Normalization PIAFS

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1 Parameters

1.1 Pump beams

Physical quantity	name in the code	usual value	comment
λ_{UV}	lUV	248nm	Pump wavelength, $\in [200, 300]$
θ	theta	0.17 pi / 180	half angle between prope beams
τ_{pulse}	tpulse	10ns	duration of the pump beam
ω_{UV}	nu	c/λ_{UV}	pump frequency
F_0	F0	$200mJ/cm^2$	pump fluence

1.2 'Derived quantities'

Physical quantity	name in the code	usual value	comment
k_{UV}	kUV	$2\pi/\lambda_{UV}$	pump beam wave vector
ω_{UV}	wUV	$k_{UV}c$	pump beam frequency
k_g	kg	$2k_{UV}\sin\theta$	grating wave vector
λ_g	lg	$2\pi/k_g$	grating wavelength
ω_g	wg	$k_g c_s$	grating frequency where c_s is the acoustic velocity for the initial conditions

1.3 Diffracted beam

Physical quantity	name in the code	usual value	comment
λ_{diff}	ldiff	532nm	Value article Michine & Yoneda
k_{diff}	kdiff	$2\pi/\lambda_{diff}$	

1.4 Gas conditions

Physical quantity	name in the code	usual value	comment
f_{CO_2}	fCO2	a few percents	CO_2 Fraction: if we have a mix of O_2 and C_O2 instead of pure CO_2
f_{O_2}	fO2	$1 - f_{CO_2}$	O_2 Fraction
f_{O_3}	fO3v	$\in [0, 0.3]$	O_3 Fraction, usually between 0 and 3% of the total gaz concentration (we assume the total concentration is the O_2 concentration since $[O_2] \ll [O_3]$
P_{tot}	Ptot	101325 Pa	O_2 Total gas pressure for 288 K
C_v	CvO2	$5/2\ k_B$	Heat capacity for O_2
M_{O_2}	mmolO2	$0.032\ kg$	O_2 Molar mass
γ	gamma	7/5	O_2 Heat capacity ratio
σ_{O_3}	sO3	$1.110^{-17} cm^{-2}$	ozone absorption cross-section in the center of the Hartley band
F_s	Fs	$h\nu/\sigma_{O_3}$	O_2 Saturation Fluence
n_{O_x}	n_Ox	$f_{O_x} P_{tot}/k_B/T_i$	Initial concentration in particle / m^{-3} of O_x where x is 2 or 3
$n_{h\nu_{max}}$	n_hnumax	$I_0/c/h/nu$	Initial photon concentration: Total laser energy divided by the energy of 1 photon
E_i	Ei	$P_{tot}/(\gamma - 1)/n_{O_2}$	Volumic initial gas internal energy in J
T_i	Ti	288 K	Initial temperature

1.5 Chemistry

Physical quantity	name in the code	usual value	comment
q	q0a, q0b etc	a few eV	O_2 Heat energy from reactions 0_a, 0_b etc
k	k0a, k0b etc	$10^{-18} - 10^{-12} m^3/s$	O_2 reaction rates from reactions 0_a, 0_b etc

2 Calculation of the viscous and heat conduction terms

From Acoustics, Allan D. Pierce, p589

Viscosity:

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + T_S}{T + T_S} \tag{1}$$

Thermal conductivity:

$$\frac{\kappa}{\kappa_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + T_A e^{-T_B/T_0}}{T + T_A e^{-T_B/T}} \tag{2}$$

where μ_0 and κ_0 correspond to temperature T_0. If these formulas hold for any given choice of T_0, they also hold for any other choice of T_0. The constants values are $T_S = 110.4K$, $T_A = 245.4K$, and $T_B = 27.6K$.

At 275K, $\mu_0 = 1.72 \times 10^{-4} g/cm^3$ and $\kappa_0 = 1.29 \times 10^{-5} cal/cm/s/K$

Bellow some values of μ/μ_0 and κ/κ_0 as a function of T, for the air.

