Aerospace Propulsion

Lecture 6

Combustion: Part IV

Combustion: Part IV

- Molecular Nomenclature
- Fuels
- Oxidizers
- Clean Fuels
- Pollutants

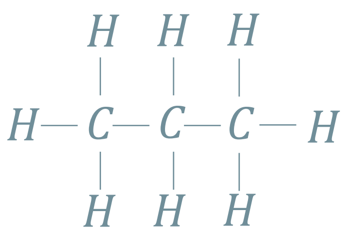
Fuels and Oxidizers

- What do we put into our aerospace vehicles?
- Aerospace fuels and oxidizers are often (but not always)
  - Complex molecules
  - Inconsistent mixtures
  - Primarily C,H,O,N
- Selected or designed to give a set of beneficial physical and chemical properties
- Generally stored in either liquid or solid form

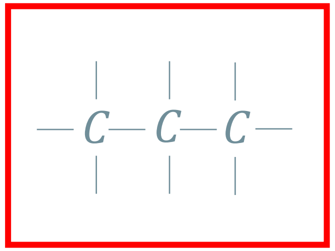
Molecular Nomenclature

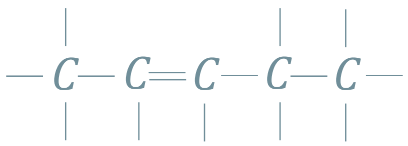
Remember the number of covalent bonds each atom can form:
H: 1 **O:** 2 **N:** 3 **C:** 4

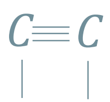
- Paraffins (Alkanes) C_nH_{2n+2}
  - Single covalent C-C bonds
  - Ends with “ane”
  - Example: *n*-propane
- Olefins (Alkenes) C_nH_{2n}
  - One double covalent C-C bond
  - Location noted with leading number
  - Ends with “ene”
  - Example: 2-pentene
- Acetylenes (Alkynes) C_nH_{2n-2}
  - One triple covalent C-C bond
  - Ends with “yne”
  - Example: ethyne (acetylene)



Common shorthand that we’ll use



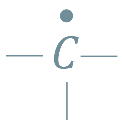




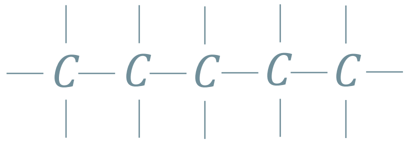
Prefix	C_n
Meth-	C_1
Eth-	C_2
Prop-	C_3
But-	C_4
Pent-	C_5
Hex-	C_6
Hept-	C_7
Oct-	C_8
Non-	C_9
Dec-	C_{10}
Dodec-	C_{12}
Hexadec-	C_{16}

Molecular Nomenclature

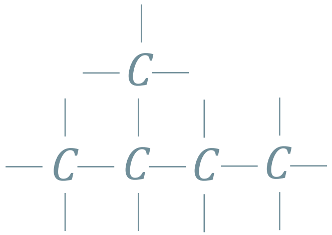
- Alkyl (ends in “yl”)
  - Alkane missing one hydrogen bond
  - Example: Methyl



- Normal Hydrocarbons (starts with “n”)
  - All carbons in a straight chain
  - Example: *n*-pentane

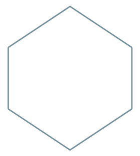


- Branched (iso) Hydrocarbons (starts with “iso”)
  - Carbon chains are branched
  - Example: iso-pentane (2-methylbutane)
  - Larger molecules have multiple branched forms

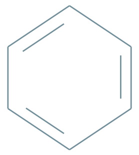


Molecular Nomenclature

- Cyclo-Hydrocarbons (starts with “cyclo”)
  - Covalent C-C bonds form rings rather than straight/branched chains
  - Example: cyclohexane



- Aromatics
  - Six-membered rings
  - Alternative single and double bonds
  - High sooting tendency when burned
  - Example: benzene



Molecular Nomenclature

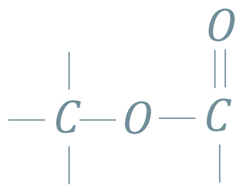
- What if we now consider molecules with oxygen?
  - Oxygen in fuel significantly lowers energy density
  - Alcohols (ends in “ol”)
    - One OH group replacing hydrogen
    - Example ethanol (ethyl alcohol)
  - Ethers
    - Hydrocarbon group on each side of an oxygen atom
    - Example: dimethyl ether (methyl-methyl ether)

$$\begin{array}{cccccc} & | & & | & & \\ - & C & - & C & - & OH \\ & | & & | & & \end{array}$$

