



Design study of a rocket-borne free-flow aerosol collector for supersonic speed deployment by means of numerical efficiency analyzes

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Abstract. The ice nuclei on which the cloud particles of mesospheric ice clouds, i.e. noctilucent clouds (NLC), form are largely unknown. Since in-situ measurements within NLC in about 85 km altitude are only possible by using sounding rockets, the careful design of an instrument to be deployed on board of the rocket is crucial. This study investigates the development of an inertia-based particle collector, which allows for sampling NLC particles during a sounding rocket flight for off-line single particle physico-chemical analyzes. Computational fluid dynamics (CFD) simulations support the design and development process in reference to a basic mechanical concept of particle sampling and sample storage, which is also presented here. Numerical studies of the supersonic flow field (Mach numbers 1.31 and 1.75) around the instrument module on the sounding rocket are carried out at different flow velocities (i.e. 300 m s^{-1} and 400 m s^{-1}) and angles of attack (i.e., at $+30^\circ$, 0° and -30°) for optimizing the aerodynamic design, arrangement, and orientation of the particle collectors. Thereby, the localization and extent of the occurring shock wave is investigated and the thickness of the boundary layer around the instrument module is determined to prevent the impairment of the particle sampling. Simulated particle trajectories based on particle radii of 0.6 nm at the lower limit of conceivable particle sizes confirm possible impactions on the collector surfaces. The investigations confirm the effectiveness of the designated particle collectors and render a yet pending rocket flight a valuable option in the investigation on the morphology, chemical composition, size, and number concentration of NLC particles and their nucleating particles.

1 Introduction

As planet Earth moves through a dusty cosmos on its orbit, dust trails are traversed that originate from sublimated comets or from the asteroid belt (Ceplecha et al., 1998; Murad and Williams, 2002), resulting in a continuous mass input of interplanetary material into the atmosphere. Plane (2012) estimates the cosmic mass input to range between 3 and 300 tons per day. Interplan-



etary solids of sufficient sizes ($> 10 \mu\text{m}$), masses ($> 10^{-7} \text{ g}$), and velocities ($> 40 \text{ km s}^{-1}$) (Plane, 2003), which penetrate the Earth's atmosphere most frequently, ablate upon atmospheric entry by reaching boiling temperatures of $> 1800 \text{ K}$, thereby releasing various volatilized meteoric constituents, where the peak altitude of the ablation is about 90 km (Plane, 2012). When they cool down in the atmosphere, the vaporous components rapidly recombine into clusters. The subsequent agglomeration is thought to lead to nanometer-sized meteoric smoke particles (MSP) (Rosinski and Snow, 1961; Hunten et al., 1980; Megner et al., 2006; Saunders et al., 2012; Plane et al., 2015; Wilms et al., 2016; James et al., 2018).

During the northern hemisphere summer months of June and July, when temperatures of $T \approx 140 \text{ K}$ or lower are reached in the mesopause region (Theon et al., 1967; Turco et al., 1982; Lübken, 1999; Rapp and Thomas, 2006; Vincent, 2015), mesospheric ice clouds known as noctilucent clouds (NLC) appear poleward of 65° N (DeLand et al., 2006) at mean altitudes of 82 to 85 km (Turco et al., 1982; Baumgarten and Fiedler, 2008; Hervig et al., 2011), which consist of water ice (Hervig et al., 2001; Eremenko et al., 2005). Due to their presumed presence at this altitude, MSP are considered potential ice nuclei (IN) for NLC particles (Hunten et al., 1980; Rosinski and Snow, 1961; Rapp and Thomas, 2006; Plane et al., 2015; Wilms et al., 2016). Little is known about MSP aside their ascribed importance for the formation of mesospheric ice particles, which, in addition to the comparatively dense and occasionally visible NLC, can also lead to the formation of faint fields of enriched ice crystal numbers. The presence of these ice particle fields and NLC is detectable by means of remote sensing methods (via back-scattered radar signals) expressed as mesospheric echoes as is for instance described by Rapp and Lübken (2004). However, specific properties of MSP would be of particular interest, such as their a) chemical composition (Asmus et al., 2014), b) particle number concentrations or size distribution, and c) shape, surface structure and morphology. Amounts of what were thought to be MSP in the mesosphere have been collected via previous direct sampling experiments (Hemenway et al., 1964a, b; Hedin et al., 2014). Observational evidence (Hervig et al., 2009a, 2012, 2017, 2021) and microphysical information (Hervig et al., 2009b) was obtained by remote sensing. Moreover, laboratory studies of heterogeneous nucleation under mesospheric conditions on potential MSP have been conducted (Duft et al., 2019), but successful collections of NLC particles or associated IN are lacking to date to support the assumption that MSP play the presumed role in NLC formation. This may be due to the challenge of conducting experimental measurements and collections at such altitudes, which are only realizable by means of sounding rockets.

The goal of this study is a proof of concept in the development process of a rocket-borne apparatus to sample NLC particles and embedded IN, which apparently is a topic of current interest as very recent, comparative studies suggest (Pineau et al., 2024). Samples will be analyzed using scanning electron microscopy and energy-dispersive X-ray analyses. These analyses have the potential to provide information on whether MSP are involved in the processes of NLC formation (MSP can be present either alongside NLC particles or embedded in a matrix of cloud particles). They can also provide information on the morphology, size, and the chemical composition of the MSP.

This is to be achieved by a rocket-borne and inertia-based aerosol collector called **Supersonic PartIcle CollEctor (SPICE)**. The work presented here is aimed at the design of such a system, with a focus on sampling optimization and optimum positioning of the SPICE instrument on the measurement platform given the restrictions of a rocket-based design. Supersonic velocities between 300 m s^{-1} and 400 m s^{-1} (at 82 km altitude, i.e. Mach numbers 1.31 and 1.75) are reached during the



55 sounding rocket flight by the so-called High Atmosphere Soarer (HAS) (Naumann et al., 2020). The HAS is characterized by its ability to perform a "hovering" flight pattern, which flattens the ballistic flight trajectory and increases the residence time of the instrument carrier in the target region. This in turn favors the scientific measurements at the altitude of 85 km (+/- 5 km) because in this way the sampling time in the NLC region is extended (where the presence of mesospheric ice particles during the rocket flight is ensured via back scattered radar signals), as is the horizontal flight distance therein. Moreover, during the flight, the HAS is stabilized against rolling, i.e. the rotation around its longitudinal axis. Due to the unique mesospheric conditions and the expected radius of the NLC particles smaller than 100 nm (Thomas, 1991; Lübken, 2005; Baumgarten and Fiedler, 2008) and of the MSP smaller than 3 nm (Horányi et al., 1999; Strelnikova et al., 2007; Rapp et al., 2010, 2012; Hedin et al., 2014; Asmus et al., 2014), one focus of this study is the sampling properties of such a system. Given the inability to carry out test flights numerical simulations are required to assess these properties. In this study, we present details of the instrument design and numerical simulations of the air stream around the instrument module including aerosol impactions. In particular, the effect of different angles of attack achieved during the hovering measurement flight of the HAS is considered.

2 Instrument Design

The SPICE instrument, in general, is a system, which works as a body impactor, i.e. it uses the flight speed and the particles' inertia to deposit them onto sampling substrates, which are exposed to the free air stream around the rocket. Figure 1 illustrates the geometry of the instrument module (see also Figure 2) with the developed design and arrangement of the SPICE instrument. The m-NLP (multi Needle Langmuir Probe) sensors and the three SPICE booms are offset from each other. The SPICE-booms, which are mechanically extended by means of a fully autonomous control system for the particle collection, are equipped with hexagonal prisms at their tips. Two transmission electron microscopy (TEM) grids each are embedded as substrates on the side panels of the prisms (substrate mounts). In this way, up to a total of 36 samples can be collected per flight at different exposure direction with respect to the outside air flow, resulting in varying collection efficiencies. After sampling and when leaving the target region, the SPICE-booms are retracted and the substrate mounts are sealed as a whole to prevent contamination of the sample during onward flight, landing or transportation to the laboratory. In addition, a same-sized gold foil is placed as backing underneath each TEM grids, for the case that the thin foil covering the TEM grids is penetrated due to a particle's kinetic energy. In this case, a remnant of this particle may be found on the gold foil, which would otherwise be lost for analysis. The small size (and inertia) of NLC particles and particularly the MSP requires a customized aerodynamic design of the impaction surfaces, hereafter denoted as substrates. The design of the substrate mounts as hexagonal prisms offers the following advantages: 1) Nanometer-sized particles very well follow streamlines up to flow velocities close to sonic speed. Due to the non-aerodynamic design, the frontal surface of the hexagonal prisms perpendicular to the direction of flow causes an abrupt deflection of the streamlines. As a result, the particle trajectories deviate from the streamlines due to the particle inertia and enable an inertia-related deposition of the particles on the substrates. 2) The other surfaces of the hexagonal substrate mounts are inclined to the main flow direction. On the one hand, this allows particles that slide off the front surface to be deposited from the decelerated airflow; on the other hand, these side surfaces become the frontal impact surface if the rocket yaws during flight. 3) The



circumferential assembly of substrates at each side of the hexagonal substrate mounts ensures sampling both within the frontal flow and in the flow shadow if, e.g., refluxes occur on the rear of the substrate mounts may lead to further particle deposition. 4)

90 The design facilitates the handling during assembly and disassembly of the TEM grids on the six sides of the substrate mount. The limited space in the SPICE compartment restricts the number of SPICE-booms to three, each of which is aligned at an angle of 120° to each other along the half-cut lines. In this way, the aerosol sampling is carried out simultaneously by three collectors.

Since the flight attitude of the High Atmosphere Soarer (cf. Figure 2) varies, the multiple sampling in different spatial
95 directions makes the sampling less dependent on the rocket's flight attitude. In this way, as confirmed later in numerical simulations, at least two of the SPICE-booms are likely exposed to a direct flow at any angle of attack relative to the zero attitude. Moreover, redundant SPICE-booms favor the success of the sampling, as the partial or complete failure of a single collector can be largely compensated for.

