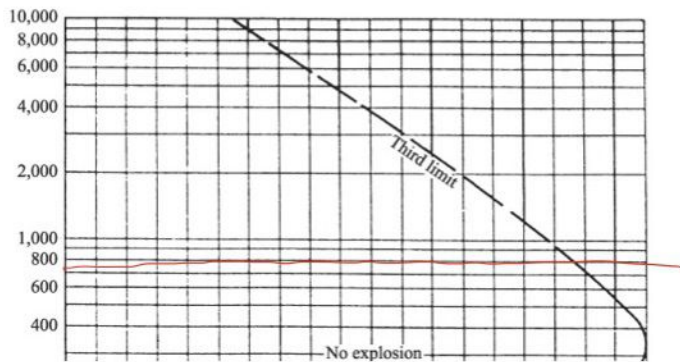
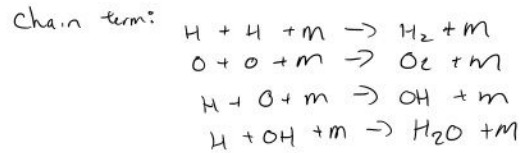
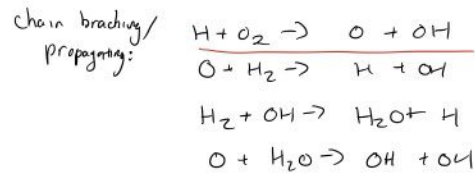
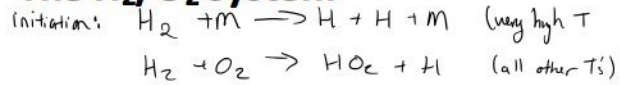