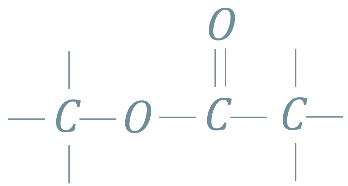
$$\begin{array}{ccccccc} & | & & & & | & \\ - & C & - & O & - & C & - \\ & | & & & & | & \end{array}$$

Molecular Nomenclature

- What if we now consider molecules with oxygen?
  - Esters (ends in “oate”)
    - Ether with a second oxygen double bonded to a carbon next to the ether oxygen
    - Example: methyl methanoate



    - Example: methyl ethanoate



    - Common in biofuels

Liquid Fuels

- What is a practical fuel made from?
  - Every batch will be different
    - Exact composition depends on petroleum, additives, etc.
  - There are standards, but these have wiggle room
  - Consider Jet-A
    - Main jet fuel used in the US
    - Representative composition (by volume) of
      - 60% Paraffins
      - 25% Cycloparaffins
      - 15% Aromatics
      - 5% Other (Often additives to achieve specific mixture properties)

Liquid Fuels

- Properties important to practical fuels
  - Density
  - Viscosity
  - Boiling point
  - Freezing point
  - Vapor pressure
  - Ignition temperature
  - Flammability limits
  - Storability
  - Price
  - …and on and on and on

Can only carry so much weight

Flame shouldn’t extinguish at altitude

Must be pumpable from storage to combustor

Fuel shouldn’t leak while in storage

Liquid Fuels

- Common jet fuels (nearly all are kerosene based)
  - Jet-A
    - Standard jet fuel in the US
  - Jet-A1
    - Standard jet fuel everywhere else (except Russia)
  - JP-4
    - USAF 1951-1995
    - 50/50 kerosene/gasoline
  - JP-8
    - US Military “universal fuel”
    - Meant to work for both turbine-powered aircraft and diesel-powered ground vehicles

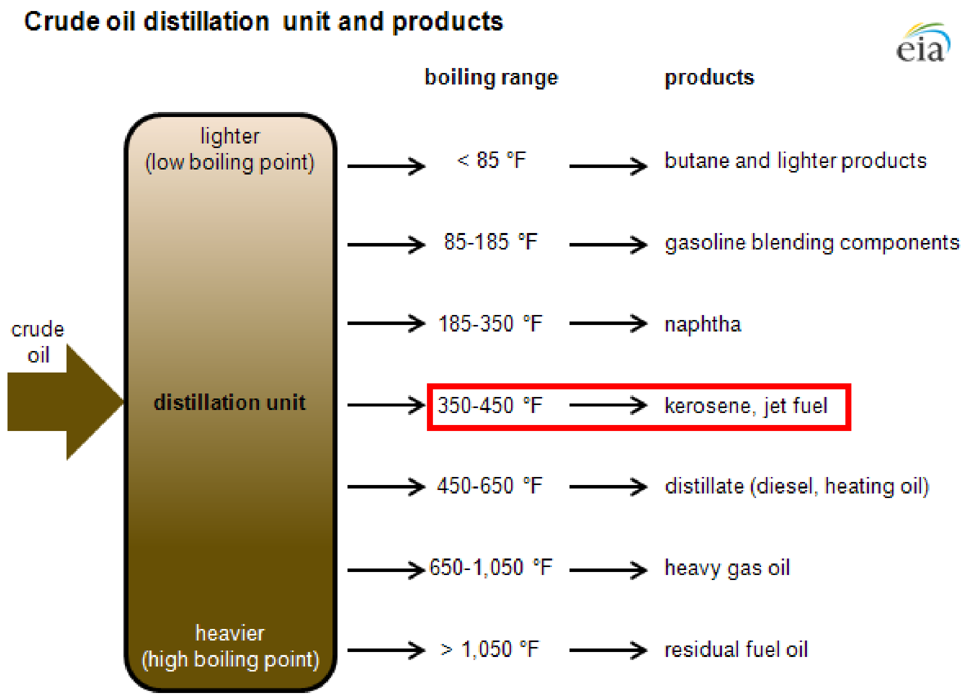
	Jet A-1	Jet A
Flash point	38 °C (100 °F)	
Autoignition temperature	210 °C (410 °F)[7]	
Freezing point	−47 °C (−53 °F)	−40 °C (−40 °F)
Max adiabatic burn temperature	2,230 °C (4,050 °F) open air burn temperature: 1,030 °C (1,890 °F)[10][11][12]	
Density at 15 °C (59 °F)	0.804 kg/L (6.71 lb/US gal)	0.820 kg/L (6.84 lb/US gal)
Specific energy	43.15 MJ/kg (11.99 kWh/kg)	43.02 MJ/kg (11.95 kWh/kg)
Energy density	34.7 MJ/L (9.6 kWh/L) [13]	35.3 MJ/L (9.8 kWh/L)