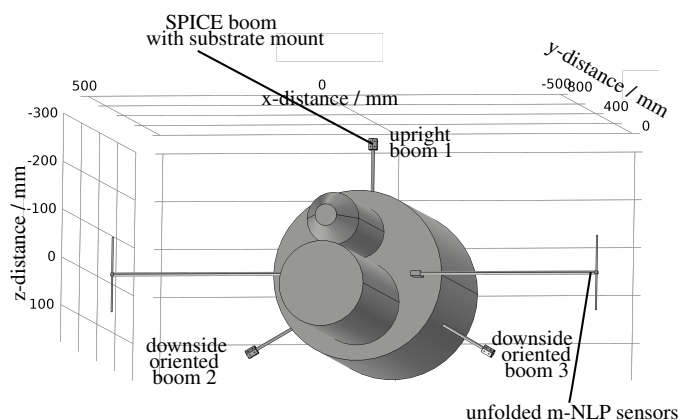


Figure 1. Geometry of the instrument module in a frontal view. The arrangement of the three SPICE booms carrying the substrate mounts (hexagonal prisms) at their tips are depicted, offset from the m-NLP sensors. The diameter of the hexagonal prisms is 20 mm with a height of 23 mm (Klug, 2024b).

3 Numerical simulation

100 At supersonic flow conditions, the aerodynamics around the rocket's instrument module were numerically investigated concerning: a) the shock wave evolving upstream of the module (at Mach numbers 1.31 and 1.75 under conditions at 82 km altitude), b) the thickness of the boundary layer at the position of the SPICE instrument to enable the particle collection ideally in the free flow and c) the optimization of arrangement, orientation, and design of the SPICE booms for the best possible particle collection efficiency. The aim is to ensure a sampling largely unaffected by the shock waves and also well outside the
105 boundary layer. This prevents flow disturbances (e.g. downwash or flow disturbances on upstream geometries or structures) from affecting the particle collection.



After completion of the numerical simulations of the flow field, this data is employed to compute the trajectories of particles of relevant sizes in the near-field of the substrate mounts. Of all the relevant particle forces (i.e. Stokes' drag force, Brownian force, gravitational force, Saffman force, pressure gradient force and additional mass force), the Stokes' and Brownian forces were considered to have non-negligible effect on the motion of the MSP (cf. Hedin et al. (2007a)), based on a preliminary study of force magnitudes. The calculated particle trajectories provide insight into whether and to what efficiency a particle collection occurs on the substrates, which also serves as proof of concept. Thereby, different particle number concentrations (from 1 cm^{-3} to 38 cm^{-3} , cf. Table 4) and different angles of attack (i.e., $+30^\circ$, 0° and -30°) were considered.

3.1 Supersonic flow modeling and simulations

The nature of the fluid dynamics during rocket-borne measurements at 82 km altitude is associated with the dimensionless Knudsen number $Kn = \lambda/L$ using the mean free path length $\lambda = 2.22 \cdot 10^{-3} \text{ m}^1$ of molecules in the atmosphere (Klug, 2024b). Together with the characteristic length $L = 0.02 \text{ m}$ for the diameter of the substrate mounts, $Kn \approx 0.1$ was obtained as relevant for an altitude of 82 km. Analogously to Dongari and Agrawal (2012), who investigated the application of classical Navier-Stokes equations (i.e., a continuum model) with conventional slip boundary conditions up to Knudsen numbers of < 10 (i.e., up to the transitional flow regime) and who found a good conformity with simulation outputs of Boltzmann equations and Direct Simulation Monte Carlo (DSMC) methods, the flow regime is regarded as continuum flow. The advantage of using the Navier-Stokes equations for the anticipated analyses lies in the availability of more advanced and mature simulation tools and a higher computation efficiency when compared to those developed on a molecular-base approach for equations like the Boltzmann equation (Dongari and Agrawal, 2012; Hadjiconstantinou, 2003). In general, a fine resolution of the mesh was achieved by an unstructured three-dimensional computational grid with mesh sizes equal to 0.5 times the mean free path. Regarding the Knudsen number of 0.1, which approximately scales the lower bound of the transition between the continuum and transitional flow regime, uncertainties arise when applying classical Navier-Stokes equations. For instance, Nourazar et al. (2005) quantified uncertainties compared to the Boltzmann equation, estimating 0.3% uncertainty in temperature, 25.03% in pressure, and 28.57% in air's mass density. The extent, to which these uncertainties quantitatively affect the simulation results presented here, ultimately remains open until an actual rocket-based sample is carried out with the SPICE instrument. It should be noted that the macroscopic modeling approach provides valid results for a flow assumed to be a continuum, which can be compared with the results based on transitional flow regime modeling to validate the uncertainties in the ambient flow conditions in the considered mesospheric altitude. Beyond the scope of this study, however, there is a strong increase in the Knudsen number with further increasing altitude and thus the shift to the transitional flow regime up to the free molecular flow needs to be considered. Since Mach numbers are $Ma > 1.3$, compressible time-dependent Navier-Stokes equations were solved. Numerical studies of the flow fields were performed, starting from zero velocity and developing until the final steady-state solution was reached. The virtual instrument setup was considered stationary and subjected to the air flow with velocities corresponding to the speed of the real HAS-flight through the mesospheric target region. The fluid flow simulations are consistently done in COMSOL Multiphysics® utilizing the High Mach Number Continuous Flow Module for laminar flows. Assuming a laminar

¹Calculated analogously to Willeke (1976), with $T = 130 \text{ K}$ and $p = 10^{-3} \text{ kPa}$.



140 flow is justified due to a low Reynolds number $Re = \frac{\rho_f |\mathbf{u}| L}{\mu_f} \approx 24$, where $|\mathbf{u}| = 400 \text{ m s}^{-1}$ is the typical velocity of the rocket, $L = 0.02 \text{ m}$ the characteristic length of the SPICE instrument, ρ_f is air's mass density, and μ_f the dynamic viscosity of air, see Table 2.

The system of Navier-Stokes equations for compressible fluids were solved,

$$\frac{\partial(\rho_f)}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}) = 0, \quad (1)$$

$$145 \quad \frac{\partial(\rho_f \mathbf{u})}{\partial t} + \nabla \cdot (\rho_f \mathbf{u} \mathbf{u}^T) = \nabla \cdot \sigma, \quad (2)$$

$$\frac{\partial}{\partial t} (\rho_f E) + \nabla \cdot (\rho_f \mathbf{u} E) = -\nabla \cdot (-k \nabla T) + \nabla \cdot (\sigma \mathbf{u}), \quad (3)$$

$$e = c_v T, \quad E = e + \frac{|\mathbf{u}|^2}{2}, \quad (4)$$

$$\rho_f = \frac{p}{R_s T}, \quad (5)$$

with the Cauchy stress tensor $\sigma = -p\mathbf{I} + \mu_f (\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I})$, air's mass density ρ_f , the fluid velocity $\mathbf{u}$, the identity matrix $\mathbf{I}$, the dynamic viscosity μ_f , the total energy E , the internal energy e , the thermal conductivity k , the specific heat capacity c_v (note that c_v is a temperature dependent variable, but is assumed here as constant. This gives an error of less than $\pm 1.1\%$ (Baumgartner et al., 2020) and is therefore negligible in terms of a linear coefficient in equation 4), and the specific gas constant R_s . Atmospheric parameters in the polar summer mesosphere, such as the mean value of temperature with local variability of $T = 130 \pm 15 \text{ K}$ (Philbrick et al., 1984; Lübken, 1999; Rapp and Thomas, 2006), or the gravitational constant of $g = 9.6 \text{ m s}^{-2}$, the static pressure at 82 km altitude of $p = 10^{-2} \text{ hPa}$ (Rapp and Thomas, 2006) were set together with the flow velocity magnitude of $u_{min} = 300 \text{ m s}^{-1}$ and $u_{max} = 400 \text{ m s}^{-1}$. The air's thermal conductivity k and the dynamic viscosity μ were calculated with Sutherland's law (Sutherland, 1893; White and Majdalani, 2006):

$$k = k_{ref} \left(\frac{T}{T_{ref}} \right)^{\frac{3}{2}} \frac{T_{ref} + S_k}{T + S_k}, \quad (6)$$

and

$$160 \quad \mu_f = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{\frac{3}{2}} \frac{T_{ref} + S_\mu}{T + S_\mu}, \quad (7)$$

where reference values of $k_{ref} = 0.0241 \text{ W (mK)}^{-1}$, $T_{ref} = 273 \text{ K}$, the Sutherland constant $S_k = 194 \text{ K}$, $\mu_{ref} = 1.714 \cdot 10^{-5} \text{ N s m}^{-2}$, $S_\mu = 111 \text{ K}$ were substituted in the equations. For the simulation setup, the geometry of the scientific payload with the unfolded m-NLP sensors (denoted as instrument module, see Figure 2) was included into the model and was located at the center of the simulation domain in which the flow field and particle simulations were conducted.

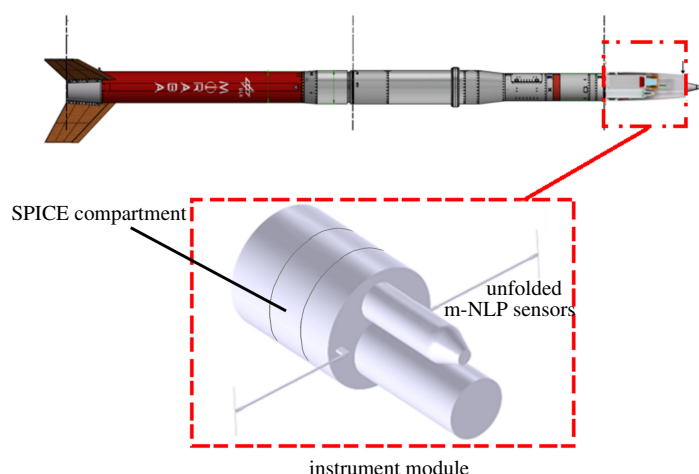


Figure 2. High Atmosphere Soarer (HAS) (Naumann et al., 2020) and geometry of the instrument module with simplified modelled structures of the measuring instruments mounted in a bay covered by the rocket's nose cone (based on Naumann et al., 2020), which is released prior to the experimental flight section by ejection of the cone cover. The rocket compartment which houses the SPICE instrument is referred to as the SPICE compartment (Klug et al., 2023).

165 The cuboid region was chosen large enough to avoid any influence of boundary conditions on the flow pattern around
the instrument module, using a hybrid boundary condition that controls the fluid stresses and applies to both subsonic and
supersonic flow conditions at the flow outlets (see Klug et al. (2023)). Geometrical structures downstream of the SPICE
compartment (cf. Figure 2) were not considered since our investigations focused exclusively on the effects resulting from
upstream assemblies on the fluid streamlines such as the unfolded m-NLP sensors and on the flow patterns in the immediate
170 vicinity of the SPICE compartment.