T[K]	μ $[kg/s/m]$	μ/μ_0	κ [W/m/K]	κ/κ_0
280	1.75×10^{-5}	1.02	2.47×10^{-2}	1.022
290	1.8×10^{-5}	1.048	2558×10^{-2}	1.055
300	1.85×10^{-5}	1.076	2.62×10^{-2}	1.087
320	1.94×10^{-5}	1.13	2.78×10^{-2}	1.151
340	2.03×10^{-5}	1.183	2.93×10^{-2}	1.213
360	2.12×10^{-5}	1.234	3.08×10^{-2}	1.275
380	2.20×10^{-5}	1.283	3.22×10^{-2}	1.335
400	2.22×10^{-5}	1.332	3.34×10^{-2}	1.394

Eventually, the x-dependence of the viscosity / thermal conductivity will be necessary for non linear situation where we have a consequent temperature modulation

The chemicals reactions in the bright interference fringes lead to a temperature modulation along x, thus an x dependence of μ and κ

Viscosity:

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

Thermal conductivity:

$$\frac{\kappa(x)}{\kappa_0} = \left(\frac{T(x)}{T_0}\right)^{3/2} \frac{T_0 + T_A e^{-T_B/T_0}}{T + T_A e^{-T_B/T}} \tag{4}$$

3 Normalizations

3.1 Basics

- Time normalized to acoustic frequency ω_g
- Space normalized to acoustic wave vector k_g
- Speed normalized to initial acoustic velocity c_s

3.2 Gas properties

- Density normalized to O_2 concentration n_{O_2}
- Pressure and energy normalized to $\omega_g n_{O_2} c_s$

In black the quantities in SI, in red the normalization.

First Euler equation:

$$\partial_t \frac{1}{\omega_g} \times \rho \frac{N_A}{M_{O_2} n_{O_2}} + \partial_x \frac{1}{k_g} \times \rho \frac{N_A}{M_{O_2} n_{O_2}} \times u \frac{1}{c_s} = 0 \tag{5}$$

Second Euler equation with viscous term:

$$\partial_t \frac{1}{\omega_g} \times \rho \frac{N_A}{M_{O_2} n_{O_2}} u \frac{1}{c_s} + \partial_x \frac{1}{k_g} \times \left(\rho \frac{N_A}{M_{O_2} n_{O_2}} \times u^2 \frac{1}{c_s^2} + p \frac{N_A}{n_{O_2} M_{O_2} c_s^2}\right) = \partial_x \frac{1}{k_g} (\mu \frac{N_A}{M_{O_2} k_g \omega_g} \times \partial_x \frac{1}{k_g} \times u \frac{1}{c_s}) \tag{6}$$

Third Euler equation with source term, viscous and heat conductivity term:

$$\partial_t \frac{1}{\omega_g} \times E \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2} + \partial_x \frac{1}{k_g} \times u \frac{1}{c_s} \times (E \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2} + p \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2}) = \frac{Q}{\gamma - 1} \frac{N_A}{w_g^2 n_{O_2} M_{O_2} c_s} + \mu \frac{N_A}{M_{O_2} k_g \omega_g} \times \partial_x^2 \frac{1}{k_g^2} \times u \frac{1}{c_s} + \partial_x(\kappa \partial_x T) \tag{7}$$

3.3 Chemistry

Normalisation of q and k:
$Q \propto q \times k \times n^2$.

$$q \frac{1}{k_g c_s^2} \times k \frac{n_{O_2}}{\omega_g} \times n^2 \frac{1}{n_{O_2}^2} \tag{8}$$

In the script, the values of q are initially in eV. qe is in J. We want q normalized to the initial internal energy. In the script, I use the normalisation e/E_i where E_i is the initial internal energy in J (not the volumic energy as in the Euler equation, hence the absence of n_{O_2} in the normalization.

