Modeling Tasks for the
3rd International Workshop on Laser-Induced Incandescence

File format:	ASCII, 49 columns, space delimited	
	first column:	time base
	other columns:	defined by Cases 1-8 given below
	Case 9 give in separate block	
	Case 10 give in header for D_{ave} or separate block for distribution	
Timescale:	Run out to at least 500 ns with a time resolution of your choice	
Laser:	wavelength:	1064 nm
	temporal profile:	see attached file
	spatial profile:	tophat, i.e., single fluence
Detection:	wavelength:	680 nm square bandpass
	time resolution:	infinitely fast
Signal collection:	don't include corrections for the solid angle element and detector quantum efficiency.	
Primary particles:	diameter: 35 nm, monodisperse	

Numbers and descriptions of simulation cases:

Melton Model with fixed parameters (see next page):
Case 1: 1650 K, 1 bar, 0.1 J/cm^2
Case 2: 1650 K, 1 bar, 0.8 J/cm^2

Free model and free parameters:
Case 3: 1650 K, 1 bar, 0.1 J/cm^2
Case 4: 1650 K, 1 bar, 0.8 J/cm^2
Case 5: 300 K, 1 bar, 0.1 J/cm^2
Case 6: 300 K, 1 bar, 0.8 J/cm^2
Case 7: 1650 K, 10 bar, 0.1 J/cm^2
Case 8: 1650 K, 10 bar, 0.8 J/cm^2
Case 9: 1650 K, 1 bar, Peak signal and peak temperature for fluences of 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.50, 0.60, 0.80, 1.00, and 1.5 J/cm^2
Case 10: evaluate average diameter or polydisperse distribution from LII signal in attached file at 1650 K, 1 bar, 0.1 J/cm^2, detection wavelength 680 nm

For Cases 1 and 2 include calculated values for
a: Particle temperature
b: Particle diameter
c: LII signal

For Cases 3-8 include calculated values for
a: Particle temperature
b: Particle diameter
c: LII signal
d: $Q_{absorption}$
e: $Q_{conduction}$
f: $Q_{radiation}$
g: $Q_{sublimation}$

Submission of the results: Please email to Hope (hamiche@sandia.gov), and/or Fengshan (Fengshan.Liu@nrc-cnrc.gc.ca), and/or Henrik (henrik.bladh@forbrf.lth.se).

Melton Model with Fixed Parameters

Energy conservation equation:

$$\frac{\pi^2 D^3 E(m)}{\lambda_l} F q(t) - \frac{2\kappa_a \pi D^2}{(D+GL)}(T-T_g) + \frac{\Delta H_v}{W_v}\frac{\mathrm{d}M}{\mathrm{d}t} - \frac{\pi D^3 \rho_s c_s}{6}\frac{\mathrm{d}T}{\mathrm{d}t} = 0 \qquad (1)$$

D: Particle diameter = 35×10^{-7} cm
λ_l: Laser wavelength = 1064×10^{-7} cm
$E(m)$: Wavelength dependent function of the soot refractive index = 0.23
F: Laser fluence in J/cm^2
$q(t)$: Laser temporal power density per unit laser fluence = $q(supplied)/q_0$ 1/s
q_0: Normalization for laser temporal profile = 1.16278×10^{-8}
κ_a: Thermal conductivity of air at 1650 K and 1 bar =9.6×10^{-4} J/(cm s K)
T: Particle temperature in K
T_g: Gas (also particle initial) temperature = 1650 K
L: Mean free path of air at 1 bar = $2.355\times10^{-8}\times T_g$ cm
G: Geometry-dependent heat transfer factor = $8f/[\alpha(\gamma+1)]$
f: Eucken factor = $(9\gamma-5)/4$
α: Thermal accommodation coefficient = 0.3
γ: Specific heat ratio of air at 1650 K = 1.3
ΔH_v: Heat of sublimation of carbon = 7.78×10^5 J/mol
W_v: Molecular weight of sublimed carbon assuming C_3 only sublimes = 36 g/mol
M: Mass of the particle in g
t: Time in s
ρ_s: Density of carbon = 2.26 g/cm^3
c_s: Specific heat of carbon = 1.90 J/(g K)

Mass conservation equation:

$$\frac{dM}{dt} = \frac{-\pi D^2 W_v p_v}{R_p T}\left(\frac{R_m T}{2W_v}\right)^{0.5} \qquad (2)$$

p_v: Vapor pressure in bar = $p_{ref}\exp[\Delta H_v(T-T_{ref})/(RTT_{ref})]$
p_{ref}: = 1 bar
T_{ref}: = 3915 K
W_v: Molecular weight of carbon vapour = 36 g/mol
R: Universal gas constant = 8.31 J/(K mol)
R_m: Universal gas constant = 8.31×10^7 g cm^2/(K mol s^2)
R_p: Universal gas constant = 83.1 bar cm^3/(K mol)

Signal calculation:

$$S = \frac{8\pi^3 D^3 hc^2 E(m)}{\lambda_s^{\,6}\left[\exp\left(hc/\lambda_s k_B T\right)-1\right]} \qquad (3)$$

h: Planck constant = 6.626×10^{-34} J s
c: Speed of light = 3.00×10^{10} cm/s
k_B: Boltzmann constant = 1.381×10^{-23} J/K
λ_s: Emission wavelength = 680×10^{-7} cm for this comparison