CHEMOSYNTHESIS AND TRANSPORT OF POLLUTANTS FROM IMPACT EJECTA REENTRY. Devon Parkos[1], Marat Kulakhmetov[1], Brandon Johnson[3], Henry J. Melosh[1,2,3] and Alina Alexeenko[1], [1]School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, USA, [2]Department of Earth, Atmospheric, and Planetary Sciences, Purdue University, West Lafayette, IN 47907, USA. [3]Department of Physics, Purdue University, West Lafayette, IN 47907, USA.

Background: Both the immediate and long-term effects of the Chicxulub impact played a crucial role in determining how life developed on Earth. The initial asteroid impact produced thermal radiation levels lethal to terrestrial life [1]; however, observations indicate this extinction was accompanied by a significant loss of ocean life that cannot be attributed to exposure to elevated thermal radiation [2].

The Chicxulub impact was sufficiently large to eject mass into low Earth orbit, which would eventually nucleate and reenter as small spherules, spreading evenly across the planet [3,4]. While this reentering mass was on the same order of magnitude as the initial impactor, the cross-sectional area increased by 8 orders of magnitude, causing significant global production of toxic chemical species during reentry.

For this reason, a new method was developed to predict the overall amount of several toxic species that were produced, and to determine whether this mechanism was responsible for the observed oceanic extinction.

Approach: The method used to determine the overall pollutant production involves several steps. Production rates for a single spherule are calculated as functions of altitude and velocity. This rate is then integrated along representative trajectories and total production from all spherules is obtained.

Production Rates: Using the direct simulation Monte Carlo (DSMC) method, flow properties and chemistry around a spherule at various flight conditions were modeled. Using the Statistical Modeling in Low Density Environment (SMILE) code [5], non-equilibrium, axisymmetric flow was modeled considering the following 5 species: *O*, *N*, *O*2, *N*2, and *NO*. The rates for the considered reactions are from Hassan and Hash [6]. The coefficients for the chemical reaction rates in high-enthalpy conditions encountered during ejectra reentry are highly uncertain, but they allow improvement beyond what is attainable from equilibrium calculations.

The drag force was obtained by integrating surface forces across the face of the spherule. By integrating the flux of each species across each domain boundary, the overall rate of production or destruction for each species was determined (see Fig. 1). The drag force and production rates for *O*, *N*, and *NO* were extracted for each flight condition and used to generate a compact model for finding properties during the trajectory integration.

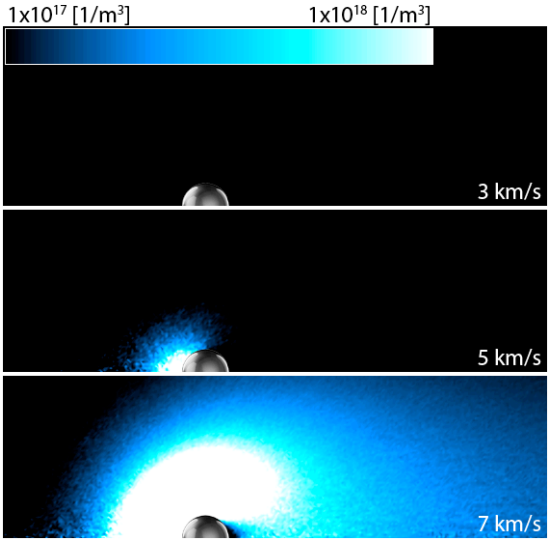

Figure 1: Nitric oxide number density for several spherule velocities. The production rate is highly sensitive to velocity.

Trajectory: The spherule diameter was chosen as 250 μm, based on the ground measurements [7]. An initial velocity of 8km/s, angled downward $\pi/4$ radians for the horizontal was chosen, based on representative conditions for a re-entry spherule [1]. The trajectory integration was performed using a 4th order, explicit Runge-Kutta method. The integration was terminated when the spherule slowed to 5 km/s, where the production rate for the species of interest dropped to negligible levels.

A total of sixteen DSMC cases were computed, for all combinations of the altitudes 66, 86, 114, and 134 km and the velocities 5.5, 7.3, 9.7, and 11.5 km/s. To calculate the values for the drag force and the species production rates, bilinear interpolation was performed between each of the DSMC results. Higher order schemes do not consistently reproduce the monotonic behavior that must be physically true (e.g. an increase in drag force from an increase in either velocity or density). Once the trajectory was determined, time integration of the rate of production yielded an altitude dependent distribution of produced pollutant density for the representative spherule, which can be convert-

ed into a total for all of the spherules [8], using the following expression

$$n_i = \frac{\dot{N}}{v}\frac{1}{4\pi(r_e + h)^2} \qquad (1)$$

where n is number density, N is the number of particles, v is the spherule velocity, r_e is the radius of the earth, and h is altitude.