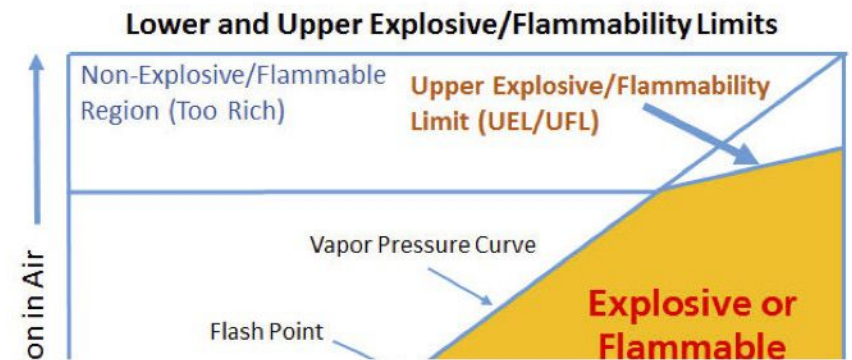
# Chemical Mechanisms

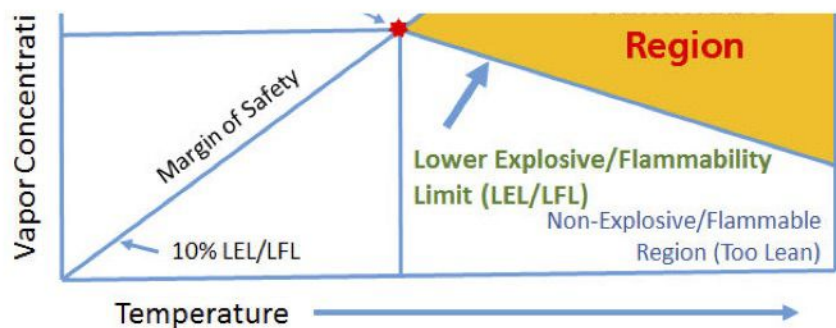
Thursday, September 28, 2017 1:05 PM

## The H<sub>2</sub>/O<sub>2</sub> system



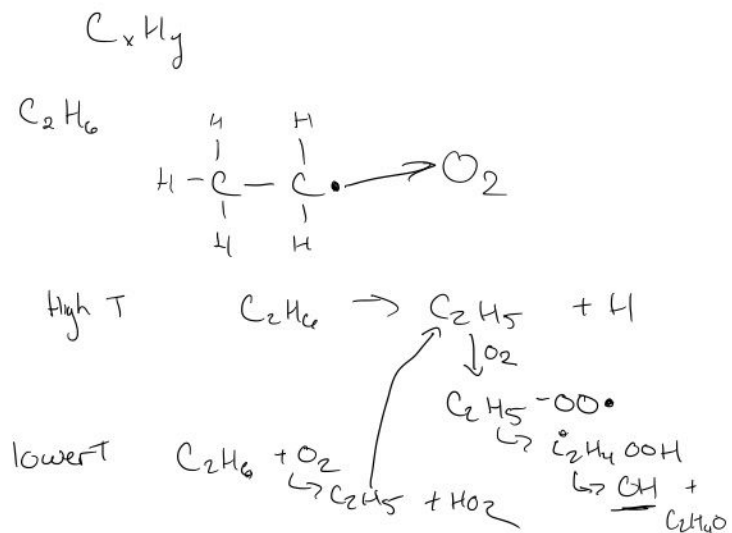
**Figure 5.1** Explosion limits for a stoichiometric hydrogen–oxygen mixture in a spherical vessel. | SOURCE: From Ref. [2]. Reprinted by permission of Academic Press.





## Combustion of Alkanes

Chemistry of Ignition:



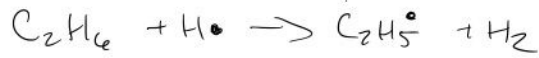
[Hydrogen Explosions \(slow motion\) - Periodic Table of Videos](#)



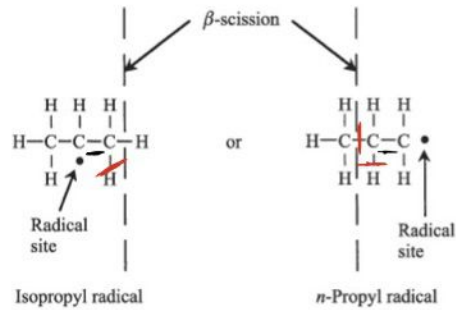
Chemistry post-ignition:

- ↳ heat release
- ↳ radical formation

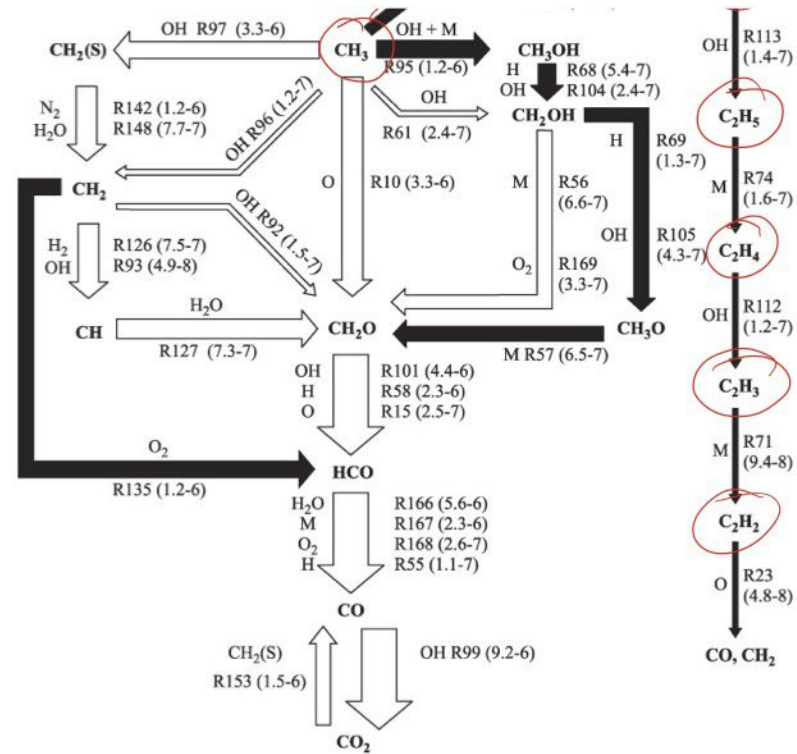
Abstraction:  $H, OH, CH_2$



fuel radicals  $\rightarrow$   $\beta$  scission



**Figure 5.3** The  $\beta$ -scission rule applied to bond breaking in  $C_3H_7$ , where the radical site occurs at different locations. Note the intervening C-C bond between the radical site and the broken bond.



**Figure 5.5** Low-temperature (< 1500 K) reaction pathway diagram for combustion of methane in a well-stirred reactor at  $T = 1345$  K and  $P = 1$  atm for a 0.1-s residence time. Reaction numbers refer to Table 5.4, and reaction rates are shown in parentheses. For example, 2.6-7 implies  $2.6 \cdot 10^{-7}$  (gmol/cm<sup>3</sup>-s). Results shown are for GRI Mech 2.11.