Liquid Fuels

- Common (liquid) rocket fuels
  - Hydrogen (H_2)
    - Massive energy release relative to burned mass
    - Low density and needs to be very cold
  - Liquid Methane (CH_4)
    - Less energetic than hydrogen, but more dense
  - RP-1 and RP-2
    - Kerosene based, more similar to jet fuels
  - Hydrazine (N_2H_4)
    - Highly toxic

Liquid Fuels

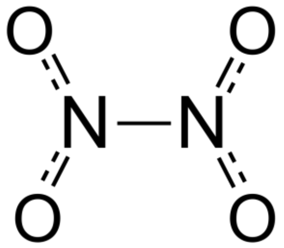
- Fuel production
  - Kerosene based (e.g., Jet-A and RP-1)
    - Distillation of crude oil
      - Dig it out of the ground, separate by weight
    - Mix components back together
      - Aim for specific fuel properties
  - Methane
    - Main component of natural gas
      - Fossil fuel from gas/oil wells
  - Hydrogen
    - Steam methane reforming ~ 50% of H_2 production
    - $CH_4 + H_2O \rightarrow CO + 3H_2$ followed by $CO + H_2O \rightarrow CO_2 + H_2$



Oxidizers

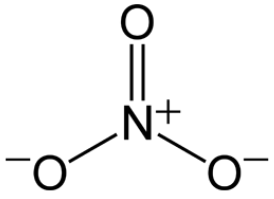
- Generally, vehicles not headed to space use air as the oxidizer
  - Doesn’t need to be stored on-board, free, and unlimited
- Space-bound vehicles usually need to bring oxidizer with them
  - No air in space, and high mass flow rates required

- Liquid oxygen (LOX)
  - Good performance, but cannot be stored long
- Nitrogen Tetroxide (N_2O_4)
  - Easy to store (most common storable oxidizer)
  - Extremely toxic

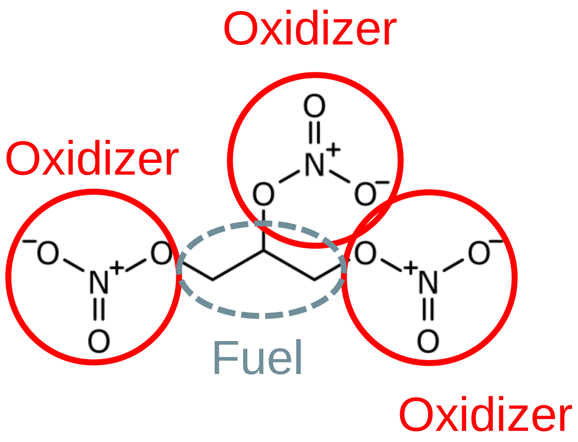


Solid Rocket Propellants

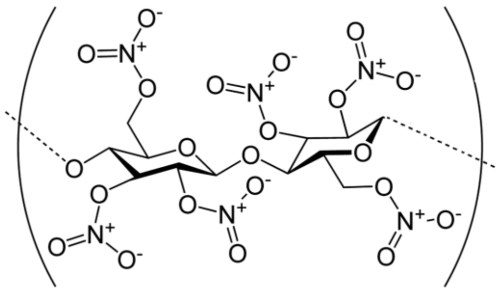
- Things get more interesting…
  - Nitrate
    - Powerful oxidizer
    - Burns well when mixed with hydrocarbon fuel



  - Can molecules have both fuel and oxidizer?



