets. The analytical framework is based on the assumption of spherical symmetric, quasisteady transport in the vapour phase. In this ideal case, the heat flux \(Q\) and vapor mass flux \(m_{vap}\) leaving the droplet are independent of the radial distance from the droplet. They are linked by the differential energy balance in the vapour phase and the energy balance of the complete droplet

\[
\dot{Q} = m_{vap} h(T) = 4\pi r^2 \lambda \frac{dT}{dr}, \quad r > r_d, \quad (6)
\]

\[
\dot{Q} = m_{vap} h(T_{d}) - m_{vap} c_{vap} \frac{dT_d}{dt} = \frac{dH_d}{dt}, \quad (7)
\]

where a uniform droplet temperature has been assumed and vapour phase properties noted without index. Classical \(D^2\)-theory applies to a cold droplet in a hot vapour. Since the droplet is first heated up \((dT_d/dt > 0, m_{vap} = 0)\) and then evaporated at constant temperature \((dT_d/dt = 0, m_{vap} > 0)\), equation (6) can be solved by direct integration. For superheat conditions, the droplet surface spontaneously drops to the boiling temperature and evaporation is controlled by droplet internal heat transfer. For low superheat \(\Delta T = T_d - T_{b}\), conduction and convection are the predominant transfer processes. For higher \(\Delta T\), these processes are drastically intensified by generation of vapour bubbles. Due to
the complexity of the phenomena, a description based on
an empirical heat transfer coefficient \( \alpha_s \) is used to quantify
internal heat flux \( \dot{Q}_i \) and associated mass flux contribution
\( \dot{m}_{\text{vap,f}} \)

\[
\dot{Q}_i = 4\pi r_d^2 \alpha_s (T_d - T_b)
\]

\[
\frac{\dot{Q}_i}{\Delta T_b} = \dot{m}_{\text{vap,f}}.
\]

Using this definition equation (6) can be integrated and re-
results in an implicit expression for the total evaporation rate

\[
\dot{m}_{\text{vap}} = 2\pi r_d \text{Nu}^* \frac{\lambda_{\text{ref}}}{c_{p,\text{ref}}} \ln \left[ 1 + \frac{B_T}{1 - \frac{\dot{m}_{\text{vap,f}}}{\dot{m}_{\text{vap}}}} \right],
\]

where the heat transfer number is defined as

\[
B_T = \frac{c_{p,\text{ref}}(T - T_b)}{\Delta h_v}.
\]

Reference values \( \lambda_{\text{ref}} \) and \( c_{p,\text{ref}} \) are evaluated at the tem-
perature \( T_{\text{ref}} = 2/3T_b + 1/3T \) and forced convection in the
vapour phase is taken into account by including the widely
used Frössling correlation

\[
\text{Nu}^* = 2 + 0.552 \text{Re}^{0.5} \text{Pr}^{0.25}.
\]

To quantify the heat transfer within the droplet, Zuo et al. suggest a correlation derived from spray evaporation
measurements in IC engines

\[
\alpha_s = \begin{cases} 760 \Delta T^{0.26}, & 0 \leq \Delta T \leq 5 \, \text{K}, \\ 27 \Delta T^{2.33}, & 5 < \Delta T \leq 25 \, \text{K}, \\ 13800 \Delta T^{0.39}, & 25 < \Delta T. \end{cases}
\]

As indicated in figure 5 the present model further includes
a size-dependent minimum value \( \alpha_{s,\text{min}} = \alpha_s / r_d \) as an or-
der of magnitude estimate for internal heat conduction.
Summarizing this model extension, flash-evaporation of a
droplet is described by the Lagrangian derivatives

\[
\frac{d\dot{m}_d}{dt} = -\dot{m}_{\text{vap}},
\]

\[
\frac{dT_d}{dt} = \left( \dot{m}_{\text{vap}} - 4\pi r_d^2 \alpha_s \right) \frac{T_d - T_b}{\dot{m}_d}.
\]

Detailed computations of single droplets evaporating in a
typical preflow environment have been presented previ-
ously.

**Spray-wall interaction**

Deposition of spray essentially depends on the local wall
temperature. In the modelling framework, a threshold
value of \( T^* = 1.05 \, T_b \) is used to separate the cold wall
mechanisms droplet deposition and splashing (partial de-
position) from the hot wall mechanisms nucleate boiling
and, exceeding the Leidenfrost temperature, reflection of
the droplet. Regarding superheated droplets, spontaneous

\[
\alpha_{s,\text{min}}:
\]

\[
\Delta T [\text{K}]
\]

0 10 20 30 40 50

\[
\alpha_s [\text{K}/(\text{m}^2 \cdot \text{K})]
\]

\[
D_d = 5 \mu m
\]

\[
D_d = 10 \mu m
\]

\[
D_d = 100 \mu m
\]

