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# SIMULATION OF COMET IMPACT AND SURVIVABILITY OF ORGANIC COMPOUNDS

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**Abstract.** Comets have long been proposed as a potential means for the transport of complex organic compounds to early Earth. For this to be a viable mechanism, a significant fraction of organic compounds must survive the high temperatures due to impact. We have undertaken three-dimensional numerical simulations to track the thermodynamic state of a comet during oblique impacts. The comet was modeled as a 1-km water-ice sphere impacting a basalt plane at 11.2 km/s; impact angles of 15° (from horizontal), 30°, 45°, 65°, and 90° (normal impact) were examined. The survival of organic cometary material, modeled as water ice for simplicity, was calculated using three criteria: (1) peak temperatures, (2) the thermodynamic phase of $H_2O$, and (3) final temperature upon isentropic unloading. For impact angles greater than or equal to 30°, no organic material is expected to survive the impact. For the 15° impact, most of the material survives the initial impact and significant fractions (55%, 25%, and 44%, respectively) satisfy each survival criterion at 1 second. Heating due to deceleration, in addition to shock heating, plays a role in the heating of the cometary material for non-normal impacts. This effect is more noticeable for more oblique impacts, resulting in significant deviations from estimates using scaling of normal impacts. The deceleration heating of the material at late times requires further modeling of breakup and mixing.

## INTRODUCTION

Comet impacts have been proposed as a mechanism for the delivery of organic compounds to the early Earth. Several authors have attempted to address these scenarios computationally, but with few exceptions, notably Pierazzo and Melosh [1], the simulations have been two-dimensional. Advances in computational power now allow three-dimensional parameter studies to be conducted. This work examines the survivability of organic compounds during comet impacts at various degrees of obliqueness using a three-dimensional shock physics code.

## Organic Survivability

Some comets have been estimated to be up to 25% organic by mass [2], but successful delivery to the Earth's surface requires that organic compounds survive the high temperatures associated with impact. This work focuses on amino acids and their thermal degradation. Under ambient conditions, amino acids can decompose at relatively low temperatures (<350°C), but gas gun experiments have shown that the high pressures and reduced times associated with shock loading result in significant survival of amino acids at shock temperatures up to 870K [3].

## COMPUTATIONAL MODELING

Calculations were performed using GEODYN, a Godunov-based Eulerian code with adaptive mesh refinement capabilities. This parallel code features high-order interface reconstruction algorithms and advanced thermodynamically consistent constitutive models described elsewhere [4] that incorporate many of the salient features of the dynamic response of geologic materials. GEODYN also utilizes high-pressure tabular equations of state to model the extreme conditions associated with shock loading.

### Problem Setup and Material Modeling

The comet impact was modeled as a 1-km diameter sphere of ice at 200K impacting a basalt half-space. The sphere impacts the surface at 11.2 km/s (Earth's escape velocity) and begins the simulation tangent to the surface; 90° (normal), 60°, 45°, 30°, and 15° impacts were undertaken. Calculations were performed with a resolution of 12.5m on the finest refinement level. The domain was a half-space centered on the impact point (due to the bilateral symmetry). The domain extended 12.8 km along the horizontal axes and 4.8 km and 3.2 km above and below the impact point, respectively. Taking advantage of the adaptive mesh refinement, the entire mesh consisted of slightly more than ten million cells.

The basalt model was developed by scaling a hard rock model calibrated to match underground explosions in granite [5]. This model includes pressure hardening, strength and failure, bulking, and porous compaction. The comet material was modeled as water; its strength was assumed to be negligible compared to basalt. Both materials were described using tabular (LEOS) equations of state to accurately capture their high pressure behavior.

### Survival Metrics

In our model, the survivability of organic compounds is tied to the condensed phases of water. This most likely is a conservative estimate–that is, our calculations provide a lower boundary estimate for survival–because, under ambient pressure, organic compounds volatilize at temperatures higher than that for water.

