CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Special features of cantera-avbp

Features specific to Cerfacs

- AVBP transport model
- ARC mechanism with custom kinetics
- Thicken a flame
- Partial Equilibrium Assumption for 2S chemistry
- Flamelet computation
- Soot computation

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What are we talking about ?

- D : diffusion coefficient [m^2/s]
- λ : thermal conductivity [$J/K/m^3$]
- μ : dynamic viscosity [Pa.s]

$$\begin{cases} \rho = \dfrac{p\bar{W}}{RT} \\ \rho\dfrac{\partial V}{\partial t} + \rho u\dfrac{\partial V}{\partial z} + \rho V^2 = \dfrac{\partial}{\partial z}\left(\mu\dfrac{\partial V}{\partial z}\right) - \lambda \\ \rho\dfrac{\partial Y_k}{\partial t} + \rho u\dfrac{\partial Y_k}{\partial z} = -\dfrac{\partial j_{k,z}}{\partial z} + \omega W_k \\ \rho C_p\dfrac{\partial T}{\partial t} + \rho u C_p\dfrac{\partial T}{\partial z} = \dfrac{\partial}{\partial z}\left(\lambda\dfrac{\partial T}{\partial z}\right) - \sum_{k=1}^{K} C_{pk} j_{k,z}\dfrac{\partial T}{\partial z} - \sum_{k=1}^{K} h_k\omega_k W_k \end{cases}$$

Two transport models exist in Cantera: Multi / Mix

They both rely on Chapman and Enskog theory for the pure properties μ_k and λ_k, and for the binary diffusion coefficients $\mathfrak{D}_{jk}$:

- For the viscosity :

$$\mu_k = \frac{5}{16}\frac{\sqrt{\pi m_k k_B T}}{\pi \sigma_k^2 \Omega^{(2,2)*}}$$

- m_k : the mass of species k
- σ_k : the collision diameter of species k
- T : temperature of the mixture
- $\Omega^{(2,2)*}$: collision integral from Lennard-Jones or Stockmayer potentials

- For the binary diffusion coefficients :

$$\mathfrak{D}_{jk} = \frac{3}{16}\frac{\sqrt{2\pi k_B^3 T^3 / m_{jk}}}{p\pi \sigma_{jk}^2 \Omega^{(1,1)*}}$$

- m_{jk} : the reduced mass
- σ_k : the reduced collision diameter
- T : temperature of the mixture
- $\Omega^{(1,1)*}$: collision integral from Lennard-Jones or Stockmayer potentials

- For the heat conductivity :

$$\lambda_k = \frac{\mu_k}{W_k}\left(f_{trans} C_{v,trans} + f_{rot} C_{v,rot} + f_{vib} C_{v,vib}\right)$$

Two transport models exist in Cantera: Multi / Mix

The differences between the models concerns the way to compute resultant gas properties and how the species diffusion are computed :

Multi

⇒ No approximation
⇒ Soret effect included

- Each Multicomponent diffusion coefficient $D_{j,k}$ is obtained through the inversion of a matrix (function of $\mathfrak{D}_{jk}$)

- The species diffusion velocities V_k depend on each other ! A system must solved

✅ Best in terms of accuracy ❌ Very very long !!

Mix

⇒ Mixing laws are used

$$\mu = \sum_k \frac{X_k \mu_k}{\sum_j X_j \phi_{kj}} \qquad \phi_{kj} = \frac{1}{\sqrt{8}}\left(1+\frac{W_k}{W_j}\right)^{\frac{1}{2}}\left(1+\left(\frac{\mu_k}{\mu_j}\right)^{-\frac{1}{2}}\left(\frac{W_j}{W_k}\right)^{\frac{1}{4}}\right)^2$$

$$\lambda = \frac{1}{2}\left(\sum_k X_k \lambda_k + \frac{1}{\sum_k X_k/\lambda_k}\right)$$

⇒ The species diffusion velocities V_k are independent of each other :

$$V_k = -D_k \frac{\nabla X_k}{X_k} \qquad D_k = \frac{1-Y_k}{\sum_{j\neq k} X_j/D_{jk}}$$

✅ Best in terms of accuracy/cost

Cantera-avbp has two additionals models: UnityLewis / AVBP

UnityLewis

⇒ Simplest model

$$Le = Le_k = \frac{Sc_k}{Pr} = 1$$

$$Sc_k = Pr = \frac{\nu}{D_k}$$

✅ Very low cost ❌ Big loss in accuracy !

