

# **SOOT MEASUREMENT AND MODELLING**

**D. Lentini, a.a. 2015/16**

- **OUTLINE:**

- **SOOT EFFECTS**
- **LIMITS OF CURRENT MODELING TOOLS**
- **EXPERIMENTAL TECHNIQUES**

## 2. SOOT EFFECTS

- PERFORMANCE:

- AMOUNT TO UNBURNT FUEL
- IN ROCKET ENGINES, MAY GIVE A  $\Delta I_{sp} \simeq 20$  s (Fortunier)

- OPERATIONAL (IN GTs):

- MAY CLOG LINER HOLES
- MAY DAMAGE TURBINE BLADES
- SOOT DEPOSITED ON TURBINE BLADES DECREASES  $\eta_t$  BY UP TO 1%

- ENVIRONMENT:

- HEALTH
- CONTRIBUTES TO GLOBAL WARMING:
  - \* DIRECTLY (AS BLACK CARBON)
  - \* INDIRECTLY (PROMOTING CONTRAILS)

### 3. MODELLING TOOLS

- SOOTING DESCRIBED IN TERMS OF A FEW STEPS:

*n.* NUCLEATION,

*g.* SURFACE GROWTH,

*a.* AGGLOMERATION,

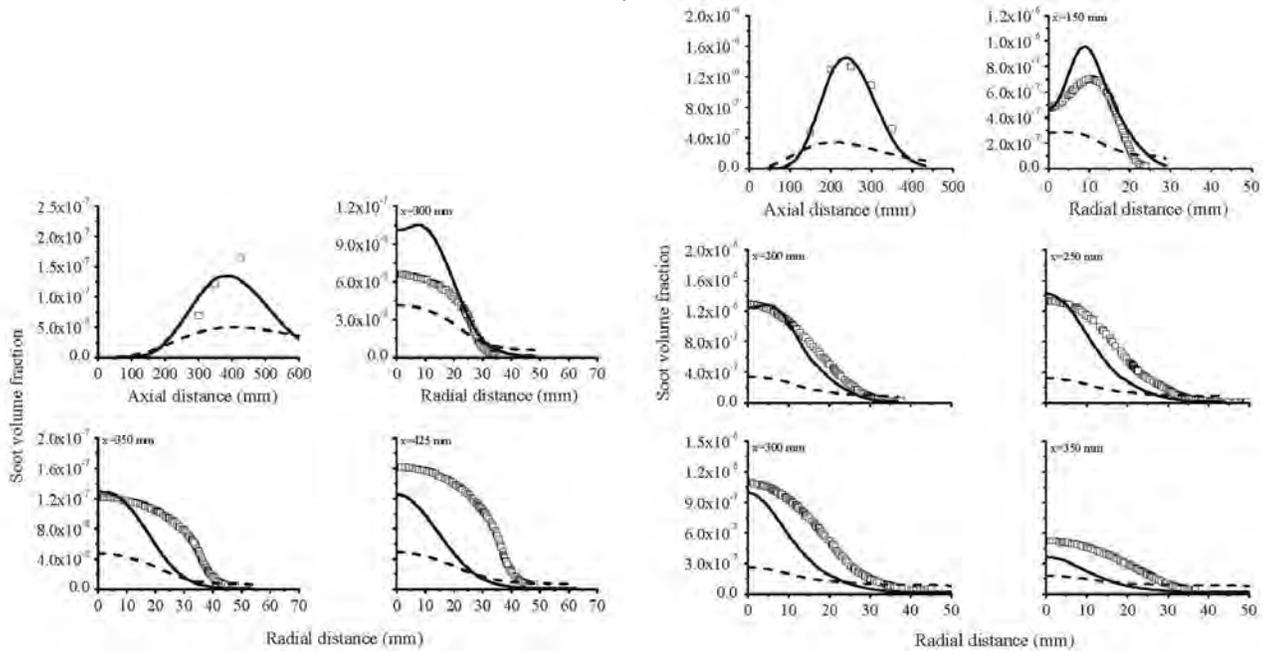
*ox.* OXIDATION

*others.* (FRAGMENTATION,...)