Here, three separate metrics are used to determine the survival:

1) *The peak temperature experienced by each material point.* This metric does not account for kinetic or pressure effects, and thus probably underestimates the survival rate. The threshold value of 870K from gas gun experiments [3] is used to indirectly account for pressure effects.

2) *The thermodynamic state of the cometary material.* This criterion assumes that any material that remains in a condensed phase survives the impact. Since the phase is dependent on both temperature and pressure, this implicitly takes the pressure effects into account. The comet is modeled as pure water, so this criterion is only effective up to the critical point of water (~650K); the phase of particular organic materials may be more relevant but involves too much uncertainty for this work.

3) *The estimated final temperature on unloading.* The state at the end of the simulation (~1s) is unloaded isentropically to ambient pressure. The resulting state is readily mapped to existing thermal decomposition data and provides an approximate upper bound for survival at a given temperature. A very conservative threshold temperature of 373K is used for this work.

## RESULTS AND DISCUSSION

The simulations were run out until comet material reached the edge of the computational domain (except in the 15° case, where the domain was extended). In Fig. 1, the peak temperature of each material point, mass averaged over the entire comet, is shown for the impact angles studied.
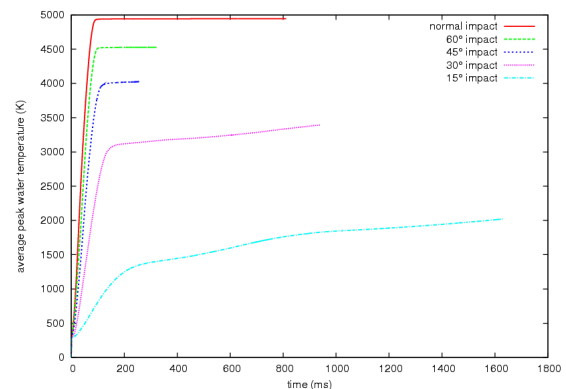


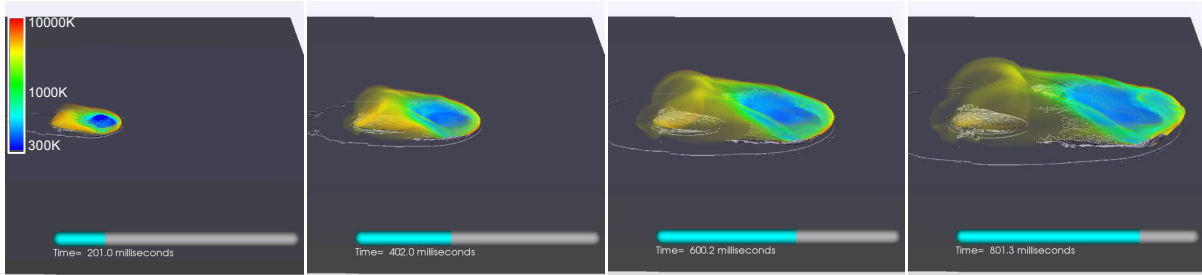**Figure 1.** Peak temperatures for various impact angles.

**Figure 2.** Volume rendering of comet temperature for 15° impact.  Temperature scale is logarithmic from 300 to 10,000K.

As expected, the peak temperatures decrease as the impact becomes more oblique.  The initial rise can be attributed primarily to the heating due to shock compression of the comet.   The peak temperature for the more normal impacts (≥45°) levels off after the initial rise, indicating that the temperature of the initial shock equal to or greater than any subsequent temperature.  For the more oblique angles (15° and 30°), however, the peak temperature continues to rise after the initial shock has passed (~200ms).  This late time heating can be attributed to the conversion of kinetic energy to internal energy as the comet decelerates after the initial impact.  Figure 2 shows a volume rendering of the comet temperature for the 15° impact.  For this low impact angle, almost no crater is formed and very little of the material remains in the crater.  Most of the material appears to "skid" along the ground, resulting in heating due to deceleration.

