Hybrid Transported-Tabulated Chemistry (HTTC) [1]

Modeling strategy: All the species which are non-zero in fresh and burnt gases are transported, and the intermediate radicals are expressed from self-similar responses.

Let us consider a mixture that involves a set A of q distinct chemical species j, interacting in a detailed chemical scheme according to N elementary reactions:

$$\sum_{j \in \mathcal{A}} \mu_{j,n}^f j \leftrightarrow \sum_{j \in \mathcal{A}} \mu_{j,n}^b j$$

 $\sum_{j \in \mathcal{A}} \mu_{j,n}^f j \leftrightarrow \sum_{j \in \mathcal{A}} \mu_{j,n}^b j \qquad \mu_{j,n}^f \text{ (resp. } \mu_{j,n}^b \text{) is the forward (resp. backward)}$ $\text{stoichiometric coefficient of the } n^{th} \text{ reaction rate.}$

Reaction rate of
$$j$$
-species: $\dot{\omega}_j = W_j \sum_{n=1}^N \left(\mu_{j,n}^b - \mu_{j,n}^f \right) \dot{\omega}_n$

nth reaction rate: $\dot{\omega}_n = \prod_{j \in \mathcal{A}} \left(\frac{\rho Y_j}{W_j}\right)^{\mu_{j,n}} A_n T^{\nu_n} \exp\left(-T_{A,n}/T\right)$ How is obtained Y_j ?

Transported species: Y_j Tabulated species: $Y_j = Y_j^{\max}(\phi) \times Y_j^+(Y_{c,j}^+(\phi))$

APPLICATION:

1. The whole kinetic mechanism is loaded

25. CH+H2O = CH2O+H

26. CH+CH2O = CH2CO+H

27. CH + CH2 = C2H2 + H

28. CH + CH3 = C2H3 + H

29. CH+CH4 = C2H4+H

30. HCO+H = CO+H2

31.HCO+O = CO+OH

2. Identification of transported species.

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3. Mass fraction of tabulated species: S2FT

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