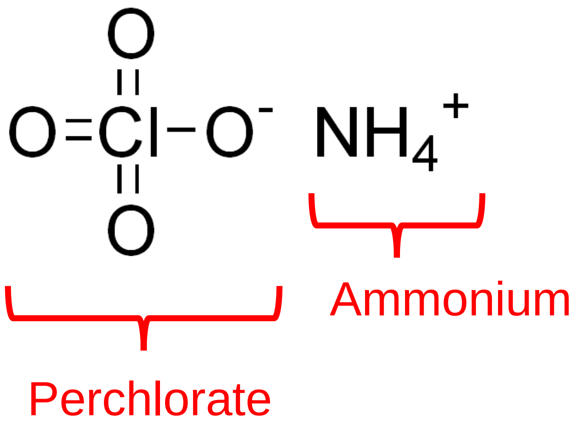
  - JPN propellant (Double-Base)
    - 51.5% Nitrocellulose
    - 43.0% Nitroglycerine
    - Each molecule is F+O



Solid Rocket Propellants

- What if we look beyond C,H,O,N?
  - Metals have desirable fuel properties
    - High energy density
    - High mass density
    - Non-toxic in solid form

  - PBAN propellant (Composite)
    - 70% Ammonium Perchlorate (oxidizer)
    - 16% Aluminum Powder (fuel)



Clean Fuels

- Increasingly strict regulations for how much CO_2 can be exhausted
  - Mainly an issue for aircraft
  - Capturing carbon after burning is tough
- Clean Hydrogen (H_2)
  - Hydrogen must be produced through renewable resources + electrolysis
  - Storage, transport, price?
- Ammonia (NH_3)
  - Easier to store and transport, potentially convert to H_2
- Biofuels (e.g., Sustainable Aviation Fuel)
  - Convert (for example) crops to fuel, no net carbon release

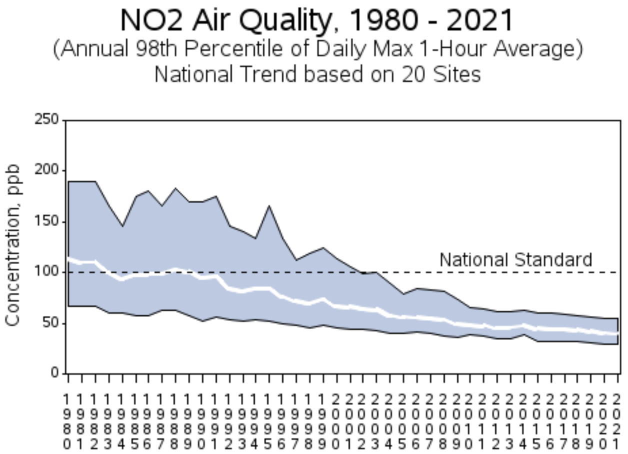
Pollutants

- Nitrogen Oxides (NO_x)
  - Primarily NO and NO_2
  - Creates ground layer ozone and photochemical smog
  - Causes and complicates respiratory problems

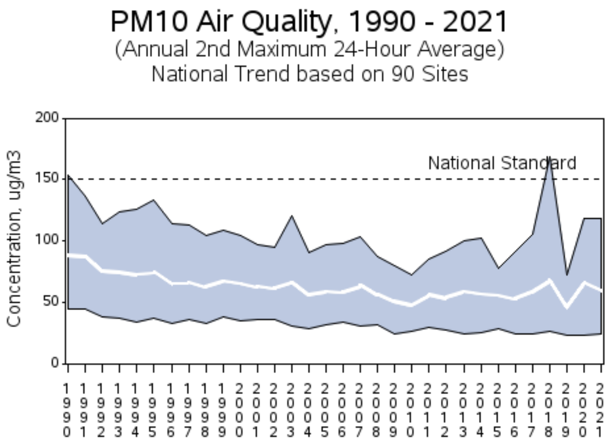
- Particulate Matter (Soot, Black Carbon)
  - Nano- to micro-scale essentially carbon particles
  - Nucleation sites for contrails and other aerosols
  - Severe respiratory and pulmonary effects

Pollutants

- Regulations
  - These emissions are tightly regulated worldwide and have been significantly reduced since the early 70's
  - Unlike CO_2, these emissions can be significantly reduced without massive technological and behavioral measures