AVBP

⇒ Constant Schmidt and Prandtl

$$Sc_k = Constant_k$$

$$Pr = Constant$$

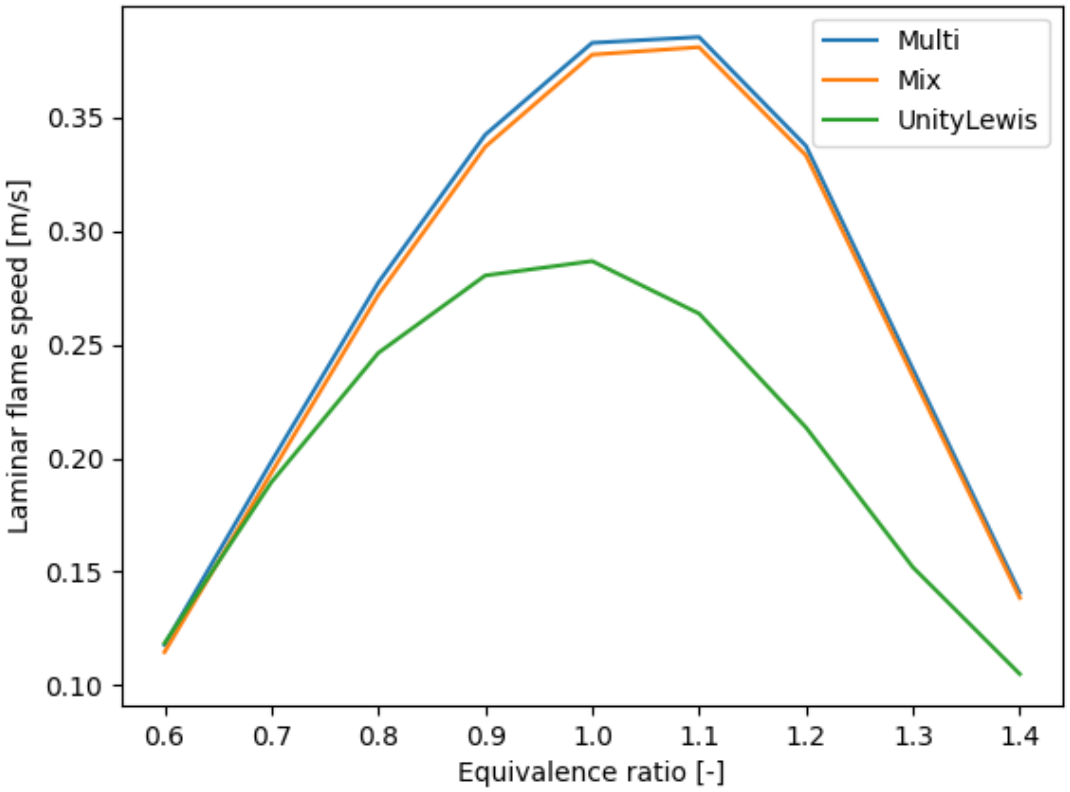
$$\Rightarrow D_k = \frac{\mu}{\rho\, Sc_k} \quad \text{and} \quad \lambda = \frac{\mu C_p}{Pr}$$

with Power law or Sutherland law

$$\mu = \mu_0 \left(\frac{T}{T_0}\right)^{\beta} \qquad \mu = \mu_0 \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S}{T + S}$$

✅ Low cost ❌ Loss in accuracy

Gri 30 at T=300K, P=1bar



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ARC mechanism with custom kinetics

ARC mechanisms are reduced mechanisms with quasi-steady state species (see ARCANE formation for more information)

⇒ It is not handled by the official Cantera !

As the objective of ARC is to be used in LES codes, especially AVBP, the mechanism file is written in Fortran (f90)

But you can use them easily in cantera-avbp :

```
kinetics = 'custom'
```

in the cti

```
import cantera as ct
ct.compile_fortran('mechanism.f90')
gas = ct.Solution('mechanism.cti')
```

in the script

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Thicken a flame

In LES codes, a common turbulent combustion model is the thicken flame model.