Transport and Precipitation: To improve the accuracy of these predictions, this work includes the subsequent reactions as the atmosphere cools and the transport of the toxins via turbulent diffusion. The effect of reactions and diffusion on the value of number density at any particular altitude is given by the following expression

$$\frac{\partial n_i}{\partial t} = \frac{\partial}{\partial y}\left(nD\frac{\partial}{\partial y}\left(\frac{n_i}{n}\right)\right) + \dot{n}_{i,rxns} \qquad (2)$$

where n is number density, t is time, y is the vertical coordinate, D is the total diffusion coefficient (the combined effect of molecular and turbulent diffusion). The subscript i denotes a property for a specific species and the last term represents the rate of change of number density for the species of interest due to chemical reactions. The diffusion from the initial profile of produced nitric oxide for the Chicxulub impact is shown in Fig. 2.

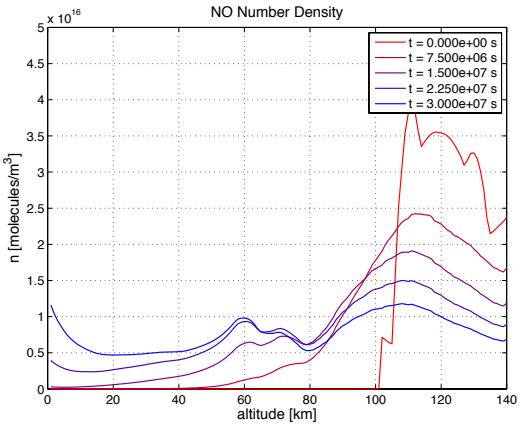

Figure 2: The initial distribution of nitric oxide at several times as it diffuses from the initial distribution.

In addition, this work includes the time required for the pollutants to be absorbed into clouds and precipitate into the ocean. An estimation of the effect of carbonate buffering in the ocean water is provided. The resulting time history for the pH level of the upper 100 meters of the ocean is calculated and this minimum pH level is then generalized for a variety of initial impactor energies and resulting ejecta masses. A sample pH history for the Chicxulub impact is shown in Fig. 3.

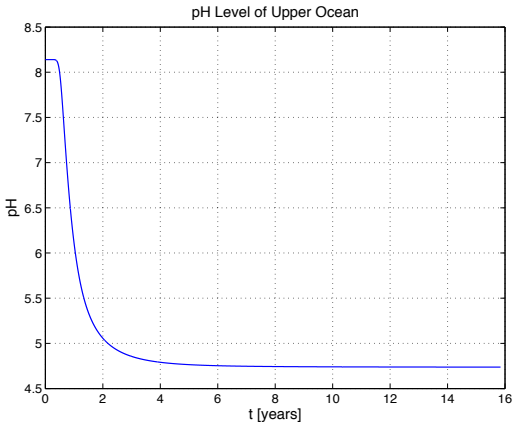

Figure 3: A sample time history for the pH level of the upper ocean neglecting the effect of buffering.

Conclusion: Ultimately, it was determined that a significant fraction of the original toxins reached the stratosphere and precipitated as acid rain, decreasing the pH level of the ocean and affecting marine life.

References: [1] Goldin, T. J., and H. J. Melosh (2009), *Geology*, *37*, 1135-1138. [2] J. Lewis, H. Watkins, H. Hartman, and R. Prinn, *Geological Society of America* (1982). [3] Melosh, H. J., N. M. Schneider, K. J. Zahnle, and D. Latham (1990), *Nature*, *343*, 251-254. [4] Johnson, B. C., and H. J. Melosh (2012), *Icarus*, *217*, 416-430. [5] M. Ivanov, A. Kashkovsky, S. Gimelshein, G. Markelov, A. Alexeenko, Y. Bondar, G. Zhukova, S. Nikiforov, and P. Vashenkov, *25th Intl. Symposium on Rarefied Gas Dynamics*, 2006, pp. 21–28. [6] H. Hassan, and D. Hash, *Phys. Fluids* 5, 738–744 (1993). [7] J. Smit, *Annu. Rev. Earth Pl. Sc.*, 1999, pp. 75–113. [8] D. Parkos, M. Kulakhmetov, B. Johnson, H. Melosh, A. Alexeenko. *28th Intl. Symposium on Rarefied Gas Dynamics*, 2012.