Impacts of Satellite Reentry on Atmospheric Composition in the Era of Mega-Constellations: Molecular Dynamics Simulations

José P. Ferreira[1], Ziyu Huang[1,1], Ken-ichi Nomura[2], and Joseph Wang[1]

[1]Department of Astronautical Engineering, Viterbi School of Engineering, University of Southern California
[2]Department of Materials Science and Chemical Engineering, Viterbi School of Engineering, University of Southern California

December 27, 2022

Abstract

The number of orbiting satellites has increased significantly and in an unrestricted and unregulated manner in recent years. This trend is expected to continue with ongoing plans from the commercial space sector to build mega-constellations of microsatellites. However, the effect of satellite demise during reentry on Earth's atmosphere has only been lightly studied, and the long-term impact remains unknown.

This poster presents, to our knowledge, the first Reactive Force Field (ReaxFF) Molecular Dynamics (MD) simulation study on the atmospheric chemical mechanisms and byproducts generated by satellite reentry. Simulations are carried out to resolve chemical reactions and byproducts for Aluminum – a typical satellite structure constituent – under reentry conditions. MD simulation results are used to estimate the presence of oxides and predict the accumulated increase of reentry byproducts in the mesosphere when compared with that from meteoroids entering atmosphere and other natural sources. A methodology to estimate the residence time of these substances in the atmosphere is also presented so as to evaluate the polluting potential of mega-constellations reentry events.

Impacts of Satellite Reentry on Atmospheric Composition in the Era of Mega-Constellations: Molecular Dynamics Simulations

José P. Ferreira, Z. Huang, K. Nomura, J. Wang
Viterbi School of Engineering, University of Southern California

AGU FALL MEETING
Chicago, IL & Online Everywhere
12–16 December 2022

Background

In 2021, the total mass of re-entering objects summed up to **280 tonnes**, doubling the figure of 2020. It is estimated that **60 to 90 % of the spacecraft mass burns** in the mesosphere.

Mega-constellation plans threaten **increasing** the number of satellites launched to date nearly **4 times**, which already faces skepticism from NASA and NSF.

FCC highlighted the **«Potential Effect on Earth's Atmosphere from Satellite Launch and Reentry»** which generates Alumina during reentry - a climate change potentiator. Lack of studies prevented further actions.

Methodology

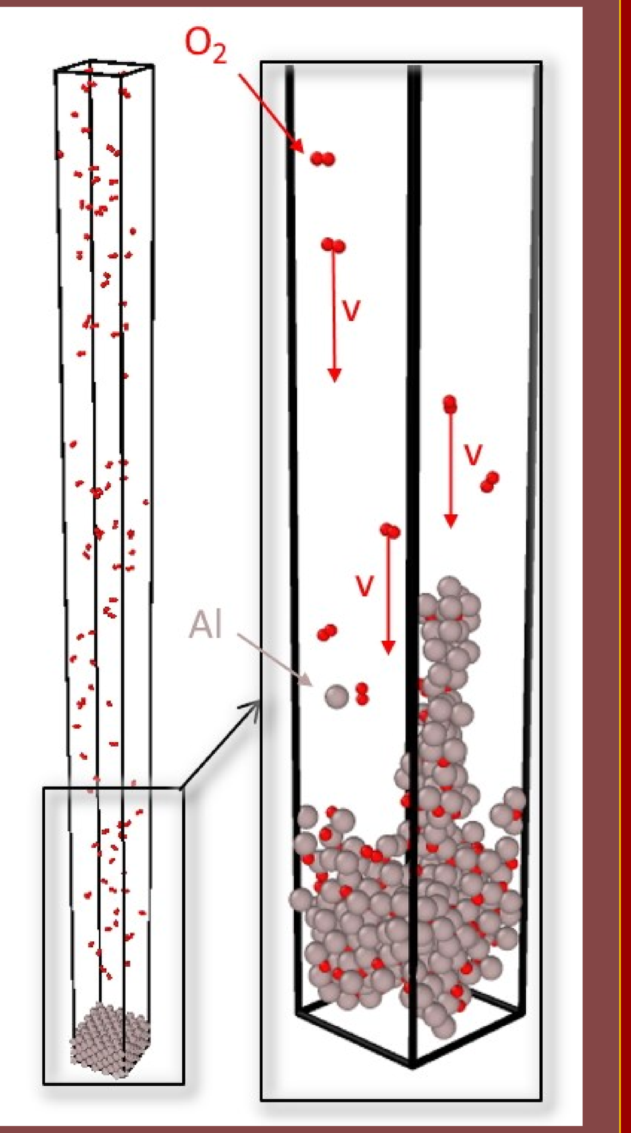
Molecular Dynamics (MD) simulations resort to empirical interatomic potentials and external forces to determine atomic trajectories at each time step. USC's RXMD framework uses ReaxFF for Aluminum-Oxygen interactions to study Aluminum Oxidation during reentry.