3.2 Particle tracking modeling and simulations

In the following, simulations of trajectories of particles in the relevant size range and mass of NLC particles and MSP and
their impaction on the substrate mounts under ambient conditions at 82 km in a supersonic flow regime are conducted. For
investigating the effectiveness and efficiency of the sample mechanism, only a short excerpt of the experimental flight segment
175 (with a duration of 0.021 s) is considered in view of the numerical effort. Due to the low particle volume fraction of NLC
particles and MSP (Elghobashi, 1994), it seems justified to consider a one-way coupling between the fluid and the particles,
hence, their influence on the ambient air is neglected. Consequently, the fluid flow and the particle motion are numerically
calculated in two separate but coupled simulation runs (COMSOL®, 2017): initially calculated flow variables are required
in the time-dependent study at the particles' positions to determine the particles' new positions and velocities in the next
180 time step. In this way, each particle can be traced, which is referred to as the one-sided Euler-Lagrangian coupling or the
Lagrangian point-particle method (Hryb et al., 2009; Gimenez et al., 2012). The corresponding equation of particle motion
is based on second Newton's law of motion and accounts for all relevant forces acting on the particles. For the examination



of force magnitudes, a distinction is made between larger NLC particles and possible ice nuclei (MSP). NLC particles are assumed as spherical ice cloud particles with a mass density of $\rho_{NLC} = 1 \text{ g cm}^{-3}$ and radius of $\leq 100 \text{ nm}$ (Rapp and Lübken, 2004; Lübken, 2005; Rapp and Thomas, 2006; Baumgarten and Fiedler, 2008; Hervig et al., 2009a)). The particle number concentration (PNC) of NLC particles is highly variable, where estimations are summarized in the left column of Table 1.

PNC of NLC / cm^{-3}	Radius of MSP / nm
29 – 133 (Baumgarten and Fiedler, 2008)	0.8 – 1.0 (Strelnikova et al., 2007)
46 – 105 (Baumgarten et al., 2008)	0.5 – 3 (Rapp et al., 2012)
23 – 1078, mean of 82 (Von Cossart et al., 1999)	0.8 – 1.4 (Horányi et al., 1999)
2 – 2668, median value 104 (Hervig et al., 2009b)	1 – 2 (Rapp and Thomas, 2006)
3 – 5342, median value 170 (Hervig et al., 2009b)	0.1 – 3 (Asmus et al., 2014)

Table 1. Particle number concentrations (PNC) of NLC particles and assumed radii of MSP.

Moreover, the right column of Table 1 depicts the assumed radii of MSP found in literature. Analogously to the investigations of Hedin et al. (2014), a MSP radius of 0.6 nm was applied in our simulations.

The nucleating particles as assumed MSP are considered with a mass density of $\rho_{MSP} = 2\text{--}3 \text{ g cm}^{-3}$ (Hedin et al., 2007b), or with $\rho_{MSP} = 2.8 \text{ g cm}^{-3}$ (Plane, 2012). To determine the relevant particle forces for the equation of particle motion, the necessary parameters of fluid and particles are summarized in Table 2. Table 3 reveals the influence of acting forces on the particle motion, the force magnitudes are evaluated based on parameters presented in Table 2. Here $\mathbf{L}_f = \mathbf{u}_r \times [\nabla \times \mathbf{u}_r]$, and $c_{am} = 0.5$ is the added mass coefficient for spherical particles (Brennen, 1982; Crowe et al., 2012; Kuerten, 2016). For the application of Brownian force a dimensionless 3D-vector $\zeta \sim \mathcal{N}(0,1)$ of independent and normally distributed random numbers, generated in each time step and for each particle is necessary. The general relevance of the Stokes' drag force and the force inherent with Brownian molecular motion for nanometer-sized particles, is shown in Table 3. Both forces are more than four orders of magnitude larger than the remaining forces potentially acting on the particles, hence only these two are included in the simulations.

To argue the application of Stokes' drag force, the particle Knudsen number is considered with $Kn_p = 2\lambda d_{NLC}^{-1} = 4.4 \cdot 10^4$, while for the mean free path the length of $2.22 \cdot 10^{-3} \text{ m}$ is applied, which results in $Kn > 1$, where the particles are assumed to be in a slip flow regime.



parameters	values	comments
ambient conditions		
μ_f	$8.99847 \cdot 10^{-6} \text{ Pa s}$	Dynamic viscosity of air at 82 km.
ρ_f	$2.6798 \cdot 10^{-5} \text{ kg m}^{-3}$	Fluid (air) density at 82 km altitude.
m_f	$2.43 \cdot 10^{-32} \text{ kg}$	Mass of fluid, displaced by a particle of $r_p = 0.6 \cdot 10^{-9} \text{ m}$.
$\frac{\partial u}{\partial y}$	650 s^{-1}	Change in velocity, estimated from fluid dynamics simulations.
$\frac{d(\mathbf{u}_f - \mathbf{v}_p)}{dt}$	$1 \cdot 10^7 \text{ m s}^{-2}$	Maximum relative particle acceleration (for $ \mathbf{u}_f = 300 \text{ m s}^{-1}$).
∇p	1.05 Pa m^{-1}	Pressure gradient (from fluid dynamics simulations).
k_B	$1.381 \cdot 10^{-23} \text{ J K}^{-1}$	Boltzmann constant.
g	9.5 m s^{-2}	Gravitational acceleration coefficient at 82 km.
particle properties		
$\mathbf{u}_r$	120 m s^{-1}	Maximum relative particle velocity (for $ \mathbf{u}_f = 300 \text{ m s}^{-1}$).
r_{NLC}	$100 \cdot 10^{-9} \text{ m}$ (Rapp and Thomas, 2006)	Max. radius of a single NLC particle.
ρ_{NLC}	1000 kg m^{-3}	Density of a NLC particle.
r_{MSP}	$0.6 \cdot 10^{-9} \text{ m}$ (Hedin et al., 2014)	Radius of a single MSP (ice nuclei).
ρ_{MSP}	3000 kg m^{-3} (Hedin et al., 2007b)	Density of a MSP.
m_{MSP}	$2.7 \cdot 10^{-24} \text{ kg}$	Mass of a single particle for $r_p = 0.6 \cdot 10^{-9} \text{ m}$ and $\rho = 3 \text{ g cm}^{-3}$.
C_c	$7.357 \cdot 10^4$	Cunningham slip corrector for particles with $r_p = 0.6 \cdot 10^{-9} \text{ m}$.

Table 2. Parameters for the simulated flow field and of the particles necessary for the evaluation of particle forces and their magnitudes (Klug, 2024b).



forces	mathematical expressions	estimated magnitude of forces / N
Brownian force	$\mathbf{F}_{Brown} = \zeta \sqrt{\frac{12 \pi \mu_f k_B T r_p}{\Delta t C_c}}$	$\sim 10^{-18}$
Stokes' drag force	$\mathbf{F}_D = 6 \pi \mu_f r_p \mathbf{u}_r C_c^{-1}$	$\sim 10^{-18}$
Saffman force	$\mathbf{F}_S = 1.615 (2r_p)^2 \mathbf{L}_f \sqrt{\rho_f \mu_f \frac{1}{ \nabla \times \mathbf{u}_r }}$	$\sim 10^{-22}$
gravitational force	$\mathbf{F}_{G,tot} = m_p \frac{\rho_p - \rho_f}{\rho_p} \mathbf{g}$	$\sim 10^{-23}$
added mass force	$\mathbf{F}_{am} = m_f c_{am} \frac{d(\mathbf{u}_f - \mathbf{v}_p)}{dt}$	$\sim 10^{-25}$
pressure gradient force	$\mathbf{F}_p = -\frac{m_p}{\rho_p} \nabla p$	$\sim 10^{-28}$

Table 3. Estimated magnitude of the forces acting on the particles. Forces highlighted in gray are excluded from the particle simulations due to their negligible impact on the particle trajectories, compared to forces associated with Brownian motion or Stokes' drag with larger order of magnitude, which therefore remain considered in the computations (Klug, 2024b).

Therefore, the Cunningham slip corrector $C_c = 1 + Kn_p[\alpha + \beta \exp(-\gamma Kn_p^{-1})]$ is taken into account in the drag force (Knudsen and Weber, 1911; Millikan, 1923; Kulkarni et al., 2011). In the literature (not significantly) different values for the dimensionless constants can be found, here $\alpha = 2.514$, $\beta = 0.8$, and $\gamma = 0.55$ were used according to Davies (1945); COMSOL® (2020).

After taking all relevant forces into account, the following equation of particle motion results:

$$m_p \frac{d^2 \mathbf{x}}{dt^2} = \zeta \sqrt{\frac{12 \pi \mu_f k_B T r_p}{\Delta t C_c}} + \frac{6 \pi \mu_f r_p \mathbf{u}_r}{C_c}, \quad (8)$$

where $\mathbf{x}$ is the position vector, and m_p and r_p denote the mass and the radius of a particle, respectively. Particle number concentrations of 1 to 38 cm^{-3} , which represents the lower limit of estimated number concentrations of NLC particles of 2 to 5342 cm^{-3} (Hervig et al., 2009b), were applied in a parametric numerical study for particle motion. By deliberately considering the lower limit of the estimated particle number concentrations in the simulations, our investigation represents a sensitivity study (i.e., if a low particle concentration proves to be effective, it will still be effective at a possibly higher concentration). The assumption of higher concentrations, and consequently higher particle impaction rates, would unnecessarily increase the computational effort required to prove the effectiveness of our particle collection concept. Moreover, lower particle number concentrations than 1 cm^{-3} , however, are not considered in our study, since in this case the statistical effects on deposition numbers are of increased dominance, which could distort the results. In the simulations, the total particle numbers to be released into the computational domain volume were chosen within the limits of $1.8 \cdot 10^4 - 6.3 \cdot 10^5$ particles (cf. Table 4).



particle numbers	PNC / cm^{-3}
18 802	1
186 370	11
280 060	17
411 180	25
633 375	38

Table 4. Chosen total particle numbers as input for different simulation runs with respective particle number concentrations (PNC) (Klug, 2024b).