1980 to 2021 : 64% decrease in National Average



1990 to 2021 : 32% decrease in National Average

Pollutants

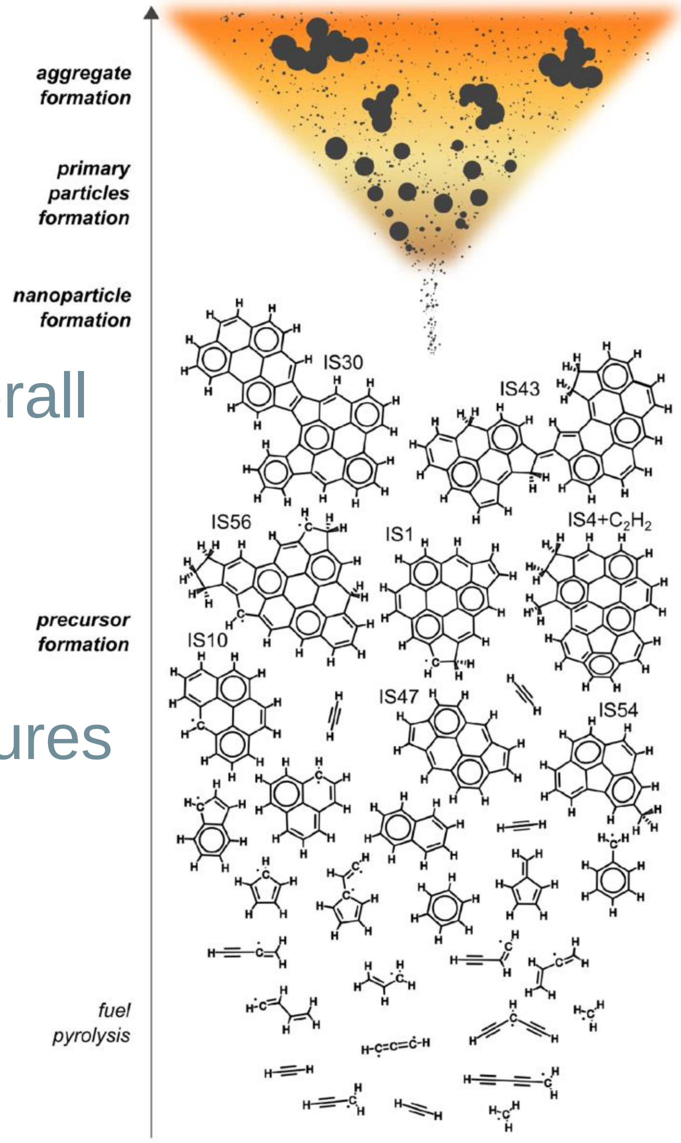
- Three rules of pollutants
  - **Rule #1**: Formation of pollutants is kinetically controlled (slow chemistry)
    - "Long" residence times (at specific conditions) are required for pollutant formation
    - Solution: Design combustion systems with short residence times
    - Complication: Short residence times increase CO and unburned hydrocarbons (UHC) due to insufficient combustion time
  - **Rule #2**: Once formed, NO_x is difficult to remove by combustion means
    - Solution (for aircraft): Avoid forming NO_x as much as possible
  - **Rule #3**: Once cold, soot is difficult to remove by combustion means
    - Solution (for aircraft): Try to destroy any formed soot before it reaches cold gases

Pollutants

- Primary NO_x formation mechanism (Zeldovich, Thermal)
  - $N_2 + O \leftrightarrow NO + N$ (very slow, rate-limiting, irrelevant at low temperatures)
  - $N + O_2 \leftrightarrow NO + O$ (fast)
  - $N + OH \leftrightarrow H + NO$ (fastest)
- Conditions conducive to NO_x formation
  - High temperatures (>1800 K)
    - Nonpremixed flames
    - Stoichiometric premixed flames
- Conditions conducive to NO_x destruction
  - None

Pollutants

- Soot evolution
  - Small gaseous molecules combining with an overall increasing C/H ratio until solid
  - Solids combine to grow in size
- Conditions conducive to soot formation
  - Very rich mixtures ($\phi > 2$) at moderate temperatures (1200 K – 1800 K) and long timescales
- Conditions conducive to soot destruction
  - High temperatures (>1800 K)
  - OH and O_2-rich gases
  - Oxidation with OH is very fast



Pollutants

- Avoiding all pollutants simultaneously is tough
- Role of fuels
  - Jet-A
    - Made of 15% aromatics which jump start soot formation
  - Hydrogen
    - No carbon so no soot
    - Burns at high temperatures so NO_x is an issue
  - Methane
    - Low C/H ratio so forms less soot
  - Biofuels
    - Presence of oxygen lowers flame temperature and suppresses soot