Setup

- Mesospheric LEO reentry simulation initiated at **86 km**.
- Oxidation process triggered by **molecular Oxygen** (O_2).
- **Thermal ablation** is dominant for steady state conditions at **2400 ºK**
- Constant attitude (null pitch)

The simulation is set for a restricted domain where **a heated Aluminum crystalline structure is impinged by O_2 molecules** at 2 km/s:

- 1024-1360 Aluminum atoms
- 100-352 Oxygen atoms



MD Simulation Setup

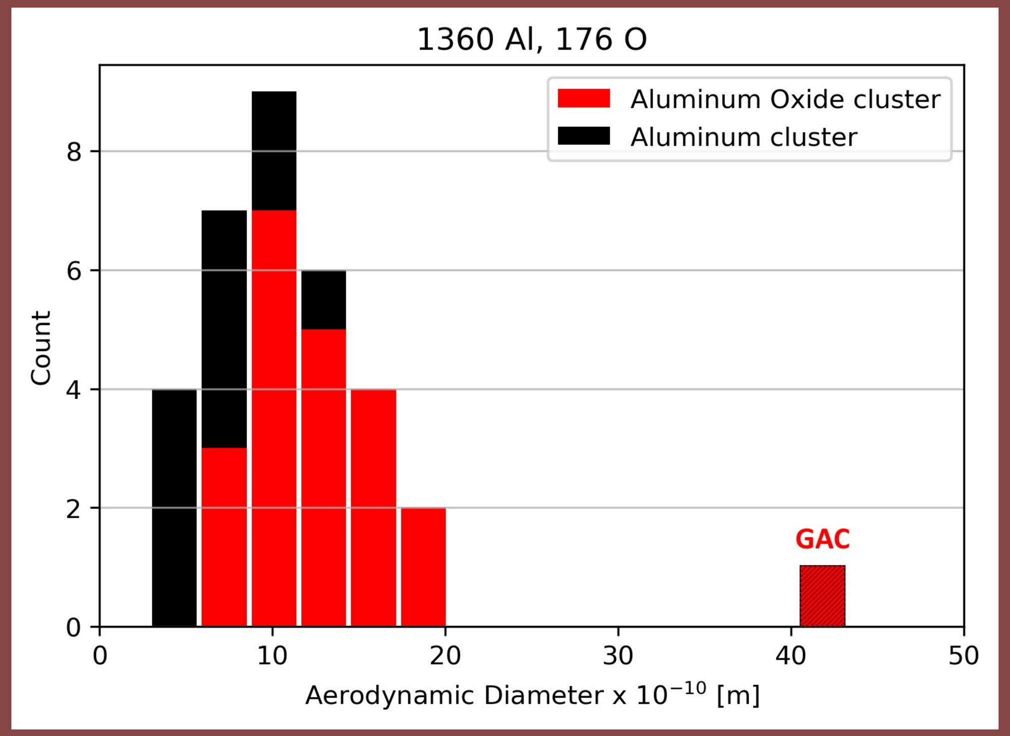
Reentry Byproducts

The visual output of the MD simulation allows identifying atomic clusters formed after the reentry event. Two species are considered bonded if Bond Order > 0.3 and if they fall below the species-wise bond cutoff distance. The average cluster atomic structure is retrieved from the Pair Separation Distance function, which is then used to compute the coordination number.

Our results show that the problem scales linearly for nanoparticles as the reaction takes place in an **oxygen-deficient environment**, generating **clusters of Aluminum Oxide and Aluminum**. Unreactive Aluminum will pile up around the Great Aluminum Cluster (GAC).

The aerodynamic diameter (D_a) is computed based on the mass of each cluster. Both clusters are well fit by a **Lognormal distribution**.