The aim of the SPICE application is to collect NLC particles - if present - as their collection is promising compared to aiming at direct collections of the significantly more mobile MSP due to the cloud elements' size and associated larger inertia (compared to those of MSP). The collection is therefore indirect with respect to MSP, but at the same time offers the possibility to attribute most impaction events (those showing visible traces of ice residues on the substrate surface) to the nuclei previously embedded in this ice - i.e. to obtain direct evidence for the ice nucleation capability of MSP (if found upon probe analysis). For this reason, a certain range of possible NLC particle number concentrations was assumed (see Table 4), corresponding to the listed particle numbers used in the simulations. However, as described in Appendix A, the NLC particles, which presumably contain the MSP, exist under unstable conditions. When approaching the substrates, the particles pass through regions of strong temperature gradients (due to the air compression in the resulting shock wave), which can lead to an abrupt subsaturation of the ambient air and thus, as shown in Appendix A, to sudden complete or partial sublimation of NLC particles. As a consequence, immediately prior to impaction, only the desired ice nucleus (i.e. one or more MSP) would be available for collection in extreme cases. Therefore, in the sense of a sensitivity study, we assume constant small particle sizes, i.e. those of the MSP with a radius of 0.6 nm, which corresponds to the lowermost limit in the range of possible MSP radii. Any as success simulated particle impaction under this assumption of extremely small particle sizes and lower limits of particle inertia allows for the unreserved conclusion that fortiori any larger particle with higher inertia will be deposited on the substrate, while smaller particles will essentially be guided around the sampler by the perturbed aerodynamics.

The presented results of particle trajectory simulations are based on fluid flow simulations with the ambient air velocity magnitude of 400 m s^{-1} and with the HAS flight attitude of 0° , and $\pm 30^\circ$. For the simulation process, the three-dimensional spatial particle distribution is projected onto the inlet plane to allow efficient time stepping of simultaneously released particles. Particles in the above defined amounts (cf. Table 4) enter the domain with their terminal velocities as planar slices with randomly distributed particle positions. Furthermore, the positions of particle entry into the domain are restricted to specific bounded areas in such a way that particle impactions can be ensured. The optimum position of the entry have been determined based on backward trajectories of impacting particles. The restriction of the bounded areas leads to a reduction in the computational effort as no integration of trajectories is performed for particles that do not reach the vicinity of the particle collectors. The simulated particle entry is defined in a distance of 0.34 m upstream of the substrate mounts as illustrated in Figure 3a (blue



markers). The selected areas of particle entry ensure that each substrate mount is entirely enveloped by the particle-loaded flow, as depicted in Figure 3b.

245 The overall performance of the substrate mount is expressed by the collection efficiency η , which is defined as

$$\eta = \frac{C_{\text{impacted}}/A_{\text{impacted}}}{C_{\text{released}}/A_{\text{released}}} \quad (9)$$

where C_{impacted} is the number of impacted particles, C_{released} is the number of released particles (cf. Table 4) and which relates to A_{released} , the total surface area through which the particles enter the domain depicted in Figure 3a as circular areas in blue, and A_{impacted} is the rectangular cross-section area of a substrate mount.

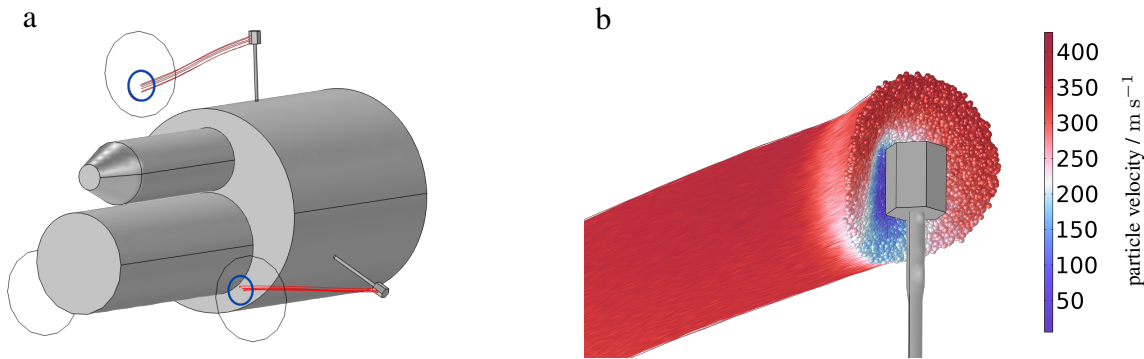


Figure 3. a: Position of the particle entry into the domain upstream of the instrument module highlighted by blue circles (Klug, 2024b), b: Simulated trajectories of an ensemble of 9401 released particles in the snapshot shortly prior to enveloping a substrate mount.

250 4 Results and Conclusions

4.1 Flow simulations

The fluid flow simulations were conducted in a rectangular computational domain with the length of 3.3 m, height of 2 m and dept of 2 m, with the instrument module embedded as an obstacle (cf. Figure 4). The computational mesh consists of up to 3.75 million tetrahedral and pyramidal elements including eight layers of boundary elements (around the vehicle fuselage) consisting of hexahedral and prismatic elements. The P1-P2 finite element method implemented in COMSOL was chosen for the spatial discretization, using streamline and crosswind diffusion as stabilization for convection-dominated regimes (Brooks and Hughes, 1982; Hughes and Mallet, 1986; Johnson et al., 1987; Semper, 1994; Hauke and Hughes, 1994; John and Schmeyer, 2009; Bayramov and Kraus, 2015). For the temporal discretization the BDF Method was applied (Hairer et al., 2000). Figure 4a shows the computational mesh elements, where smaller mesh elements (with smallest sizes of $1.15 \cdot 10^{-3}$ m) were generated in regions where strong gradients of the flow velocity occur. Larger element sizes of up to 0.1 m are represented in the far field. Eight layers of boundary elements (mesh elements around the vehicle fuselage) turned out a sufficiently high resolution to visualize the relevant viscosity-induced flow development of the boundary layer.

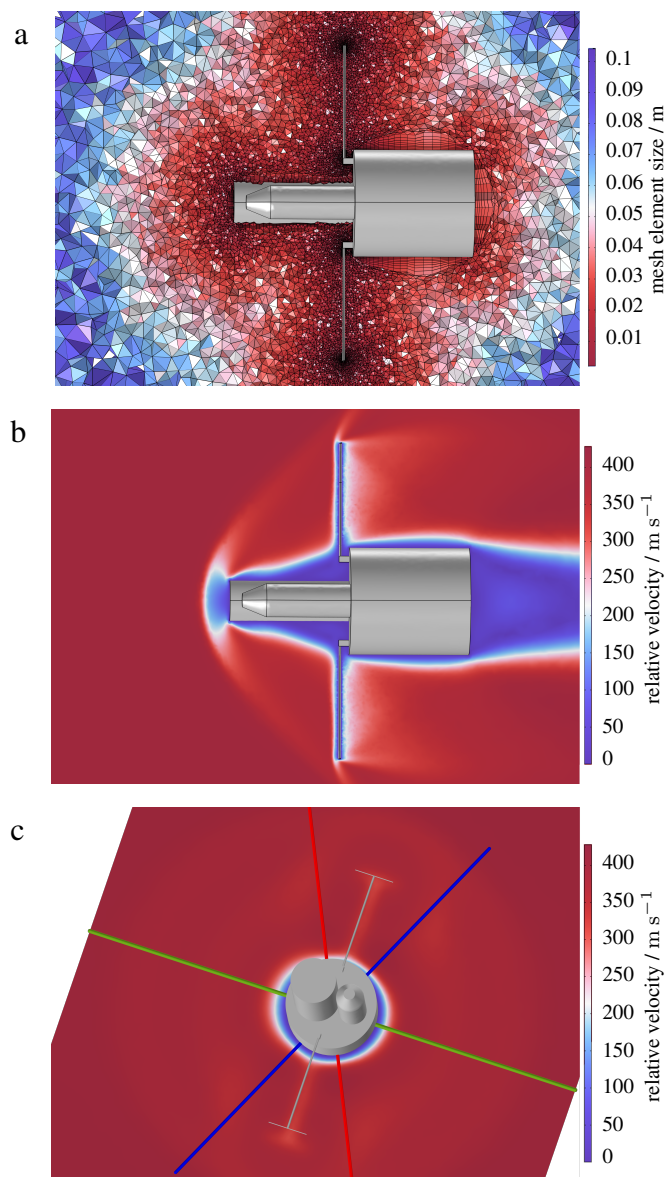


Figure 4. Panel a: Computational mesh for fluid flow simulations around the instrument module. The mesh sizes are refined in the vicinity of the flow obstacle, and boundary layer elements were generated at the instrument module hull. Panel b: The stationary flow field around the instrument module with the bow shock at the instrument module tip for the incident velocity of 400 m s^{-1} is depicted on a longitudinal cut plane. The simulated air flow originates on the left side of the image with the flow direction towards the right. Panel c: Velocity field depicted on a cross-section in the plane of the SPICE instrument. The colored lines mark potential orientations of the SPICE instrument booms.

Figure 4b illustrates the simulated flow field around the instrument module at the flow velocity of 400 m s^{-1} and depicts the bow shock evolved upstream of the instrument module's tip, which interferes with further shock waves caused by the tips of the m-NLP sensor. Downstream of the m-NLP, the disturbance of the flow field is pronounced (slowed velocities),



however, the influence of the m-NLP is limited to the slipstream of the sensors as illustrated in Figure 4c. Further flow field analyses downstream of the instrument module are not covered here, as we focused exclusively on the effect of the SPICE compartment's fore-build structures. With regard to the alignment of the potential SPICE booms positioned downstream of the m-NLP sensors, an alignment in the slipstream of the sensors was to be avoided. Possible orientations for the SPICE booms unaffected by any flow disturbance caused by the m-NLP sensors are shown in Figures 4c and 5, where three cut lines 1 (blue), 2 (green), and 3 (red) are illustrated. Along these cut lines, the flow velocities in the flow region adjacent to the module surface were analyzed. The results are depicted in Figure 6 for the incident flow velocity of 300 m s^{-1} in panel a and for 400 m s^{-1} in panel b. The zero point denotes the starting point of the cut lines on the rocket module surface, the positive values on the x-axis indicate distances of the cut line points to the surface point, the negative x-values represent distances to the counterpart surface point traveling the cut lines in the opposite direction. Crosshair symbols indicate the mesh nodes, at which the flow velocities were computed.

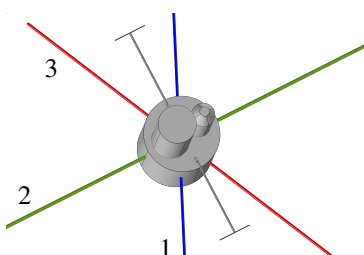


Figure 5. Representation of the instrument module. Three cut lines 1 in blue, 2 in green and 3 in red are shown along which the velocity values are analyzed.