Then the normalization for the chemistry equations are:

$$n_c = n \frac{1}{n_{O_2}} + \partial_t \frac{1}{\omega_g} \times (k \frac{n_{O_2}}{\omega_g} \times n_x \frac{1}{n_{O_2}} \times n_y \frac{1}{n_{O_2}} + ...) \tag{9}$$

where n_c is the concentration of n at time n+1

4 Navier–Stokes Equations

The 1D Navier–Stokes equations in dimensional form (Tannehill & Anderson) are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \tag{10a}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + P\right) = \frac{\partial}{\partial x}\left[\frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right)\right], \tag{10b}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}(E + P)\,u = \frac{\partial}{\partial x}\left[\frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right)u\right] + \frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right), \tag{10c}$$

where

$$E = \frac{P}{\gamma - 1} + \frac{1}{2}\rho u^2, \qquad P = \rho R T. \tag{11}$$

Normalization Rewriting (10),

$$\frac{\rho_{\text{ref}}}{t_{\text{ref}}}\frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \frac{\rho_{\text{ref}} c_s}{x_{\text{ref}}}\frac{\partial}{\partial \tilde{x}}(\tilde{\rho}\tilde{u}) = 0, \tag{12a}$$

$$\frac{\rho_{\text{ref}} c_s}{t_{\text{ref}}}\frac{\partial}{\partial \tilde{t}}(\tilde{\rho}\tilde{u}) + \frac{\rho_{\text{ref}} c_s^2}{x_{\text{ref}}}\frac{\partial}{\partial \tilde{x}}\left(\tilde{\rho}\tilde{u}^2 + \tilde{P}\right) = \frac{\mu_{\text{ref}} c_s}{x_{\text{ref}}^2}\frac{\partial}{\partial \tilde{x}}\left[\frac{2}{3}\tilde{\mu}\left(2\frac{\partial \tilde{u}}{\partial \tilde{x}}\right)\right], \tag{12b}$$

$$\frac{\rho_{\text{ref}} c_s^2}{t_{\text{ref}}}\frac{\partial \tilde{E}}{\partial \tilde{t}} + \frac{\rho_{\text{ref}} c_s^3}{x_{\text{ref}}}\frac{\partial}{\partial \tilde{x}}\left(\tilde{E} + \tilde{P}\right)\tilde{u} = \frac{\mu_{\text{ref}} c_s^2}{x_{\text{ref}}^2}\frac{\partial}{\partial \tilde{x}}\left[\frac{2}{3}\tilde{\mu}\left(2\frac{\partial \tilde{u}}{\partial \tilde{x}}\right)\tilde{u}\right] + \frac{\kappa_{\text{ref}} T_{\text{ref}}}{x_{\text{ref}}^2}\frac{\partial}{\partial x}\left(\tilde{\kappa}\frac{\partial \tilde{T}}{\partial \tilde{x}}\right), \tag{12c}$$

where the subscript ref denotes a reference quantity, and $\tilde{cdot}$ are the normalized variables. Based on the previous section, we have the following basic quantities:

$$\begin{aligned}
&R = \frac{N_A k_B}{M_{O2}} \approx 259.7\,\mathrm{J\,kg^{-1}\,K^{-1}}, \quad c_p = 918.45\,\mathrm{J\,kg^{-1}\,K^{-1}} \ \left(\mathrm{O_2 \text{ at } 288\,K}\right),\\
&x_{\text{ref}} = \frac{1}{k_g}, \quad T_{\text{ref}} = T_i = 288\,\mathrm{K}, \quad \rho_{\text{ref}} = \frac{P_{tot}}{R T_{\text{ref}}} = 1.356\,\mathrm{kg\,m^{-3}},\\
&\mu_{\text{ref}} = \mu_{O2}\left(T_{\text{ref}}\right) = 1.99 \times 10^{-5}\,\mathrm{kg\,s^{-1}}\,m^{-1}, \quad \kappa_{\text{ref}} = \kappa_{O2}\left(T_{\text{ref}}\right) = 2.70 \times 10^{-2}\,\mathrm{W\,m^{-1}\,K^{-1}}.
\end{aligned} \tag{13}$$

and the following derived reference quantities:

$$c_s = \sqrt{\gamma R T_{\text{ref}}} = 323.59\,\mathrm{m\,s^{-1}}, \quad t_{\text{ref}} = \frac{x_{\text{ref}}}{c_s}, \quad P_{\text{ref}} = \rho_{\text{ref}} c_s^2. \tag{14}$$