The GAC is identified as an outlier. As some Oxygen atoms are trapped within, it is classified as an Aluminum Oxide cluster, which suggest that it will likely oxidize with atmospheric decay.



Cluster Size Distribution

We can estimate that a **single reentry** of a small spacecraft of **250 kg** generates around **30 kg of Aluminum Oxide** clusters and **51 kg of Aluminum**.

Settling Time

The U.S. Standard Atmosphere 1976 model is used, and a simple force balance including the **weight** of the cluster (F_g) and the **viscous force** (F_v) as per Stokes' Law corrected for high Knudsen numbers using the Cunnigham Correction factor yields to 1-D acceleration (a).

$$\vec{F_g} + \vec{F_v} = m\vec{a}$$

Position is then retrieved, and the **settling time** is calculated by equating a reference altitude. Values of reference are computed for nano and microparticles.

Cluster Settling Time

D_a [m]	Time
10 x 10^{-10}	40 000 years
41.5 x 10^{-10}	9500 years
1 x 10^{-6}	13.5 years
50 x 10^{-6}	5.3 hours
1 x 10^{-3}	30.6 min

Outcomes

Considering current and future reentry rates:

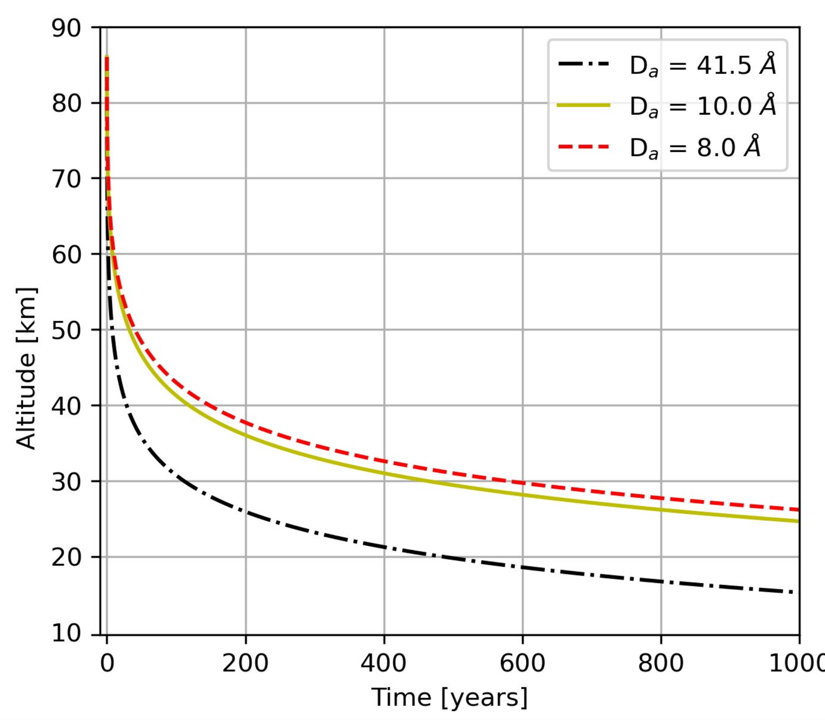
- **2021**: 43 % increase in Aluminum above natural levels (TOA), **33.9 tonnes** of Aluminum Oxide clusters
- **Future**: 640 % increase in Aluminum (TOA), **509 tonnes/year of Aluminum Oxide clusters**

The **settling time** of nanoparticles is reportedly long, hence Brownian motion prevails. However, such particles may get to the upper **stratosphere in 20 to 100 years after reentry.**

Considering the ozone depletion potential of Aluminum Oxide clusters, the **possibility of a cascade reaction with the ozone layer is concerning**.

As to **Aluminum clusters**, considering its smaller D_a, they are expected to **endure at higher altitudes**.

Larger microparticles will reach hypersonic velocities and likely undergo a thermal ablation process.



Nanoparticle Altitude Profile

Conclusion

Nanoparticles

- 12 % of reentry mass turns into Aluminum Oxide clusters, likely reacting with the ozone layer in 20 to 100 years and thus increasing shortwave radiative forcing.
- 20 % of reentry mass turns into Aluminum clusters which may undergo secondary oxidation, but also decrease longwave radiative forcing.

Microparticles

- Likely to ablate and converge to stratospheric altitudes

jose.ferreira@usc.edu