The outermost edge of the flow region adjacent to the module surface is recognizable. Figure 6a shows maximum flow velocities along cut lines 1 and 3 (these run through regions with comparatively high flow velocities), which are up to 25 m s^{-1} higher than values along cut line 2. Since the focus is on the region in the immediate vicinity around the instrument module, the extent of the diagrams is limited to a range in which the free flow velocities have not yet been reached. Certain conclusions can be drawn from the comparison of the various results:

- The deviant pattern in Figure 6b compared to Figure 6a at velocities of 400 m s^{-1} can be explained by the Mach cone represented in Figure 4b, which is narrower at higher incident velocities.
- Noticeably, velocity values along cut line 2 compared to 1 and 3 deviates by some extent, which can be explained by the course of the cut lines through the simulation geometry: for cut lines 1 and 3, the geometry of the instrumentation in the upstream instrument module is almost symmetrical to the zero point, whereas it is asymmetrical for cut line 2.
- Concerning the boundary layer thickness: the maximum flow velocities for the 400 m s^{-1} incident velocity simulation are reached at slightly lower distance from the fuselage compared to the 300 m s^{-1} - simulation (i.e., at higher incident velocities the boundary layer is thinner).



290 – No measurable influence on the flow pattern due to the expansion of the m-NLP sensors is observed at the selected cut
line positions.

In conclusion, it seemed reasonable to position the SPICE booms according to the cut line orientation. To ensure an efficient
particle sampling in the largely undisturbed free flow around the rocket's body, the length of the SPICE booms was set at more
than 120 mm. This specification is subject to a compromise between the shortest boom length (due to limited space in the
295 instrument module), the highest mechanical stability (against vibrations, dynamic pressure and lateral accelerations) and the
exceeding of the flow region adjacent to the module surface.

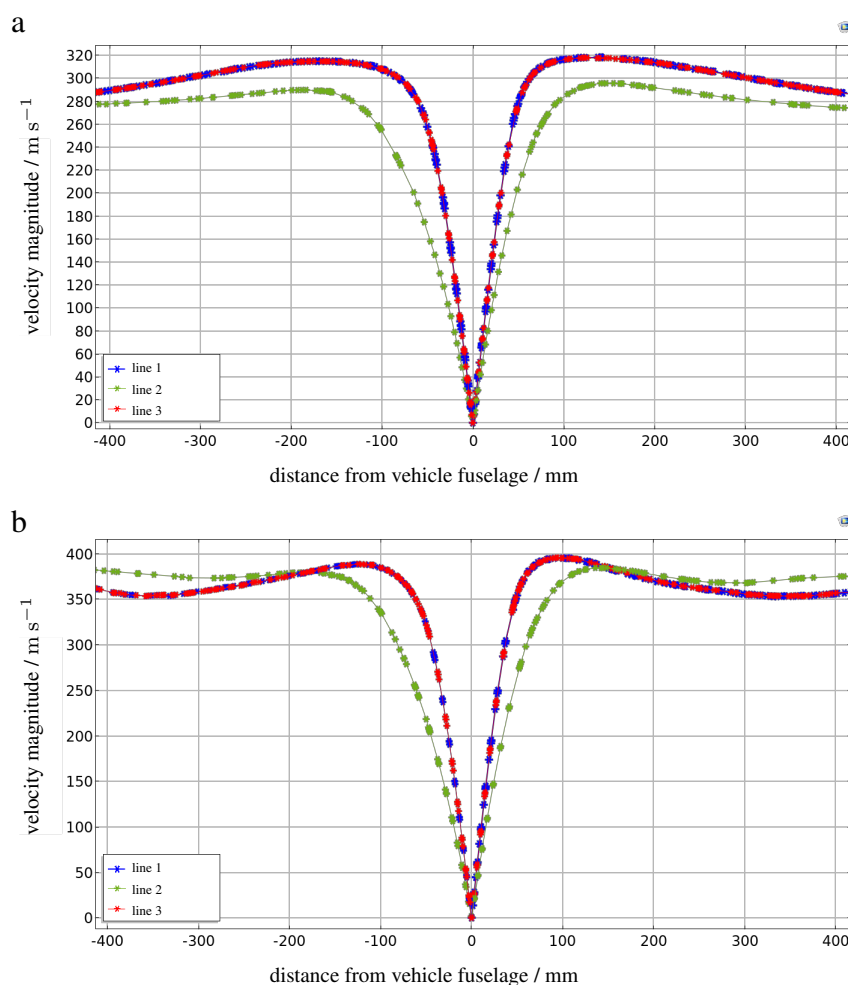


Figure 6. Panel a: Flow velocity as a function of distance to the rocket's fuselage surface (0 mm) at incident flow velocities of 300 m s⁻¹ (Klug, 2024b) and panel b: 400 m s⁻¹ (Klug et al., 2023) evaluated along cut lines 1 (blue), 2 (green), and 3 (red). Crosshair symbols indicate data points at analyzed mesh nodes of the simulation.



4.1.1 Sensitivity tests

Subsequent simulations focused on the flow profile around the instrument module under varying angles of attack of the HAS during the experimental flight section. Thereby, the extremes in the range of possible angles of attack are $\pm 30^\circ$, and the horizontal position of 0° were considered. First, it was investigated whether the substrate mounts remain unaffected by the surface adjacent flow region of the instrument module on different angles of attack. In the following simulations the m-NLP sensors were not considered for simplification, as the neglect of these structures saved computational costs (the m-NLP had no measurable influence on the flow profile at the SPICE boom positions, see Section 3.1). A mesh of 3.75 million elements was used and is shown in Figure 7, where the mesh resolution around the instrument module was enhanced, especially in the vicinity of the substrate mounts the mesh was refined with particular focus on their wake region to resolve the flow patterns there with high accuracy. Again, eight levels of boundary layer elements yielded an adequate resolution of the surface adjacent layer. The minimum size of a boundary layer element was $1.15 \cdot 10^{-3}$ m. For a 0° flight attitude of the HAS, Figure 8a depicts the velocity magnitude on a cross-sectional cut plane at the level of the SPICE booms, whereas panel b shows the flow velocity on a cut plane aligned along the longitudinal axis of the instrument module, both for the incident flow velocity of 400 m s^{-1} .

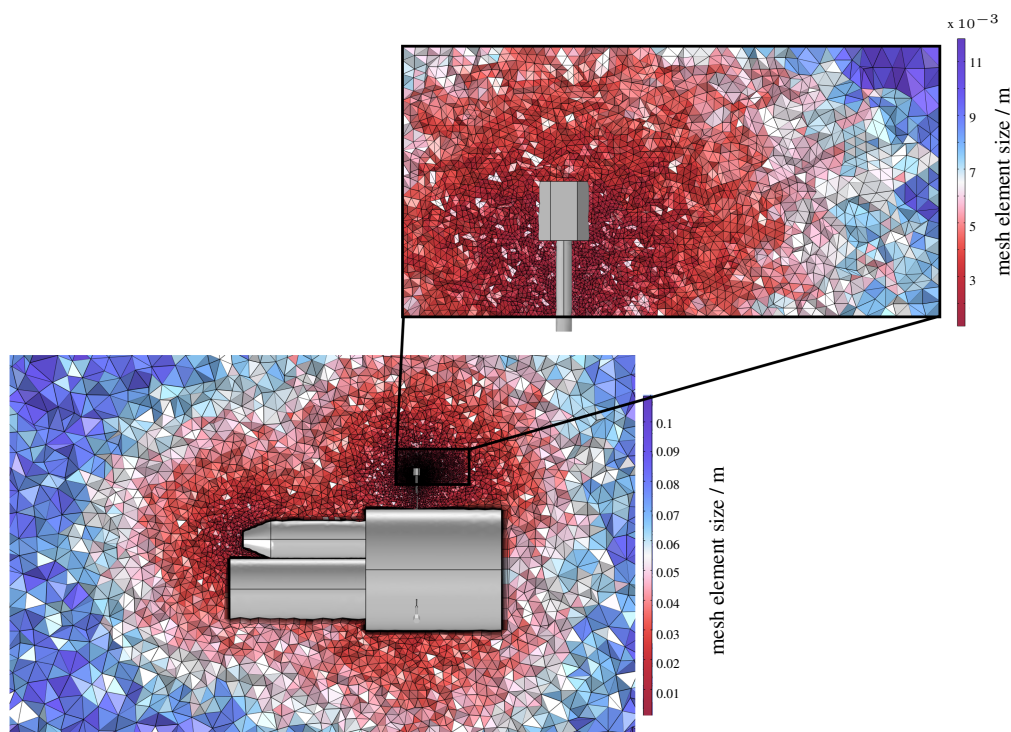


Figure 7. Computational mesh for fluid flow simulations around the entire geometry of the instrument module, including the SPICE compartment and one representative boom with substrate mount. The close-up shows a high-resolution mesh for the upright SPICE boom in detail, which has been created around each of the substrate mounts.

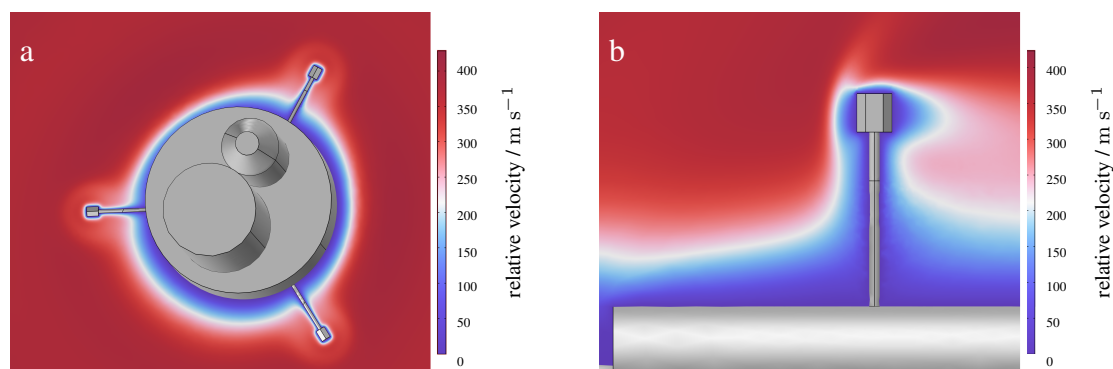
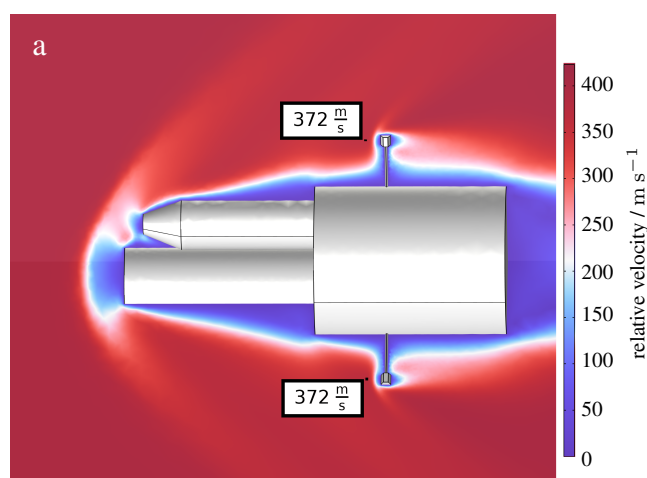


Figure 8. Panel a: Frontal view of the HAS instrument module and the velocity magnitude at the level of the SPICE instrument at an incident flow speed of 400 m s^{-1} . Panel b: corresponding side view of one SPICE boom with substrate mount (Klug, 2024a). Both views hold for an angle of attack of 0° .

