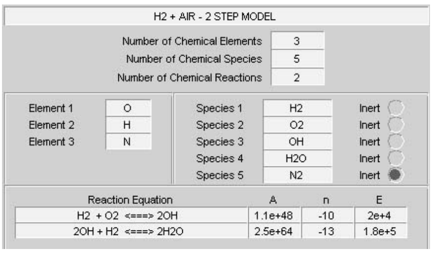
CAESIM chemical reaction models can be applied to situations involving combustion, power generation, propulsion systems, and chemical vapor deposition, among others. **CAESIM** offers seven types of reaction models with varying degrees of complexity and generality.

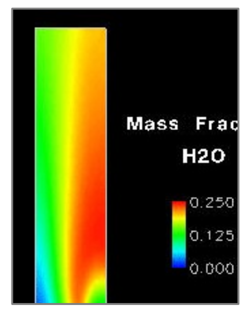
Reaction Model	Description
Frozen	Solves for chemical species transport without reaction (mixing only)
Instantaneous	"Fast chemistry" mixture fraction model for situations where the reaction time scale is much less than that of the flow.
Equilibrium	Specialized "fast chemistry" model for two-way reactions, products based solely on thermodynamic state of the system.
Mixture Fraction	Specialized finite-rate, single-step chemistry model designed primarily for oxidation/combustion problems.
Finite Rate	Full finite-rate, multi-step chemistry model with kinetic source terms. The most general of all CFD2000 reaction models. Useful for situations where reaction time and flow time scales are comparable.
CVD	Finite-rate, multi-step chemistry model for chemical vapor deposition. Activates a Soret diffusion term in the species conservation equation
Surface Reactions	Reactions occurring at a gas-solid, gas-liquid, or liquid-solid interface. Catalytic or combustion reactions can be modeled.

CAESIM includes a library of pre-defined finite rate reaction models. Most of these reactions involve at least two "steps", and a few require thirty or more. Required inputs for these models include the reaction equations, the reaction collision coefficient **A**, the collision factor exponent **n**, the activation energy **E**, and the values of any third body coefficients M.



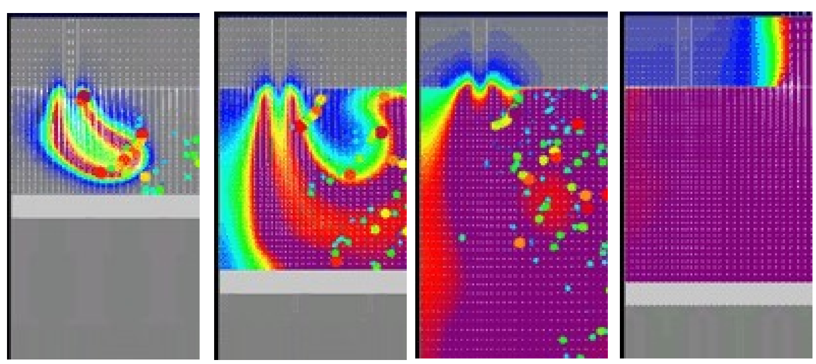
Arrhenius Equation: $$k_f = AT^N \exp\left(-\frac{E_a}{R_0 T}\right)$$

The figure to the right shows a supersonic jet diffusion flame solution. A compressible, turbulent, reacting flow is assumed, and the chemical reaction type is set as "Finite Rate," with "H2 + Air - 2 Step" selected as the model that represents the combustion process. The transport equations for the H2, O2, OH, H2O and N2 species are solved. "Generic Mixture," which assumes ideal gas behavior, is selected as the default fluid for the model. Values for the gas constant, specific heat and ratio of specific heats are computed from local concentrations.



CAESIM Application Examples

Flow and combustion inside an engine cylinder is simulated. The fuel (methane) and oxygen enter the cylinder chamber through separate outlet ports. During the intake stage, the piston head moves down and combustion occurs. The residual gases are ejected from the cylinder chamber through the outlet port during the upstroke of the piston head.



Intake and combustion start **Combustion end and exhaust**

The figure to the right depicts high speed compressible flow and secondary flash phenomena for a G3 weapon blast using a 10-step finite-rate chemical reaction model. Shock heating, air entrainment, and chemical reactants/products are determined.