

Chemical Libraries: Mechanism Construction & Reduction

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Combustion chemistry is one of the pillars of combustion science. Unfortunately, the chemical mechanisms by which fuel is converted into energy (simultaneously producing pollutants and sometimes also desirable materials) are so complex that they are hard to construct, and these large mechanisms challenge conventional methods of peer review and debugging. Often the chemistry is so complex that it is not feasible to solve the exact chemical kinetic equations, particularly in complex fluid-dynamic situations, and approximate reduced chemistry models must be used. Producing a suitable reduced model can be a challenge, and it is hard to know how much error has been introduced by approximating the chemistry in this way. Despite considerable work in the literature that indicates that these issues are solvable, the broad combustion community does not yet have access to cyber-tools that make this convenient, and the conventional data models for mechanisms are not completely satisfactory. Here we will discuss two recent attempts to provide some of these cyber-tools, and to develop data models suitable for cyber-collaboration: the RMG mechanism-generation and RIOT mechanism-reduction packages. We will also present a vision for how combustion science could be done in the future, using these mechanism-tools in conjunction with cyber-databases and other cyber-tools.