Combustion modeling with Comsol4.2a

Limitation for model

- for gas phase combustion in 3D (no 2D or 2D-axi)
- valid only for turbulent, non-premixed diffusion flame

Used physics in Comsol

Needed physics in Comsol.

- Turbulent Flow, k-ε
- Transport of Diluted Species
- Heat Transfer in Fluids

CFD-module cover all these physics. Chemical Reaction Engineering Module is not necessary needed.

Reaction according Eddy dissipation model ("mixed is burnt" assumption)

Reaction is assumed to be controlled by mixing not gas kinetics.

Combustion reaction:

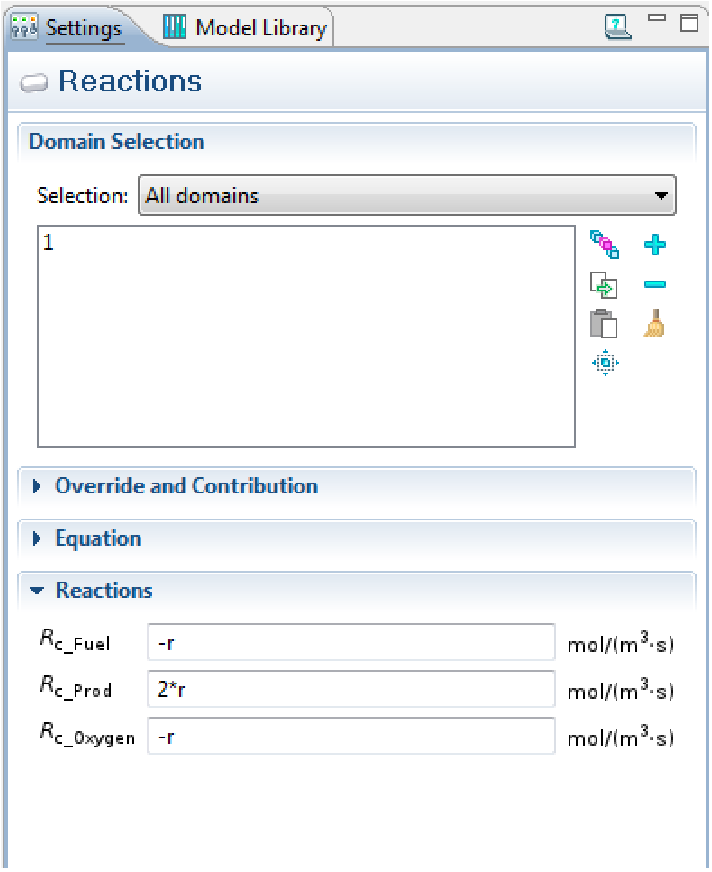
Fuel + v*Oxygen => (1+v)*Product

Reaction rate:

$$r = A_{EB}\frac{\varepsilon}{k}min\left[C_F,\frac{C_O}{\nu},B_{EB}\frac{C_F}{1+\nu}\right]$$

Model constant A_{EB}=4 and B_{EB}=0.5 can vary depend on combustion type
ε is turbulent dissipation rate (ep in Comsol)
k is turbulent kinetic energy (k in Comsol)
C is concentration of fuel (F), oxidiser (O) and product (P)
v is stoichiometric ratio

Reactions are defined under "Transport of Diluted Species" physics in "Reactions" domain. For example if v is 1 reaction domain look like this:



Picture 1 Reaction domain

On other hand, kinetic reaction component can added to model. Reaction is now controlled by smaller reaction rate (=> $r=\min(r_{kin},r_{mix})$). Kinetic reaction rate is usually Arrhenius type function. Suitable functions can be found in literature.

Heat production of combustion

Heat production is defined to Heat Transfer module under domain "Heat Source":

$$Q = r * H$$

where r is reaction rate and H is enthalpy of reaction

Enthalpy of reaction can be define by formula

$$H(T) = \Delta H_f * (h(T) - h(298K))$$

where ΔH_f is enthalpy of reaction at temperature 298 K and h is enthalpy of reactants. Thermodynamic data can be found for example here: www.me.berkeley.edu/gri-mech

More useful information

www.cfd-online.com/Wiki/Combustion	General information about CFD and combustion
www.me.berkeley.edu/gri-mech	Thermodynamic data
www.sandia.gov/TNF/abstract.html	Turbulent combustion research