310 The inference of the two depictions is that the chosen length of the SPICE booms allows for particle collection outside the instrument module's boundary layer (confirming the boom length of 120 mm as sufficient). However, additional boundary layer structures also form around the substrate mounts themselves. Figure 9 illustrates the simulation results of the velocity magnitude around the instrument module under consideration of the shock waves forming at the module's tip and the HAS attitudes of 0° and $\pm 30^\circ$. The panels a, b and c hold for the incident flow velocity of 400 m s^{-1} with the defined flow entry into the domain on the left-hand side of each picture. Clearly visible are the differently pronounced (asymmetric) shock waves at the HAS angles of attack of $\pm 30^\circ$, whose shape and extent vary dependent on the geometry structure facing the flow. The various structures (protrusions, bulges, edges) of the instrument module contribute to the deformation of the shock wave and the formation of slipstream zones. The flow velocities downstream of the shock wave, however, remain in the supersonic range. The results of the simulations show a significant variation in the approach flow towards the substrate mounts at the different

315

320 angles of attack:



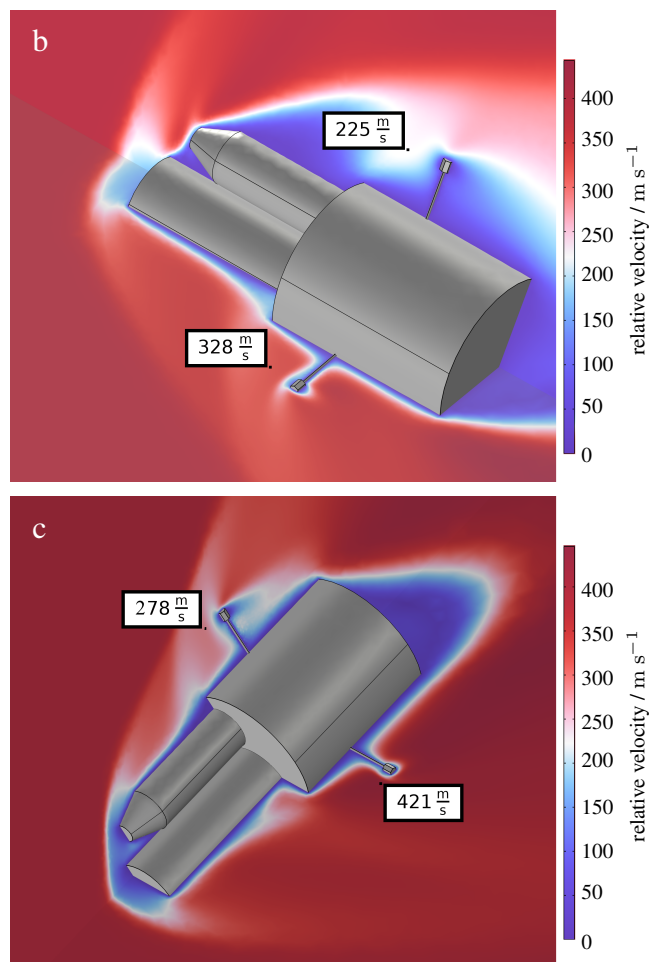


Figure 9. Panel a: Representation of flow velocities in the vicinity of the instrument module for the angle of attack of 0° , panel b: for $+30^\circ$, and panel c: -30° for the flow velocity of 400 m s^{-1} (Klug, 2024a).

At 0° all three SPICE booms are exposed to an almost undisturbed flow. The flow velocities in the immediate vicinity of the substrate mounts (indicated in the following figures as markers with velocity data) are consistent at the three boom positions. However, at an angle of attack of $+30^\circ$, the upright substrate mount is shielded from the free flow by the upstream geometry of the instrument module, expressed in a steeply decreased flow velocity of 225 m s^{-1} . In contrast, both of the downside oriented substrate mounts exceed any slipstream region and are still positioned well within the shock wave's cone, hence still largely unaffected from the wave edge, at decelerated flow velocities of 328 m s^{-1} . At the angle of attack of -30° , the upright substrate mount is almost directly affected by the shock wave front. Here, the incident flow velocity is decreased to values of 278 m s^{-1} .

The downside oriented substrate mounts, however, are exposed to even increased flow velocities of 421 m s^{-1} as compared to the incident flow speed, but neither the shock wave nor any shielding affects the flow pattern in the booms' vicinity. In essence, the chosen arrangement of the three SPICE booms allows the particle collection to remain as unaffected as possible



over a wide range of potential HAS flight attitudes. Even at extreme angles of attack, at least two of the substrate mounts are always directly exposed to the almost undisturbed flow. However, each additional and simultaneous particle collection represents a redundant safety backup, which is well justified in view of the shortness and cost of the measurement time in the target region.

4.2 Particle impaction



Figure 10. Pattern of 2703 impacted particles distributed over the entire surface of a substrate mount at an initial particle number concentration of 11 cm^{-3} corresponding to a total number of about $1.9 \cdot 10^5$ particles. Panel a: Frontal view of a substrate mount, panel b: angled side view (Klug, 2024b).

A result of the particle trace modelling is shown in Figure 10, where impaction positions of 2703 particle hits are depicted from two different perspectives. Analogous simulation results of particle impactions for each particle number concentration (cf. Table 4), for each of the three substrate mounts, and angle of attack are evaluated and presented later on (see Figure 11).

4.2.1 Efficiency of the inertia-based particle collection

For analyzing the collection efficiency of the individual substrate mounts in dependence of flight attitudes and particle number concentrations (cf. Table 4) for symmetry reasons only one of the two downside oriented SPICE booms is considered in numerical simulations of particle trajectories (cf. Figure 1). Consequently, the upright substrate mount is referred to hereafter as substrate mount 1 and a downside oriented one as substrate mount 2. The simulation results are shown in Figure 11, wherein the vertical bars represent the statistical variability of the model output from four independent simulation runs. The left column of Figure 11a₁, b₁, and c₁ depicts the number of impacted particles as a function of released particle number concentration for the HAS angles of attack of 0° in a₁, -30° in b₁, and $+30^\circ$ in c₁. Qualitatively consistent for both substrate mounts (1 and 2), an increase of released particle number concentrations goes along with a linear increase in the particle impactions. However, the slopes of the linear relationship for both substrate mounts differ slightly for the zero angle of attack, cf. Figure a₁. The difference in the impaction frequency as a function of the released particle concentration becomes more pronounced with a negative angle of attack of -30° , cf. Figure b₁. While the behavior of the substrate mount 2 (downward directed) hardly changes compared to the zero angle of attack, the effective impact rate on the substrate mount 1 (upward directed) is significantly reduced with



this attitude. With a positive angle of attack $+30^\circ$, cf. Figure c_1 , the effective impact rate on the substrate mount 1 is reduced even further, while the impaction behavior on the substrate mount 2 still remains almost unchanged.

355 For the substrate mounts 1 and 2 the resulting efficiency η (see equation 9) in collecting particles of released number concentrations is depicted in Figure 11 as a slope of the impaction particle curves, see right column. In general, each of the efficiency curves shows an almost constant behavior over the entire range of released particle concentrations. The individual deviations depending on the collection position and the angle of attack confirm the previous findings concerning the flow pattern. In the zero angle of attack, the particle collection with substrate mount 1 occurs (slightly different from substrate
360 mount 2) with a constant efficiency of 13%, which is almost halved at a negative inclination of -30° , cf. Figure b_2 and reduced to only 2 impacted out of 100 released particles at a positive attitude of $+30^\circ$, cf. Figure c_2 . For the three angles of attack, the collection efficiency of substrate mount 2 (downwards oriented) remains almost constant at around 11 – 12%, regardless of the flight attitude. An almost constant sampling efficiency can be observed over all released particle number concentrations per flight attitude, although the variability of this efficiency increases at lower particle number concentrations,
365 indicating that it is a statistical feature (as impaction processes are sensitive to the position of particle release). These variations disappear especially for higher concentrations.

Figure 12 shows simulated streamlines enveloping the substrate mounts for the angles of attack of 0° in panel a, and $\pm 30^\circ$ in panels b and c together with the course of the shock waves (marked as black contour in each panel). Streamlines are colored with reference to the incident velocity of 400 m s^{-1} . In general, a higher flow velocity implicates a higher number of particle
370 impactions, since an increased number of particles cannot circumvent the obstacle (substrate mount) due to their enhanced velocities and inertia at higher flow speeds. Apparently, the substrate mounts are subjected to different flow patterns for the angles of attack of $\pm 30^\circ$.