### Estimated Survivability

Table 1 shows the fractional survival estimated using each of the three criteria.  By 200 ms (around the time that the initial shock has passed), only the 15° impact simulations shows any surviving material using the first two criteria.  For the less oblique cases, the initial impact vaporizes the entire comet, heating the entire mass above the 870K survival threshold.  The third criterion was only applied to the impact angles of 15°, 30°, and 90°, but again only showed survival for the most oblique case.
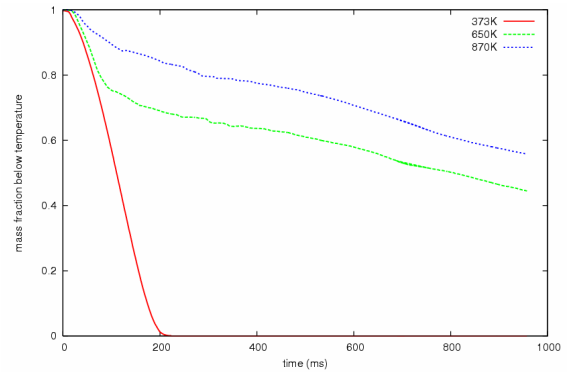


**Figure 3.** Fraction of material below various peak temperature thresholds for 15° impact.

Figure 3 shows the fraction of material with a peak temperature below various thresholds as a

**TABLE 1.** Fractional survival of organic compounds estimated using various criteria.

| | IMPACT ANGLE | | | | |
|---|---|---|---|---|---|
| | 15° | 30° | 45° | 60° | 90° |
| *Fractional Survival at 200 ms* | | | | | |
| **CRITERION 1: Peak temperature < 870K** | 82% | 0% | 0% | 0% | 0% |
| **CRITERION 2: Condensed phase** | 75% | 0% | 0% | 0% | 0% |
| *Fractional Survival at  end of simulation,        time =* | *1100 ms* | *900 ms* | *250 ms* | *300 ms* | *800 ms* |
| **CRITERION 1: Peak temperature < 870K** | 55% | 0% | 0% | 0% | 0% |
| **CRITERION 2: Condensed phase** | 25% | 0% | 0% | 0% | 0% |
| **CRITERION 3: Isentropic release to 1 atm, T < 373K** | 44% | < 1% | - | - | < 1% |

function of time for the 15° impact. The initial shock heats all of the comet material above the normal boiling point of water (373K). This material is not initially vaporized due to the high shock pressures. Figure 3 shows the condensed mass fraction as a function of time.
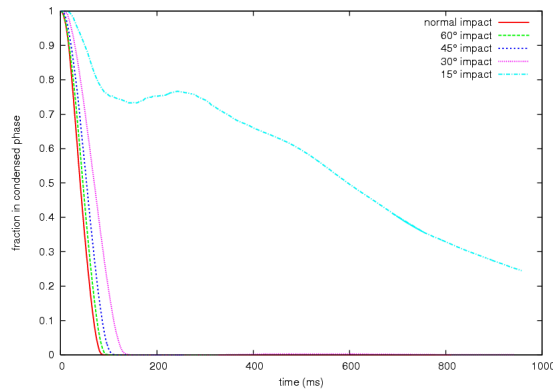


**Figure 3.** Mass fraction remaining in condensed phase for various impact angles.

Though a significant fraction of the material survives the 15° impact to 1 second, this fraction would decrease with time due to deceleration heating. This heating will continue until the material has come to rest. However, this deceleration heating is heavily dependent on droplet formation and breakup, as well as gas phase mixing, which become important beyond one second. The relevant physics for these phenomena are not modeled in this work, but should be included to estimate final survivability.

## CONCLUSIONS

High resolution three-dimensional calculations of comet impacts at various angles have been performed. For the configuration examined (1-km diameter sphere at 11.2 km/s impacting basalt), organic materials are only expected to survive for impact angles lower than 30°. For oblique angles, deceleration heating was found to be important, indicating that scaling of the shock temperatures may be insufficient for low impact angles. At 1 second, a significant fraction of the material is estimated to survive a 15° impact, but estimating the effect of deceleration heating at later times

requires further modeling of droplet formation/breakup and gas phase mixing.

## REFERENCES

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