A35Q-1876 - Garbage-In Garbage-Out (GIGO): The Use and Abuse of Combustion Modeling and Recent U.S. Spacelaunch Environmental Impacts

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🕐 **15:00 - 17:00**
📍 **Convention Center - Poster Hall, D-F**

Background: Garbage-In, Garbage-Out (GIGO) combustion calculations are defined here as the use of a detailed Arrhenius chemical-kinetic reaction/combustion suite for _some of the_ chemical species which are present in real-world combustion, but the exclusion _by choice_ of detailed reactions of other crucial chemical species known to be present. In the simplest instance, a detailed H_2+O_2+CO reaction suite combined with a single kerosene _overall- or net-reaction_ (pseudoreaction) can produce valid LOX/RP-1 (kerosene) combustion chamber pressures and temperatures for engine-design purposes, but the results _cannot_ produce data on the hydrocarbons relevant to nozzle efficiency and mandated environmental assessments, because it ignores the complex hydrocarbon chemistry dependent upon trace-O_2 hydrocarbon _cracking_ and _oligomerization reactions_ (e.g., Christardo [2009], Seshardi [1982], VanKamp [1984], Speight [2003]) which ultimately produce the soot observed in real-world combustion. Non-GIGO chemistry for these key species in LOX/RP-1 combustion modeling has been available for decades (e.g., Marinov [1998]); see figure), and reproduces known LOX/RP-1 measurements: Large quantities – _up to several percent of total fuels flow_ – of complex hydrocarbons are typical; benzene, butadiene, and polycyclic aromatic hydrocarbons (PAH) such as anthracene, fluoranthene, etc. (Thompson, _Rocketdyne_ [1966]; figure). These hydrocarbons are the well-known _soot-precursor_ species, and are therefore necessarily formed concomitantly with soot (e.g, Pugmire [2001]). The direct observation of large quantities of soot in a rocket plume is thus _diagnostic of low combustion-efficiency and the presence of these chemical species_, and low overall engine-efficiency due to rocket nozzle thermodynamics. The latter is due inefficiency in extracting molecular vibrational energy from the expansion of large polyatomic molecules such as benzene and PAH (Clark [1972]). Examples are provided. Additionally, legal limits have since been established on the production of these class-1 carcinogens from internal combustion engines (rocket engines), and appropriate employee and civil protections established, making these species important to model and measure directly in the lack of afterburning (see below). These considerations apply to both the open-cycle fuel-rich gas generators and main engine combustion chamber fuels and film-coolants in LOX/RP-1 engines since the products distribution is largely thermodynamically controlled.

During the decades of government-funded launch vehicle development, liquid fueled engines for space launch were typically designed for high efficiency to maximize, for instance, mass-to-orbit. To this end, pre-burners and high-energy fuels atomization (via high-energy swirl or impinging injectors) have been used to minimize fuel droplet starting size, maximizing gasification rate, and increasing _gas-phase_ combustion efficiency and therefore engine/nozzle efficiency (Clark; Sutton; Sutton/Yang). Recent private LOX/RP-1 rocket engine development in the U.S. (SpaceX), and a strikingly similar Korean engine (Hanwha), favor particularly _low_-combustion-efficiency by eschewing fuel atomization in favor of Pintle-style injectors (Son [2016], Seedhouse; _Springer_ [2013], Mueller [2012], Zarchan [2004]). The resulting low gasification rate of the characteristically large RP-1 fuel droplets maximizes the yield of large hydrocarbons (e.g. benzene, PAH, PM2.5, tars, and cokes), lowering gas-generator/nozzle/engine efficiency. Egregious GIGO errors can be seen, for instance, in recent U.S. Environmental Assessment/Impact documents (45th Space Wing [2007], U.S. Army [2007], Nelson Eng. [2013], F.A.A. [2014], Sierra Eng. #_2003-001_ [2003], Song [2017]) wherein GIGO calculations _de facto_ instruct computer combustion models to _ignore PAH formation known to be present_. Examples are provided. _Awareness of the above combustion science is essential knowledge for research personnel involved in understanding launch vehicle upper-atmospheric impacts and climate disruption._

Impacts: During flight in the Troposphere, a sufficient atmospheric partial pressure of O_2 is present to burn-off the PAH and soot generated by low-efficiency rocket engines, ignited by the hot rocket plume. This so-called "afterburning" of the excess hydrocarbons (soot, tars, PAH, etc.) gives rise to the _brilliant_ appearance of an inefficient LOX/RP-1 plume shortly after lift-off in these engines; however, above the troposphere, and on the launch stand during water-deluge, afterburning ceases and the predominant quantities of these species are directly deposited and persist. Examples are provided. Low-efficiency launch vehicles also need significantly larger liftoff fuels loads (a factor of >1.2) to achieve similar orbital mass, further increasing the per-launch yield of complex hydrocarbon tars and stable PAH free radicals. These are deposited directly into launch trajectories, including the launch pad, stratospheric ozone layer, mesosphere, and above. Increasing launch rates of these new, low-efficiency engines must therefore have an increasing cumulative impact on critical and poorly-understood upper-atmosphere chemistry systems (Ross/Sheaffer [2014]; Sheaffer [2016]). For instance; the ozone reactions of gas- or condensed-phase hydrocarbon tars combined with PM2.5 have not yet been studied in detail, and potentially represent an unrecognized class of ozone-depleting compounds. The direct deposition of PAH tars during orbital maneuvers in populated orbits and orbital stations is of potential concern to the satellite remote-sensing community. The solar absorption of these species is much higher than that of the background atmosphere, and converts UV/Visible insolation into upper-atmospheric heat.

Benzene yield of >1% in non-GIGO hydrocarbon combustion (e.g., Marinov [1998]) modeled under very low O_2 conditions, chemistry similar to that of engine film coolants and in fuel-rich gas generators combustion. Benzene formation is one of the key initial steps along the chemical pathway to the formation of soot in low-combustion-efficiency, fuel-rich internal combustion engines. (e.g., Pugmire [2001]) Due to the chemical process of soot formation, the observation of soot is diagnostic for the presence of benzene, PAH, PM2.5, tars, and cokes.