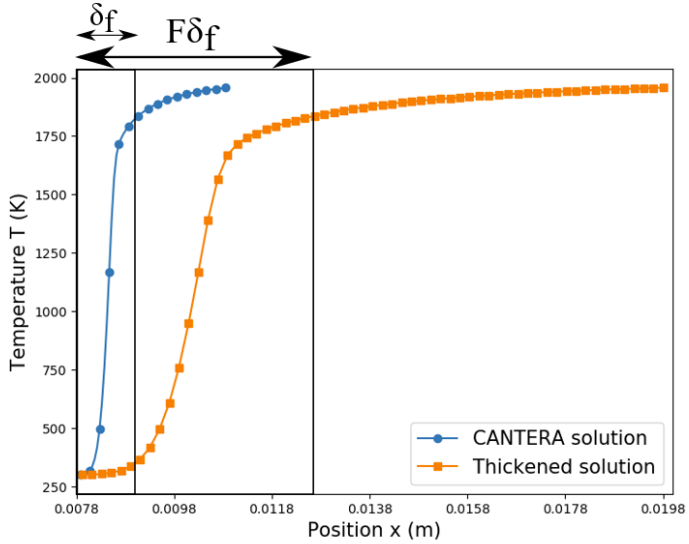
The objective of the method is to thicken the flame in order to have sufficient number of points in the flame front while keeping the flame velocity constant :

$$D_k \rightarrow D_k F \quad \Rightarrow \quad s_L \rightarrow F\, s_L$$

$$+ \quad \Rightarrow \quad s_L \rightarrow s_L$$

$$\dot{\omega}_k \rightarrow \dot{\omega}_k / F$$

In Cantera: `f.flame.thick = value`



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Partial equilibrium assumption (PEA)

For BFER mechanisms, a partial equilibrium assumption is made to apply a correction for rich conditions:

The 2S_KERO_BFER scheme is based on the two following reactions:

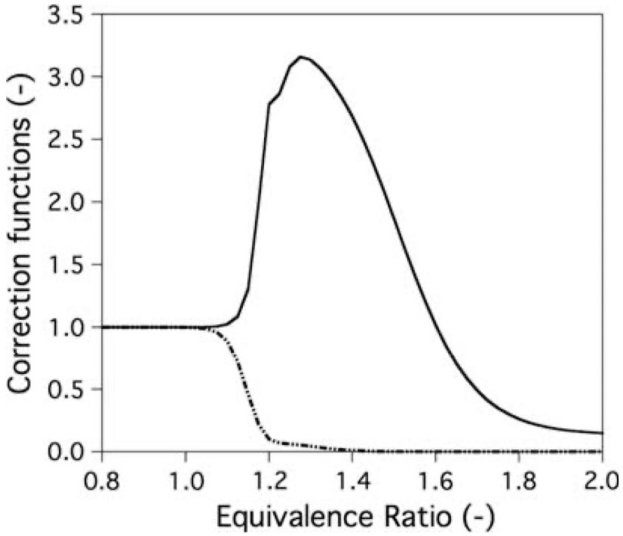
$$KERO + 10\ O_2 \Rightarrow 10\ CO + 10\ H_2O \quad (9)$$

$$CO + 0.5\ O_2 \Leftrightarrow CO_2 \quad (10)$$

where the forward reaction rates for reactions (9) and (10) are written as:

$$k_{f,1} = A_1 \boxed{f_1(\phi)} e^{(-E_{a,1}/RT)} [KERO]^{n_{KERO}} [O_2]^{n_{O_2,1}}, \quad (11)$$

$$k_{f,2} = A_2 f_2(\phi) e^{(-E_{a,2}/RT)} [CO]^{n_{CO}} [O_2]^{n_{O_2,2}}, \quad (12)$$



f_1 (–) and f_2 (-···-)

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Useful for diffusion flames, it consists in a change of space:

x (position) to z (mixture fraction)

✅ Faster computations (20s instead of 200s)
✅ Better stability in Cantera
❌ No return possible to x-space

In Cantera: `f = ct.Flamelet()`

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- Cantera-soot uses a Discrete Sectional Method (DSM) following the work of [1] implemented by E.Lameloise in Cantera
- Soot is described solving the Population Balance Equation (PBE):

