Potential Explosion Hazard of Carbonaceous Nanoparticles:

Explosion Parameters of Selected Materials

Supplemental Material

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**Statistical Correlations of the Explosion Parameters**

As discussed in our first paper [Turkevich et al. 2014], the explosion severity index, K(500), is highly correlated with the maximum explosion overpressure, Pm(500) [Figure 5 of Turkevich et al. 2014]; this high degree of correlation is confirmed (R2 = 0.9) between the global explosion severity index, KSt, and the global maximum explosion pressure, Pmax

The minimum explosive concentration, MEC, is also highly correlated with both Pmax (R2 = 0.7) and with KSt (R2 = 0.8)

As expected, the more explosive powders (high Pmax, high KSt) exhibit a lower concentration threshold (MEC) for explosion.

However, the minimum ignition energy, MIE, is poorly correlated with both Pmax (R2 = 0.2) and with KSt (R2 = 0.3)

Although the correlation is poor, the trend is as expected, namely the more explosive materials (high Pmax, high KSt) exhibit a lower ignition threshold (MIE) for explosion. It is not surprising that there is a similar lack of correlation (R2 = 0.2) between MIE and MEC

Again, while the correlation is poor, the trend is as expected, namely, the materials with a low concentration threshold (MEC) also exhibit a low ignition threshold (MIE).

Similar behavior obtains for the minimum ignition cloud temperature: MITcloud is reasonably correlated with both Pmax (R2 ~ 0.6) and KSt (R2 ~ 0.7)

with the more explosive powders (high Pmax, high KSt) exhibiting a lower temperature threshold (MITcloud) for explosion. There is poor correlation (R2 ~ 0.3) between MITcloud and MEC and also (R2 ~ 0.3) between MITcloud and MIE

Again, while the correlation is poor, in both cases, the trend is as expected, namely, that materials with low concentration (MEC) and ignition (MIE) thresholds for explosion also exhibit a low temperature threshold (MITcloud) for explosion.

**Statistical Correlation with Aggregate Particle Size.**

We believe that aggregation of the primary particles is not a significant determinant of the explosion parameters. As indicated in the main paper, there is no evidence of any tightly bound aggregates from our electron micrographs (either before or after explosion). We believe that aggregation has, at best, a minimal effect on the explosion parameters of the carbonaceous nanomaterials.

As discussed in the main paper, we have measured aggregate particle size distributions with light scattering (CILAS 1064). We have attempted to correlate the various parameters that characterize those distributions with the measured explosion parameters. The aggregate size distributions are all broad and multimodal (main paper, Figure 1). Statistically, we may identify a mean size, dmean, and the size of the mode (cumulant midpoint), d50; qualitatively, we may also identify the size, ddom, of the dominant mode, as well as the sizes, dmax and dmin, of the largest and smallest modes, respectively. As most of the weight is at the upper end of the distributions, the parameters, dmean, d50, ddom, dmax are essentially equivalent.

There are weak statistical correlations (R2 ~ 0.6) of Pmax with dmean, d50, ddom, dmax

There are similar weak statistical correlations (R2 ~ 0.6) of KSt with dmean, d50, ddom, dmax

Statistically, the smaller the aggregate, the less explosive is the material—i.e. smaller Pmax and smaller KSt. However, under the NanoSafe hypothesis, the smaller aggregates should be more explosive. Thus the NanoSafe model is not supported by the statistical correlation.

With such a limited data set, it is impossible to deconvolute the effect of aggregate particle size from the effect of allotrope on explosion severity; e.g. on the above correlation plots, the most explosive material, fullerene (Pmax = 8 bar, KSt = 199 bar-m/s), is always upper right, and the least explosive material, graphite (Pmax = 6.3 bar, KSt = 64 bar-m/s), is always lower left. Given the established dependence of explosion severity on allotrope [Turkevich et al. 2014], it is difficult to extract any additional influence of aggregate particle size on the severity of the carbonaceous explosions.

For completeness, we have also examined the potential correlation with the lower end of the distribution, dmin; there is poor correlation of both Pmax (R2 ~ 0.1) and KSt (R2 ~ 0.2) with dmin

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Similarly, we have attempted to correlate MEC with aggregate particle size. The correlation is weak (R2 ~ 0.6) for dmean, d50, ddom, dmax

Again, the weak statistical correlation contradicts the NanoSafe hypothesis, namely, while the smaller aggregates should be more explosive, statistically, the smaller aggregates exhibit a higher threshold MEC for explosion.

There is no correlation of MEC with dmin (R2 ~ 0.1)

We have not attempted to correlate the more limited data sets for MIE, MITcloud with the aggregate particle size distribution parameters.