**Results**

Using the oxidizer Nitrogen Tetroxide (NTO) which is
employed in many spacecraft propulsion applications, the
preflow is computed for the three initial size spectra sum-
marized in table 1. Combustion chamber and expansion
nozzle are discretized by a structured 113 × 30 × 15 grid,
of which only a fraction is illustrated in figure 2. Per
vapour-spray iteration cycle, 70000 trajectories from pri-
mary spray droplets are computed. Depending on the ini-
tial size spectrum, secondary effects can double to triple
this number. To ensure global convergence of the iterative
Euler-Lagrange method, only a fraction of the spray source
terms is updated for the flow solver employing the follow-

-1
0.1
1
10
100
1000
10000
100000
1000000

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ing underrelaxation procedure

$$\overline{S}_j = \alpha S_j + (1-\alpha)\overline{S}_{j-1}, \quad \alpha = 5\%. \quad (16)$$

As illustrated in figure 6 (left) the static pressure in the combustion chamber is nearly constant exhibiting a slight decrease towards the nozzle throat due to the increasing flow velocity. Accordingly, rapid evaporation within a short distance from the baseplate establishes a nearly constant value of the vapour mass fraction in the chamber. Further evaporation can be associated to the steep pressure drop imposed by the accelerating flow. The effect of droplet sizes is reflected in the adaption of the vapour mass fraction to the pressure drop imposed by the accelerating flow. The trend towards local equilibrium is most pronounced for the 50 µm-spray.

The total effect of spray phenomena such as transport, evaporation, secondary effects on the size spectrum is characterized by the evolution of the Sauter mean diameter $D_{32}$ shown in figure 6 (right). Up to the throat, $D_{32}$ exhibits a slightly decreasing trend. Fluctuations are more pronounced for the coarse spray, which, due to the distinct inertia of large droplets and the wide angle atomization characteristics, is more prone to wall-interaction. The fine spray, on the other hand, is rapidly entrained by the vapour flow. Accordingly, wall-interaction and, to a lesser extent, aerodynamic droplet breakup are responsible for the substantial drop of $D_{32}$ in the throat region. Effectively, the nozzle acts on droplet size as a low-pass filter. In this context it is interesting to note, that the pressure level in the chamber appears to be linked to the droplet sizes (and thus evaporation characteristics) in the expanding nozzle flow, which are almost equivalent for the 100 µm and 150 µm-sprays due to the filtering effect.

Contour plots of static temperature are depicted in figure 7. For the fine spray a nearly homogeneous distribution in the chamber is achieved. Despite of the large number of evenly distributed injectors on the baseplate, the flow field generated by the coarse spray is characterized by significant temperature streaks, which indicate delayed evaporation of individual spray plumes. Regions of elevated static temperature occur towards the baseplate. This effect can be attributed to low flow velocities due to delayed vapour formation (see also figure 6, left). Evaluation of the Mach number indicates that the subsonic region of the two-phase

Figure 6 Pressure on centerline and vapour mass fraction (left), Sauter mean diameter on centerline (right)

Figure 7 Vapour temperature and sonic line in a longitudinal section of the 3D flow field
flow can extend significantly far into the divergent part of the nozzle. As illustrated in figure 7, this effect is most pronounced for the fine spray.

Spray deposition on chamber walls is characterized by a bimodal character. As illustrated in figure 8, liquid oxidizer is deposited on the cylindrical part of the liner mainly due to spray impingement from the peripheral row of injector elements. Caused by wide-angle flash-atomization of the injected liquid, this massive spray deposition significantly contrasts the behaviour at nominal operation of the engine. A second region of increased deposition occurs at the converging part of the nozzle. This effect is mainly due to larger spray components which are not able to follow the contracting flow (compare \( D_{32} \) in figure 6, right).

### Table 2 Averaged deposit mass flow density \( \bar{\Sigma}_{m,d} \) [kg/(m\(^2\)s)]

<table>
<thead>
<tr>
<th>( D_{32.0} [\mu m] )</th>
<th>50</th>
<th>100</th>
<th>150</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseplate</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Cylindrical part</td>
<td>13.38</td>
<td>18.00</td>
<td>18.65</td>
</tr>
<tr>
<td>Converging part</td>
<td>18.09</td>
<td>22.79</td>
<td>20.98</td>
</tr>
</tbody>
</table>

The averaged deposit mass flow density on various engine parts is given in Table 2, indicating the dependency on the initial size spectrum. Accumulation on the baseplate could not be assessed in the present study due to the limited resolution of the computational grid which does not allow for capturing of small-scale recirculation zones and hence the possible entrainment and deposition of droplets.

### Conclusions

In contrast to nominal operation of a storable propellant upper-stage rocket engine, the low-pressure oxidizer preflow is characterized by intense phase transfer due to flashing of injected superheated liquid. The presented computational analysis addresses this issue by an empirical description of flash-atomization and a semi-empirical extension of \( D^2 \)-theory to flash-evaporation of individual spray droplets. A consistent implementation of spray source terms ensures numerical stability of the flow solver within the coupled Euler-Lagrange approach. The analysis indicates that pressure and temperature level in the chamber are further controlled by spray-wall interaction including flash-evaporation of wall-deposit. It is demonstrated that the typical wide-angle character from flash-atomization causes massive oxidizer deposition on the cylindrical part of the combustion chamber. Further improvement of the analysis can be expected from detailed research on flashing phenomena and development of physical models.

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### References