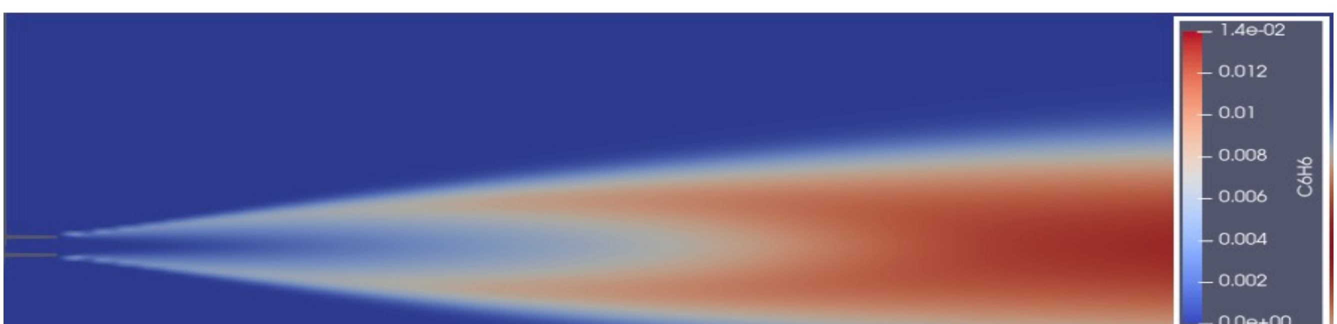
A35Q-1876 - Garbage-In Garbage-Out (GIGO): The Use and Abuse of Combustion Modeling and Recent U.S. Spacelaunch Environmental Impacts

Wednesday, 15 December 2021
15:00 - 17:00
Convention Center - Poster Hall, D-F

Background: Although detailed Arrhenius chemical-kinetic reaction/combustion suites for were not readily available for LOX/kerosene combustion modeling until ca. 1990 (e.g., Marinov [1998]; see figure), it was already known from mass-spectrometer measurements during the early Apollo era that fuel-rich liquid oxygen + kerosene (RP-1) gas generators yield large quantities – *up to several percent of total fuels flow* – of complex hydrocarbons such as benzene and butadiene, and polycyclc aromatic hydrocarbons (PAH) such as anthracene, fluoranthene, etc. (Thompson, *Rocketdyne* [1966]). Although most of these have not been characterized, many are known to be class-1 carcinogens. These are well-known *soot-precursor* chemical species, and are therefore *necessarily formed concomitantly with soot* (e.g, Pugmire [2001]). Significant soot in a rocket plume is therefore *diagnostic of low combustion efficiency, and therefore low engine efficiency,* due to fundamental rocket nozzle thermodynamics, yielding low overall launch-vehicle efficiency (Clark [1972]). This is due to the inability of the nozzle to extract energy from the expansion of large molecules, such as PAH. Examples are provided. As early as the 1960's, the detrimental impact of low combustion efficiency on the governing rocket-nozzle efficiency factor had been empirically well-understood. Also at that time the U.S. EPA had not been established, nor had legal limits been set on the production of class-1 carcinogens by internal combustion engines (rocket engines). This discussion applies directly to both open-cycle fuel-rich gas generators and main engine combustion chamber fuels and film coolants in LOX/RP-1 rocket engines.

During the decades of government-funded launch vehicle development, liquid fueled engines for space launch were typically designed for high efficiency in order to maximize orbital parameters and mass-to-orbit while minimizing fuels and structural masses. To this end, pre-burners and high-energy fuels atomization (via high-energy swirl or impinging injectors to pre-atomize fuels) have been used to decrease fuel droplet size and thereby increase *combustion efficiency / nozzle efficiency*, maximizing system launch and orbital-maneuver capability (Clark; Sutton; Sutton/Yang). Recent private LOX/RP-1 rocket engine development in the U.S. (SpaceX) and Korea favor particularly low-combustion-efficiency, with no fuels atomization incorporated due to the use of Pintle-style injectors (Seedhouse; *Springer* [2013], Mueller [2012], Zarchan [2004]). The resulting very low RP-1 gasification rate in the combustion chambers maximizes the yield of high-molecular-weight hydrocarbons (e.g. benzene, PAH, PM2.5, and cokes), via thermal cracking and oligomerization of unburned hydrocarbons, lowering nozzle efficiency. Additionally, the combustion community has long been aware that specific Arrhenius chemical-combustion suites are *required* to validly estimate the yield of these hydrocarbons; nevertheless, egregious GIGO errors can be seen, for instance, in many recent U.S. EPA Environmental Assessment/Impact documents (45^{th} Space Wing [2007], U.S. Army [2007], Nelson Eng. [2013], F.A.A. [2014], Sierra Eng. *2003-001* [2003]) wherein a H_2+O_2+CO mechanism is used to *de facto* instruct computer combustion models to *ignore PAH formation*, which are nonetheless *known to be present* due to the presence of significant soot. *Knowledge of these facts is <u>essential</u> for valid atmospheric pollution research, especially in the upper atmosphere.*

It is therefore the *environmental impacts* of the above considerations which are the primary goal of this document: During rocket flight *in the lower Troposphere only*, a sufficient atmospheric partial pressure of O_2 is present to burn off the PAH and soot generated by low-efficiency rocket engines in the hot rocket plume; however, at all altitudes above the lower troposphere, and on the launch stand during water-deluge, these species persist and are directly deposited. Examples are provided (see also figure, modeled after Marinov [1998]). Low-efficiency launch vehicles also need significantly larger fuels loads to achieve the same launched mass, further increasing the yield of complex hydrocarbon tars and stable PAH free radicals deposited along launch trajectories, including the launch pad, stratospheric ozone layer, mesosphere, and above. Increasing launch rates of new low-efficiency engines must therefore have an increasing cumulative impact on critical, poorly-understood upper-atmosphere chemistry systems (Ross/Sheaffer [2014]; Sheaffer [2016]). For instance; the ozone reactions of gas-phase or condensed 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 orbital stations is also of potential concern to the satellite remote-sensing community.



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