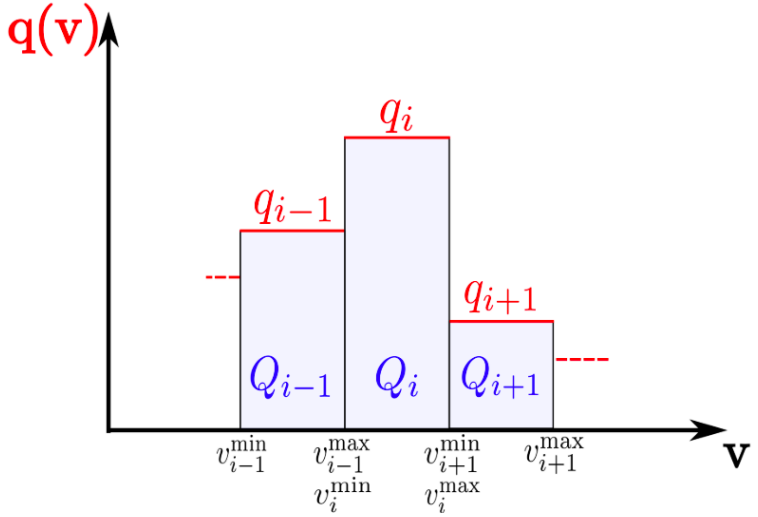
$$\begin{aligned} &\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{u}n) - \nabla \cdot \left(C_{\text{th}} \nu \frac{\nabla T}{T} n \right) = \nabla \cdot (D_s \nabla n) + \dot{n}_s \\ \Leftrightarrow \quad &\frac{\partial n}{\partial t} + \nabla \cdot ((\mathbf{u} + \mathbf{v_T})\, n) = \nabla \cdot (D_s \nabla n) + \dot{n}_s \end{aligned} \tag{1.8}$$

where:

- $\mathbf{v_T} = -C_{\text{th}} \nu \frac{\nabla T}{T}$ is the thermophoretic velocity,
- ν is gas kinematic viscosity,
- D_s is the particles soot diffusion coefficient,
- $\dot{n}_s$ is the source term of the volume distribution $n(v)$. It accounts for particles dynamics (nucleation, condensation and coagulation) and particles reactivity with the gaseous phase (surface growth and oxidation).

[1]Rodrigues, P., Franzelli, B., Vicquelin, R., Gicquel, O., & Darabiha, N. (2018). Coupling an LES approach and a soot sectional model for the study of sooting turbulent non-premixed flames. *Combustion and Flame*, *190*, 477–499. https://doi.org/10.1016/j.combustflame.2017.12.009

- Particle Size Distribution divided in n_sections
  - Soot volume fraction of the section i $Q_{s,i}$ and particle number density N_i



$$Q_{s,i} = \int_{v_i^{\min}}^{v_i^{\max}} q(v)dv = q_i \left(v_i^{\max} - v_i^{\min}\right)$$

$$N_i = \int_{v_i^{\min}}^{v_i^{\max}} n(v)dv = q_i \int_{v_i^{\min}}^{v_i^{\max}} \frac{dv}{v} = q_i \ln\left(\frac{v_i^{\max}}{v_i^{\min}}\right)$$

$$f_V = \int_0^{\infty} q(v)dv = \sum_{i=1}^{N_{\text{sect}}} Q_{s,i} = \sum_{i=1}^{N_{\text{sect}}} q_i \left(v_i^{\max} - v_i^{\min}\right)$$

$$N_{\text{part}} = \int_0^{\infty} n(v)dv = \sum_{i=1}^{N_{\text{sect}}} N_i = \sum_{i=1}^{N} q_i \ln\left(\frac{v_i^{\max}}{v_i^{\min}}\right)$$

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Soot computation

- The soot mass fraction can be written as:

$$\frac{\partial \rho Y_{s,i}}{\partial t} + \nabla \cdot (\rho(\mathbf{u} + \mathbf{v_T}) Y_{s,i}) = \nabla \cdot (\rho D_{s,i} \nabla (Y_{s,i})) + \rho_s \dot{Q}_{s,i}$$

- And $\dot{Q}_{s,i} = \rho \dot{q}_{s,i}$; $\dot{q}_{s,i} = \dot{q}_{\mathrm{nu},i} + \dot{q}_{\mathrm{cond},i} + \dot{q}_{\mathrm{sg},i} + \dot{q}_{\mathrm{ox},i} + \dot{q}_{\mathrm{coag},i}$