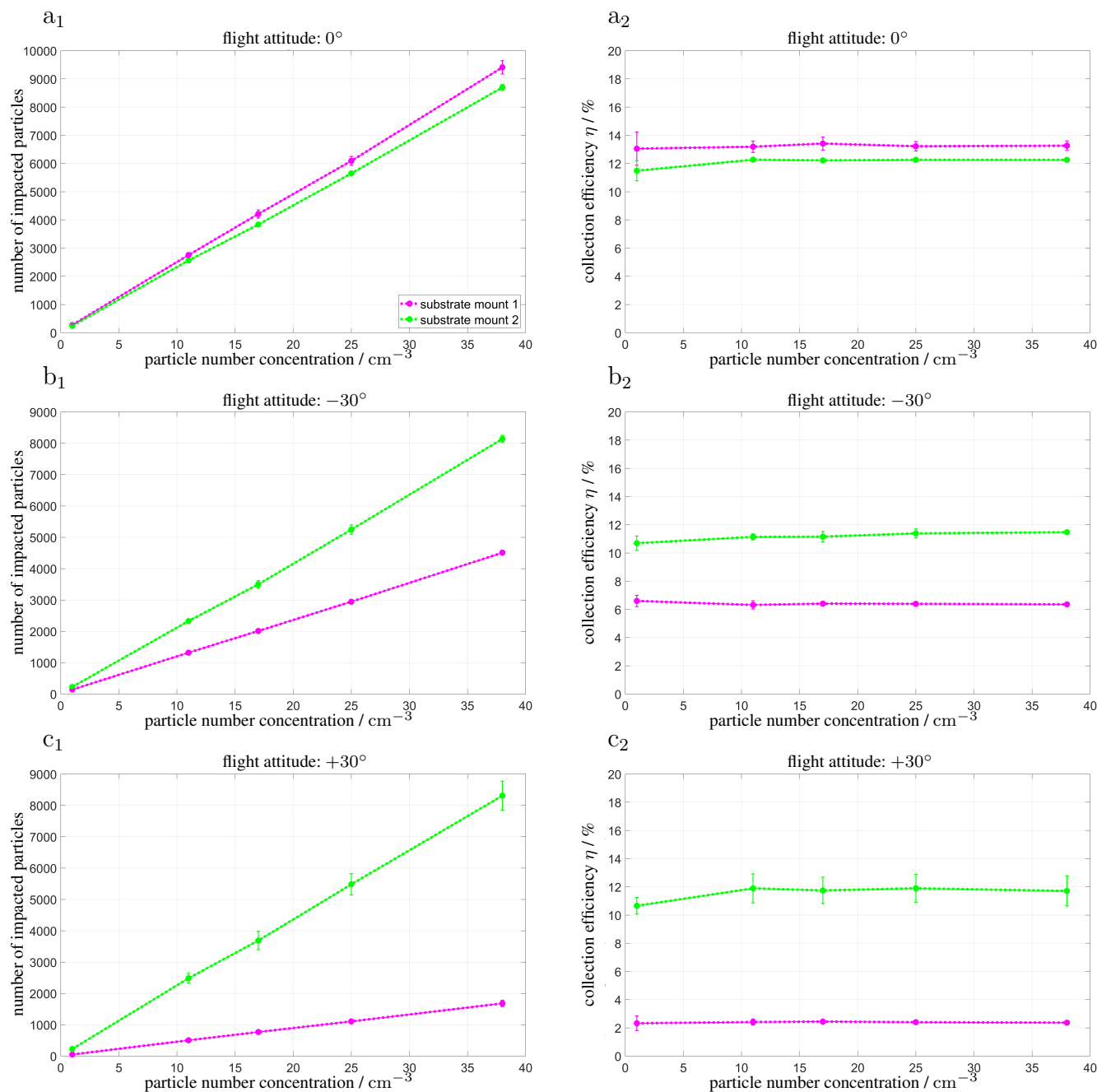


Figure 11. Left column: Relationship between the number of particles (with particle radius 0.6 nm) impacted on SPICE substrate mounts and the released particle number concentrations at two different collection positions dependent on the HAS flight attitude. Right column: Resulting collection efficiency η for various particle number concentrations released under corresponding flight attitudes. The statistical variability of four independent simulation runs is marked by vertical bars (Klug, 2024b).

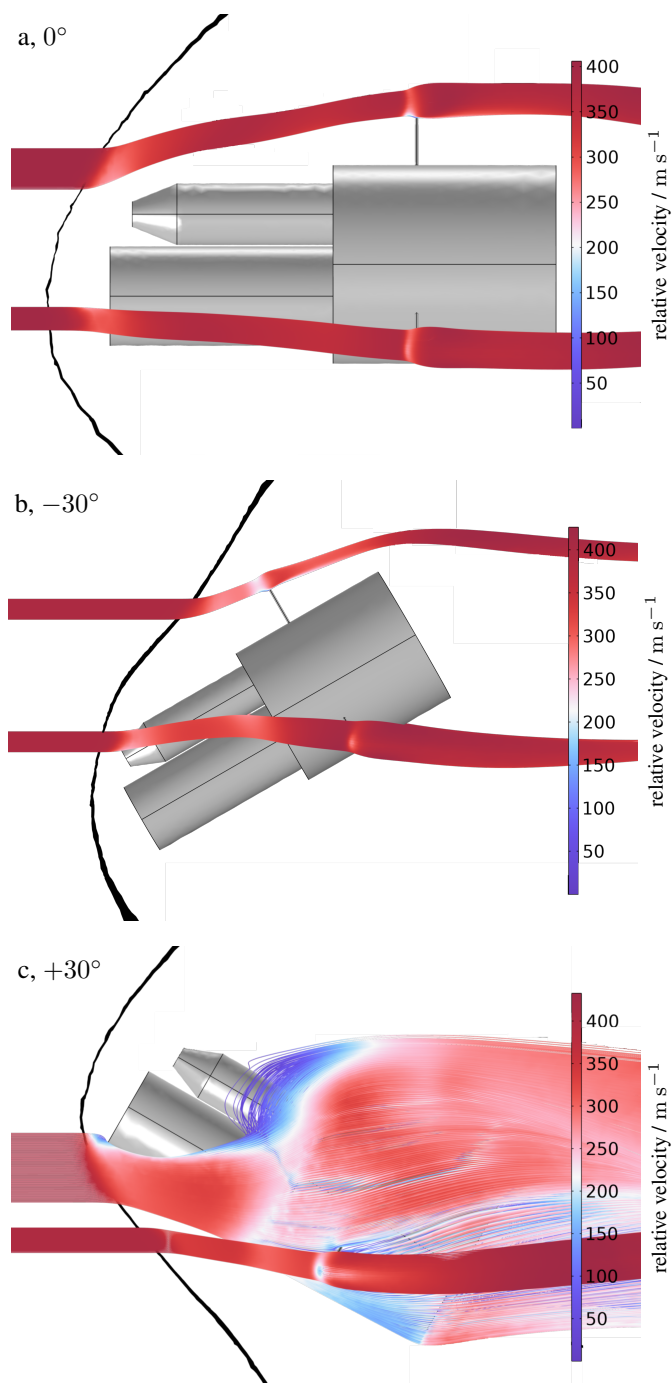


Figure 12. Panel a: Streamlines enveloping the substrate mounts for the angles of attack of 0° , panel b: -30° , and panel c: $+30^\circ$, for the incident flow velocity of 400 m s^{-1} . Streamlines are colored with reference to incident velocity values. For illustration purposes, the contour of the shock wave front is indicated in black.



However, according to the results exhibited in Figure 12a, the flow velocities in the near field upstream of both substrate mounts (1 and 2) at 0° correspond to each other, and are about 350 m s^{-1} to 400 m s^{-1} . This is reflected by almost equal collection efficiencies of substrate mounts 1 and 2, cf. Figure 11a₂), which differ by about 1%. This slight discrepancy is explainable again by the asymmetric tip of the instrument module upstream of the SPICE booms. Corresponding results for the simulation under different angles of attack of -30° and $+30^\circ$ are shown in Figure 12b and Figure 12c, respectively.

The flight attitude of -30° causes reduced flow velocities (with respect to the incident flow) to up to 270 m s^{-1} at a position upstream of substrate mount 1 (very close to the shock wave front), for which η is thus reduced by 5% in comparison to substrate mount 2. In addition, the downward oriented substrate mount is exposed to maximum flow speeds of 420 m s^{-1} (Figure 12b). Therefore, despite the negative angle of attack, the sampling efficiency η remains almost stable at the downwards oriented substrate mounts, while the upward collection decreases in efficiency at this flight attitude.

Under the positive flight attitude of $+30^\circ$, cf. Figures 11c₂ and 12c, the significantly decreased η for substrate mount 1 is due to shielding from the free flow that is caused by the tip of the instrument module. At this position, the flow speeds are reduced to about 220 m s^{-1} . As a consequence, due to the geometry-related deflection, a significantly reduced number of particles arrive in a position favorable for impaction since the decelerated flow in the near field upstream of substrate mount 1 allows many particles to circumvent the obstacle. At this flight attitude, however, the two downward oriented substrate mounts are still exposed to the almost free flow at velocities of 320 m s^{-1} . In this regard, the resulting η discussed above (cf. Figure 11c₃) correspond to the flow pattern observed in Figure 12c.

5 Final conclusions

5.1 Flow simulation and particle collection efficiencies

Generally, the presented particle simulations confirmed the effectiveness of the developed SPICE instrument. In this numerical study the substrate mounts as hexagonal prisms are hit by particles with radii of 0.6 nm and mass densities of 3 g cm^{-3} . Thus, the particle trace modelling based on simulated flow dynamics predicts the suitability of the developed aerodynamic design and the chosen arrangement of the substrate mounts for the collection of considered nanometer-sized particles in the mesosphere: The substrate mounts (with a boom length of 120 mm) are located outside the boundary layer around the fuselage of the instrument module. The simulated particle collection occurs mostly unaffected by the shock wave evolving at the tip of the instrument module. The conducted simulations allowed for estimating the particle collection efficiency η within the target altitude. The analyses of η at the respective collection position of each substrate mount show its clear dependence on the particular SPICE boom orientation and to the especially considered angle of attack of the HAS. According to these simulations, the collection efficiencies of the downwards oriented substrate mounts range from 10% to 12% at angles of attack of 0° and $\pm 30^\circ$ and is thus less sensitive to the flight attitude than the collection efficiency of the upright substrate mount, which ranges from 2% to 13% at these angles of attack. There are at least two of the three SPICE booms permanently exposed to the almost undisturbed flow during the collection phase regardless the flight attitude of the HAS. According to the computed trajectories, particle impactions onto designated collection surfaces are highly probable. In comparison to Pineau et al. (2024), where the



rocket-based particle sampler MESS (MEteoric Smoke Sampler) is designed to collect the particles during the sounding flight at the rocket tip, i.e. frontally aligned against the airflow within the forming bow shock, our SPICE instrument is located downstream of the rocket tip, where the single booms are radially adjacent to the HAS and almost unaffected by the shock wave. Another distinction between both approaches lies in the rocket velocity: Pineau et al. (2024) states that lower velocities
410 result in more efficient particle collection. While their rocket achieves speeds of up to 1000 m s^{-1} , the velocity range of the HAS that is to carry the SPICE system is limited to $300 - 400 \text{ m s}^{-1}$. However, one major advantage of the envisaged HAS flight pattern with SPICE is that the rocket remains at the target altitude for an enhanced duration compared to the MESS rocket. Thus, hovering at this altitude at lower rocket speeds enables longer measurement times at NLC levels and, in this way, facilitates the investigation of the spatial distribution of NLC constituents. In essence, however, both concepts of a particle
415 sampler would allow for collocative measurements to obtain complementary samples if both instruments were deployed on the same sounding rocket.