Thus, omitting the ˜ symbol for convenience, (12) is:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0, \tag{15a}$$

$$\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2 + P\right) = \left(\frac{\mu_{\rm ref}}{\rho_{\rm ref} c_s x_{\rm ref}}\right)\frac{\partial}{\partial x}\left[\frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right)\right], \tag{15b}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}\left(E + P\right)u = \left(\frac{\mu_{\rm ref}}{\rho_{\rm ref} c_s x_{\rm ref}}\right)\frac{\partial}{\partial x}\left[\frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right)u\right] + \left(\frac{\kappa_{\rm ref}}{\gamma R \rho_{\rm ref} c_s x_{\rm ref}}\right)\frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right). \tag{15c}$$

Note that

$$\left(\frac{\kappa_{\rm ref}}{\gamma R \rho_{\rm ref} c_s x_{\rm ref}}\right) = \left(\frac{\kappa_{\rm ref}}{\gamma R \mu_{\rm ref}}\right)\left(\frac{\mu_{\rm ref}}{\rho_{\rm ref} c_s x_{\rm ref}}\right) = \left(\frac{\kappa_{\rm ref}}{\left(\gamma - 1\right) c_p \mu_{\rm ref}}\right)\left(\frac{1}{Re}\right) = \frac{1}{\left(\gamma - 1\right)\ Pr\, Re}, \tag{16}$$

where Pr is the Prandtl number and Re is the Reynolds number. Therefore, the normalized Navier-Stokes equations (as implemented in `PIAFS2D`) are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0, \tag{17a}$$

$$\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2 + P\right) = \frac{1}{Re}\frac{\partial}{\partial x}\left[\frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right)\right], \tag{17b}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}\left(E + P\right)u = \frac{1}{Re}\frac{\partial}{\partial x}\left[\frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right)u\right] + \frac{1}{\left(\gamma - 1\right)\ Pr\, Re}\frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right). \tag{17c}$$

Normalizing the equation of state (11),

$$P = \left(\frac{\rho_{\rm ref} R T_{\rm ref}}{\rho_{\rm ref} c_s^2}\right)\rho T \quad \Rightarrow \quad \gamma P = \rho T. \tag{18}$$

The normalized coefficients of viscosity and conductivity are computed by normalizing (1) and (2):

$$\mu = \frac{T}{T_0}^{\frac{3}{2}}\left(\frac{T_0 + T_S}{T + T_S}\right), \qquad \kappa = \frac{T}{T_0}^{\frac{3}{2}}\left(\frac{T_0 + T_A e^{-\frac{T_B}{T_0}}}{T + T_A e^{-\frac{T_B}{T}}}\right), \tag{19}$$

where the constants are all normalized by $T_{\rm ref}$.

Implementation in `PIAFS2D` The following parameters should be specified in the `physics.inp` file:

$$Re = \frac{\rho_{\rm ref} c_s x_{\rm ref}}{\mu_{\rm ref}} \approx \frac{1.36 \times 323.59 \times 6.65 \times 10^{-6}}{1.99 \times 10^{-5}} = 1.47 \times 10^2 \quad \text{(Reynolds number)} \tag{20a}$$

$$Pr = \frac{c_p \mu_{\rm ref}}{\kappa_{\rm ref}} \approx \frac{918.45 \times 1.99 \times 10^{-5}}{2.70 \times 10^{-2}} = 0.68 \quad \text{(Prandtl number)} \tag{20b}$$