CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Cantera

Special features of cantera-avbp

Several features are coded in cantera-avbp

1. AVBP transport model
2. The use of custom kinetics
3. Thickening a flame
4. Alternative remeshing possible
5. Partial Equilibrium Assumption for 2S chemistry
6. Flamelet computation
7. Soot equations

1. Transport

What are we talking about ?

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

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

You have anyway in cantera, based on Lennard-Jones potentials :

- 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

$$\mu = \sum_k \frac{X_k \mu_k}{\sum_j X_j \phi_{kj}}$$

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

- For the heat conductivity :

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

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

https://www.cerfacs.fr/avbp7x/HELP/MOULINETTE/XML2AV/xml2av.pdf

- For the diffusion :

1. Multi

Inverse a diffusion matrix to each coefficient D_{jk}.

Best in terms of accuracy.

Very very long !!

gas.transport_model = 'Multi'

Or transport = 'Multi' in the .cti

2. Mix

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

- p : pressure
- m_{jk} : reduced molecular mass $m_{jk} = (m_j m_k)/(m_j + m_k)$
- σ_k : the collision diameter of species k
- T : temperature of the mixture
- $\Omega^{(1,1)*}$: collision integral

$$D_{km} = \frac{1 - Y_k}{\sum_{j \neq k} X_j / D_{jk}}$$

Best in terms of accuracy/cost.

Still costly if used in 3D codes.

gas.transport_model = 'Mix'

3. Lewis ($Le_k = \frac{Sc_k}{Pr} = 1$)

Very low cost.

Big loss in accuracy !

Simplified expression

$$D_{km} = \frac{\lambda}{\rho C_p}$$

gas.transport_model = 'UnityLewis'

4. AVBP ($Le_k = \mathrm{c}^{\mathrm{te}}$)

Low cost.

Loss in accuracy, you have to check !

Power law or **Sutherland law**

$$\mu = \mu_0 \left(\frac{T}{T_0}\right)^{\beta}$$

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

Simplified expression from Sc_k

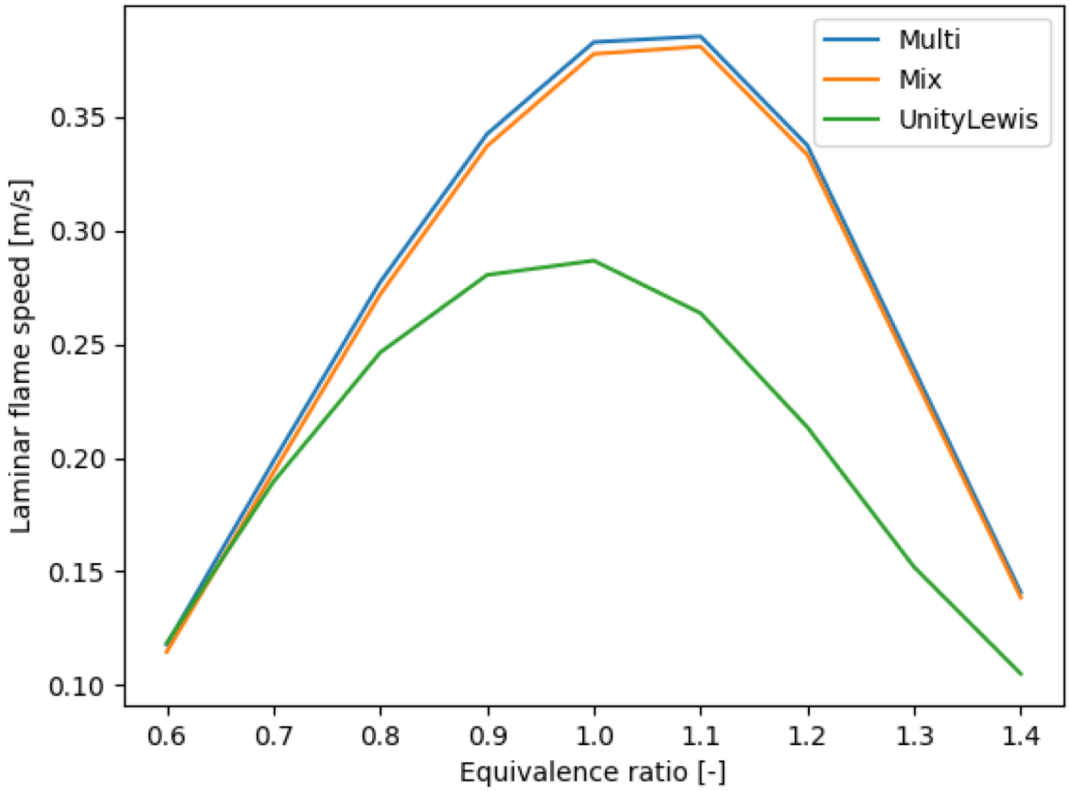
$$D_k = \frac{\mu}{\rho Sc_k}$$

Simplified expression from Pr

$$\lambda = \frac{C_p \mu}{Pr}$$

gas.transport_model = 'AVBP'

Gri 30 with T=300K, P=1bar.



2. Customkinetics

If you want to give another thing to CANTERA than the information provided in a .cti.