With the help of performed computational fluid dynamic and particle simulations, a design concept for the successful fundamental feasibility of carrying out the planned collections in the mesosphere was confirmed. In the meantime, however, the actual rocket flight with the finalized prototype of the SPICE instrument is still pending, which will provide the verification of
420 the numerically predicted sampling effectiveness.

6 Outlook

6.1 Flow modeling and simulations

A validation of the presented modeling approach on the macroscale, underlying compressible and supersonic conditions and using Navier-Stokes equations at the flow transition value of $Kn = 0.1$, can be addressed, for example, by different modeling
425 approaches on the mesoscale via the Boltzmann equation or statistical microscopy approaches of the free molecular flow using DSMC methods to assess the uncertainties.

6.1.1 Instrument design improvements

In the current state of development, the SPICE booms are not designed to be rotatable, and due to the HAS stabilization against rotation around the longitudinal axis, the boom positions remain the same. For the most efficient particle collection,
430 however, it would be conceivable to keep one impact surface of the substrate mount continuously facing against the flow direction during the measurement flight. Such an orientation (i.e., with substrate mounts perpendicular to the flow) yields a non-aerodynamically positioned frontal surface that forces the surrounding streamlines to change their direction steeply, which in turn promotes inertia deposition of particles onto the substrates as presented in Figure 10. Such a rotation mechanism could be achieved by using suitable bearings in the booms and by adding fin-tails to the hexagonal substrate mounts (acting like an
435 oar). However, the fin-tails complicate the design of the SPICE booms; the fin-tails must be extended and retracted during the short duration of the measurement phase, and their space requirements must be considered in the design of the mechanically



extendable booms. The fin-tails would also increase the sensitivity of SPICE booms towards vibrations that occur during the flight.

Appendix A: Investigation of the particle size

At an altitude of about 85 ± 5 km, unique atmospheric conditions persist in the summer mesopause region, where the ambient temperature falls far below the frost point, leading to supersaturation and the sublimation of water vapor on available surfaces, which forms ice particles. The radius of these particles is typically measured and estimated to range from 38 to 100 nm (Von Cossart et al., 1999; Rapp and Lübken, 2004; Rapp and Thomas, 2006; Baumgarten and Fiedler, 2008). Due to the limited thermodynamic range for supersaturation in the mesosphere, small temperature variations significantly impact ice particle formation and persistence.

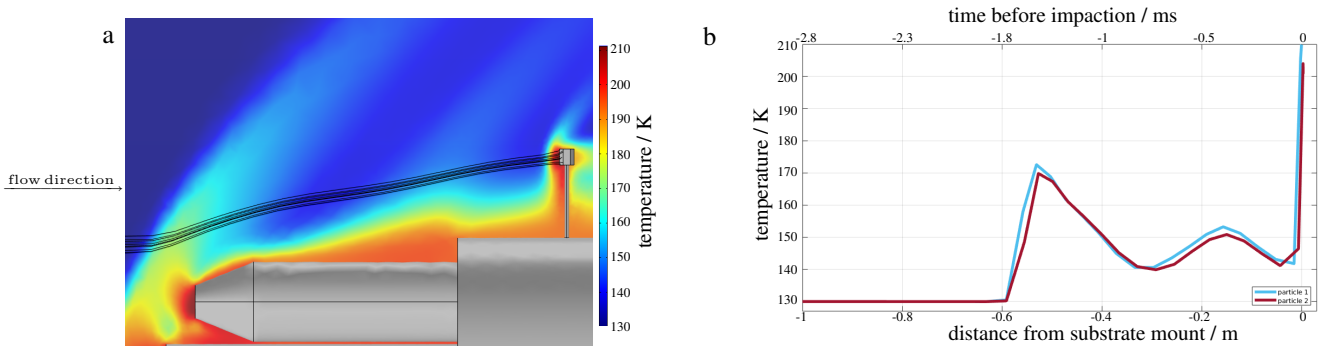


Figure A1. Panel a: Enlargement of the temperature field (in K) around the instrument module, showing the temperature increase generated by the shock waves at the incident flow velocity of 400 m s^{-1} . Additionally, the trajectories of individual impacting particles are illustrated in black. Panel b: Temperature profile along the trajectories of two particles are represented in blue and red. The origin of the x -axis (zero) marks the location of particle impact on the substrate mount. (Klug, 2024b)

Supersonic flights through the mesosphere generate shock waves, i.e., regions of air congestion, causing a temperature rise that could initialize the sublimation of the ice particles as they pass these regions on their way to the substrate mounts, which is depicted in Figure A1a. The temperature evolution along two exemplary particle trajectories is illustrated in Figure A1b, where the simulations with an incident flow velocity of 400 m s^{-1} show a temperature increase of up to 80 K. This rapid heating may impact the particles' masses upon their approach towards the substrate mounts, where the mass evolution is calculated based on

$$\frac{dm_{ice}}{dt} = \frac{2\pi}{R_v} \alpha_d D_v 2r \left(\frac{p_v}{T_{air}} - \frac{p_s}{T_{ice}} \right) \quad (\text{A1})$$

(Stephens, 1983), with

$$\frac{dT_{ice}}{dt} = \frac{L_s \frac{dm_{ice}}{dt} + 4\pi r k (T_{air} - T_{ice})}{m_{ice} c_{ice}} \quad (\text{A2})$$



455 (Lohmann et al., 2016), with the diffusion coefficient D_v of water vapor, which is calculated by

$$D_v = 2.11 \cdot 10^{-5} \left(\frac{T_{air}}{T_0} \right)^{1.94} \left(\frac{p_0}{p} \right) \quad (A3)$$

(Pruppacher et al., 2010). Here p is the air pressure, T_{air} is the ambient temperature, p_v is the partial pressure of environmental water vapor, p_s is the saturation pressure over a curved ice surface (as, e.g., presented by an cloud ice particle), $T_0 = 273.15$ K, and $p_0 = 101325$ Pa are reference values, r is the particle radius, R_v is the gas constant for water vapor, T_{ice} is the surface temperature of the ice particle, L_s is the latent heat for the sublimation, k is the thermal conductivity in air, c_{ice} is the specific heat capacity of ice, and α_d is the deposition coefficient of ice particles. In the literature, a wide range of measured deposition coefficients α_d is reported, varying from 0.005 to 1 (Magee et al., 2006; Pruppacher et al., 2010). To account for the inherent uncertainty, conducted simulations use different values of α_d , such as 0.1, 0.5 (Spichtinger and Gierens, 2009), and 1, resulting in varying model outputs, as depicted in Figure A2a to c, where considered NLC particle radii lie in the range of 25 nm to 150 nm. Note, that only pure ice particles are considered, excluding any nucleating particles. Results reveal that larger ice particles with radii of up to 75 nm may sublime entirely for $\alpha_d = 1$, where in reality only the nucleating particles for the impactions would remain. However, in cases of $\alpha_d = 0.5$ and $\alpha_d = 0.1$, ice particles with radii of up to 50 nm and up to 25 nm, respectively, would sublime entirely. Regarding the uncertainty of α_d , a worst-case scenario assumes the complete sublimation of even larger ice particles. Thus, after sublimation, only the nucleating particles, applied with a radius of 0.6 nm, remain available for impaction. Due to their low inertia, these small particles are likely to be guided around the sampler by aerodynamic perturbations. Consequently, if these nuclei are deposited on the substrate mounts, it can be deduced that larger particles with greater inertia will also impact. The conducted particle simulations, therefore, assume a constant MSP radius of 0.6 nm with a mass density of 3 g cm^{-3} . As shown in Figure A1, the maximum temperatures reach around 210 K. The nucleating particles, initially embedded in ice, remain unaffected over the entire observed temperature range in general agreement with Pineau et al. (2024). Furthermore, the heating caused by the particle impact clearly exceeds all other heating processes.

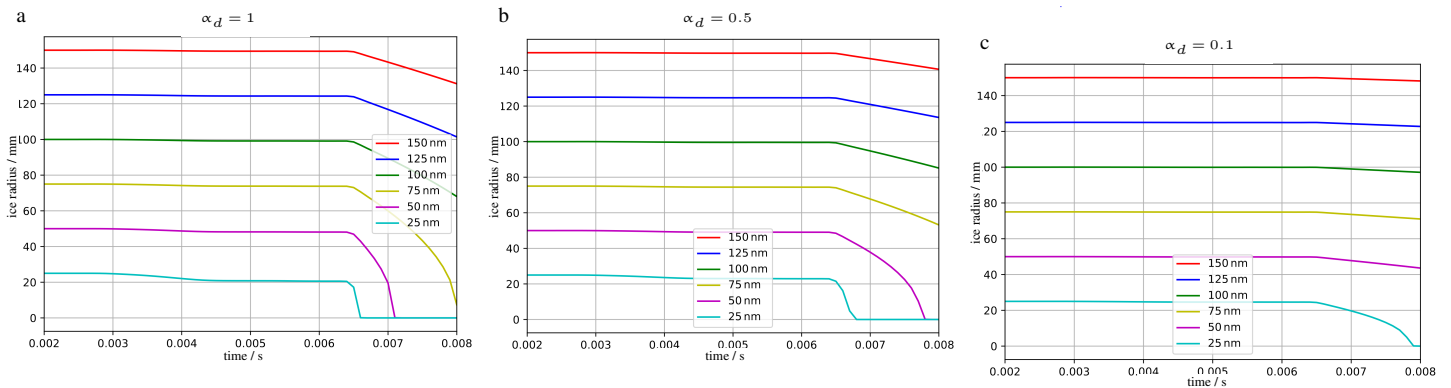


Figure A2. Simulated mass loss of ice particles of different sizes based on varying values of α_d , (Klug, 2024b).



Author contributions. BK established the flow model and its generalization for compressible fluids in the supersonic flow regime with contributions by AH and RW. BK conducted the numerical simulations as well as the analysis, visualization, and documentation of the results, and drafted the manuscript, which was critically reviewed, commented and revised by RW and with contributions from all co-authors. The design development of the SPICE instrument was primarily driven by RW, BK, TB, KDW, and TK. MR was the project initiator, OD (inter alia) supported this study with technical rocket-related information and by extensive discussions. CAD models were prepared by TB. MB performed calculations on the simulated mass loss of ice particles of different sizes. KK contributed significantly to the design development and the physical model of the particle simulation process.

Competing interests. Markus Rapp is a member of the editorial board of AMT



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