- Soot mechanisms:
  - Nucleation through dimerization (PAH + PAH -> DIMER) ; DIMER + DIMER -> SOOT
  - Condensation : PAH + soot (growth)
  - Coagulation : soot + soot (growth)
  - Surface growth : Soot – H + C2H2 (HACA) (growth)
  - Oxiadation : Several species involved : O2, OH, HCO … (not growth)

[1]Rodrigues, P., Franzelli, B., Vicquelin, R., Gicquel, O., & Darabiha, N. (2018). Coupling an LES approach and a soot sectional model for the study of sooting turbulent non-premixed flames. *Combustion and Flame*, *190*, 477–499. https://doi.org/10.1016/j.combustflame.2017.12.009

Soot computation

- To sum up:

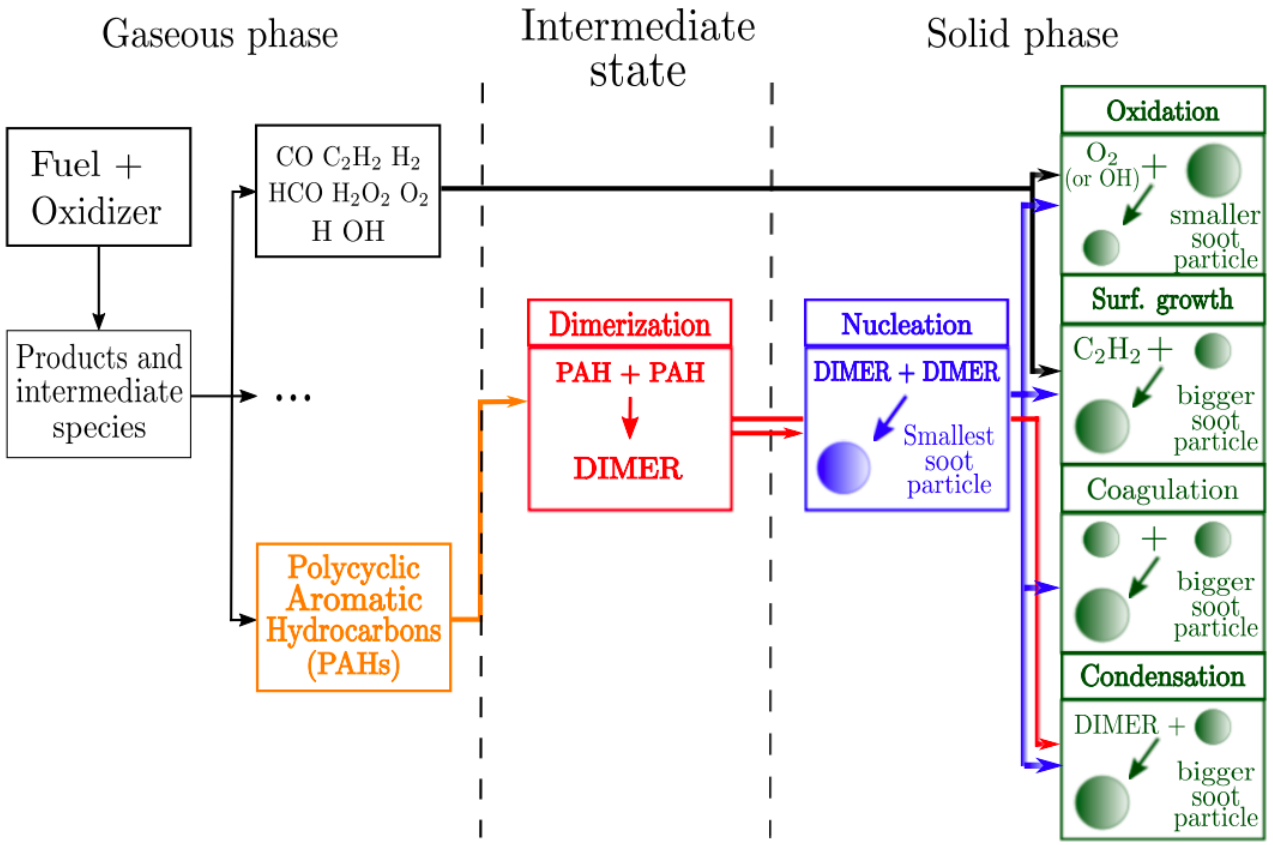

Figure 1.4: *Schematic representation of soot formation processes*

More info : *https://cerfacs.fr/chemistry-repo/priv/cantera_soot/Handbook_cantera-soot.pdf*

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