- A f90 to be included in the code
- Useful if you want to have a special handling of the kinetics (ex: algebraic relations between species)

```
kinetics = 'custom'
```
in the .cti

```
import cantera as ct
ct.compile_fortran('mechanism.f90')
```
in the script

3. Thickening

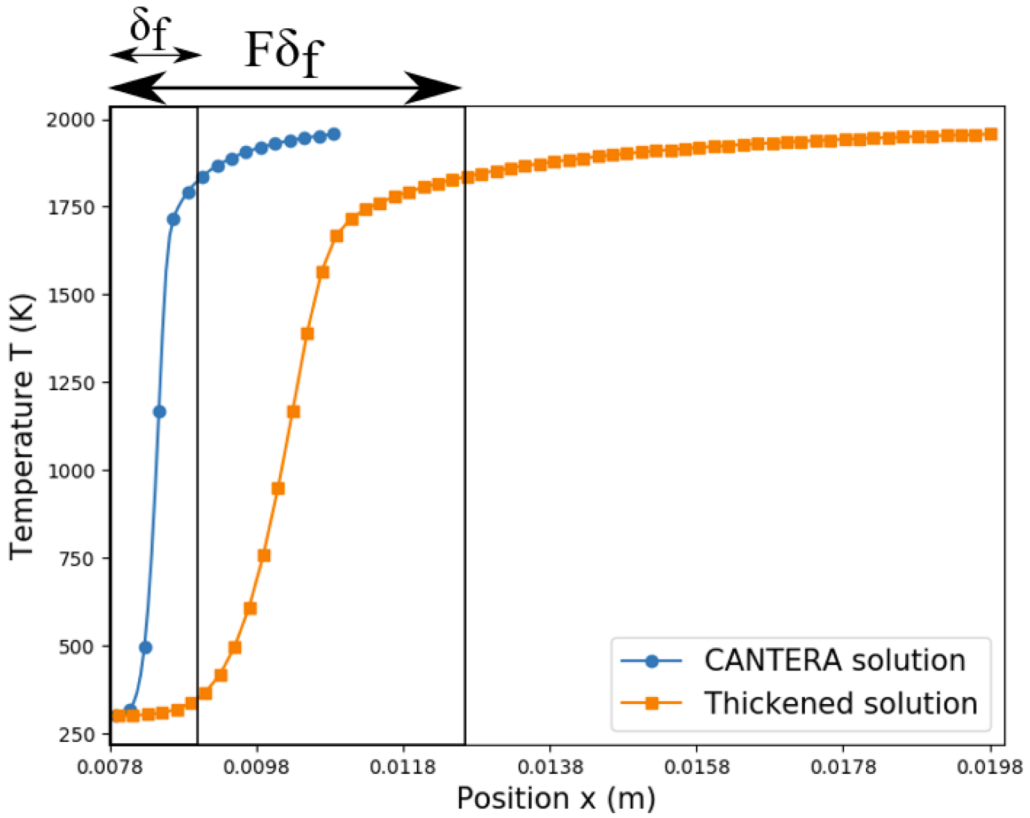
To be able to test the chemistry for

```
f.flame.thick = value
```

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

$D_k \rightarrow D_k F$

$s_L \rightarrow s_L$



https://cerfacs.fr/chemistry-repo/pub/cantera_jypnb/Thickening.html

4. Alternative remeshing

Three options for “refine_grid” parameter:

- “***disabled***” : no refinement. Can be useful if one wants to test a regular-spaced grid.
- “***refine***” : default refinement method of CANTERA. Is very useful to refine more the flamefront than the edges.
- “***remesh***” : CERFACS method, useful to go from one grid to another.

```
refine_grid = 'remesh'
f.solve(loglevel, refine_grid)
```

5. Partial Equilibrium Assumption (PEA)

- Special to BFER -> correction for the rich part.
- Only available with AVBP format.

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:

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

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

https://cerfacs.fr/chemistry-repo/pub/cantera_jypnb/Pea.html

6. Flamelet computation

Mixture fraction variable : z

Trick : change of space from
x (position) to **z (mixture fraction)**

Faster computations (20s instead of 200s).

Better stability (CDF is very capricious.

No return possible to x-space.

```
f = ct.Flamelet()
```

https://cerfacs.fr/chemistry-repo/pub/cantera_jypnb/CDF-Flamelet.html

7. Soot equation

- Enables the computation of soot after a flame in cantera

$$\frac{\partial n}{\partial t} + \underbrace{\nabla \cdot (\mathbf{u}n)}_{\text{Convection}} - \underbrace{\nabla \cdot \left(C_{th} \nu \frac{\nabla T}{T} n \right)}_{\text{Thermophoresis}} = \underbrace{\nabla \cdot (D_s \nabla n)}_{\text{Diffusion}} + \underbrace{\dot{n}_s}_{\text{Source}} \qquad (1)$$

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

Bonus: Cantera as an input of AVBP

- It is possible to generate a 1D flame from Cantera and make an initialization for AVBP

```
f.write_AVBP('name_of_file.csv')
```

- It is possible to generate a *gas_out* with the help of Cantera.
- It is possible to use Cantera to calculate evaporation with *evol_evap0D*.
- It is possible to create the mixture_database.dat with the *xml2av* tool.

Bonus 2: Cantera as an input of AVBP

- You have a separate git called cantera-tools
  - Initialize 3D AVBP calculations with cantera
  - Optimize Schmidt & Prandtl numbers

https://chemistry.cerfacs.fr/en/avbp/avbp-tools-for-chemistry/

BACKUP

http://www.cmap.polytechnique.fr/~giovangi/convergent.pdf

https://chemistry.cerfacs.fr/en/cantera/cantera-tutorials/