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 Gaz 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	$0.032\ kg/m^3$	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

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 Normalizations

2.1 basics

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

2.2 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:

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

Second Euler equation:

$$\partial_t \frac{1}{\omega_g} \times \rho \frac{N_A}{M_{O_2} n_{O_2}} u \frac{1}{c_s} + \partial_x \frac{1}{k_g} \times \rho \frac{N_A}{M_{O_2} n_{O_2}} \times u^2 \frac{1}{c_s^2} + p \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2} = 0 \tag{2}$$

Third Euler equation with source term:

$$\partial_t \frac{1}{\omega_g} \times E \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2} + \partial_x \frac{1}{k_g} \times u \frac{1}{c_s} \times (E \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2} + p \frac{N_A}{k_g n_{O_2} M_{O_2} c_s^2}) = \frac{Q}{\gamma - 1} \frac{N_A}{w_g^2 n_{O_2} M_{O_2} c_s} \tag{3}$$

2.3 chemistry

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

$$q \frac{1}{k_g c_s^2} \times k \frac{n_{O_2}}{\omega_g} \times n^2 \frac{1}{n_{O_2}^2} \tag{4}$$

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:

$$n_c = n \frac{1}{n_{O_2}} + \partial_t \frac{1}{\omega_g} \times (k \frac{n_{O_2}}{\omega_g} \times n_x \frac{1}{n_{O_2}} \times n_y \frac{1}{n_{O_2}} + ...) \tag{5}$$

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