- AND A FEW VARIABLES, e.g.,
  - \*  $Y_s$  SOOT MASS FRACTION
  - \*  $n_s$  SOOT NUMBER DENSITY

## 4. PERFORMANCE OF CURRENT MODELS

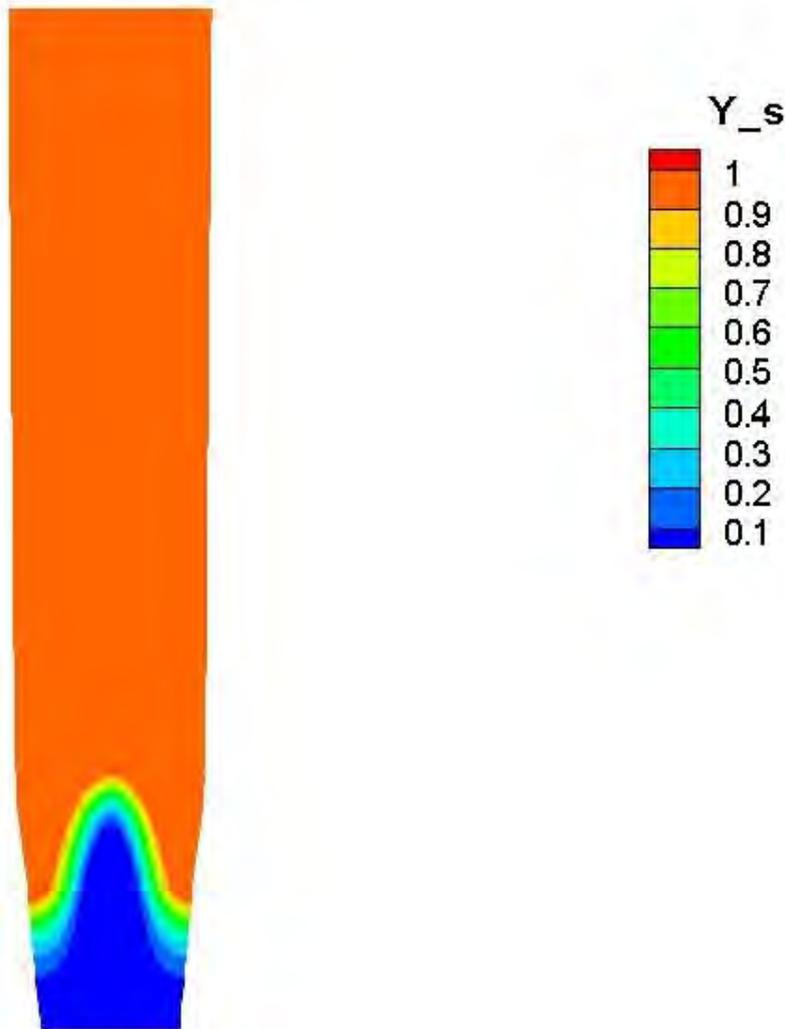
- METHANE/AIR FLAME at 1 (left) to 3 (right) bars,  $T_{max} \simeq 1700$  K (Woolley *et al.*, 2009):



- ORDER OF MAGNITUDE MORE OR LESS CAPTURED

## 4.2 PERFORMANCE OF CURRENT MODELS (2/2)

- METHANE/OXYGEN FLAME at 10 bar,  
 $T_{max} \simeq 3000$  K (Lentini and Mazzone, 2011):



- UNPHYSICAL RESULTS

## 5. LIKELY CAUSES FOR FAILURE

- GENERAL:

- JUST 2 MODEL EQS. TO DESCRIBE:

- \* > 500 REACTION STEPS;

- \* AGGLOMERATION BY van der WAALS and ELECTROSTATIC FORCES;

- \* FRACTION OF ACTIVE SITES ON PARTICLE SURFACE;

- \* ...

- SPECIFIC TO HIGH- $T$ , HIGH- $p$  APPLICATIONS:

- VERY INTENSE SOOT FORMATION, BUT...

- NO ACCOUNT FOR GAS-PHASE CARBON DEPLETION BY SOOTING;

- MODEL UNDER DEVELOPMENT, EXPERIMENTAL DATA AT HIGH- $T$ , HIGH- $p$  NEEDED FOR VALIDATION

- MEASUREMENTS IN CLOSED CHAMBER

## 6 QUANTITIES TO BE MEASURED

● ...

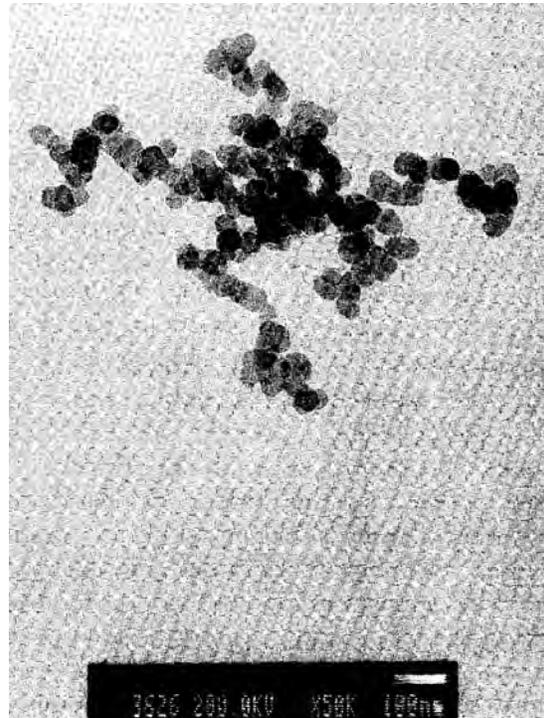
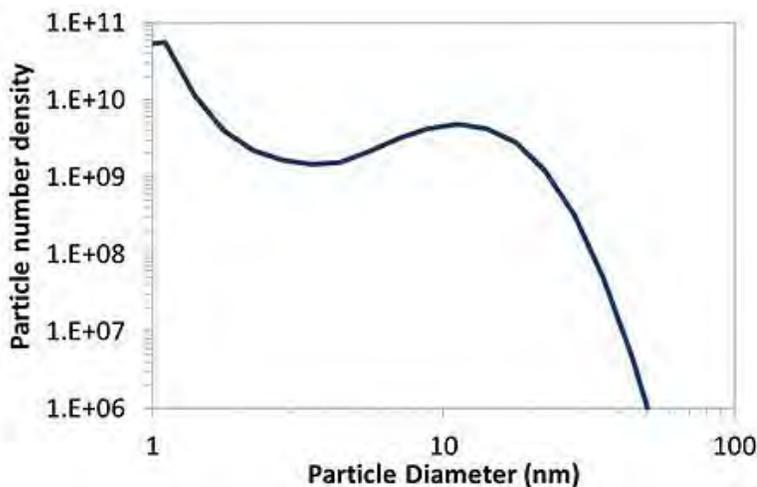
- SOOT VOLUME FRACTION  $f_v$
- PARTICLE SIZE DISTRIBUTION
- MORPHOLOGY
- CHEMICAL COMPOSITION

$$f_v = \frac{\rho_{mixture} \cdot Y_s}{\rho_{soot}}$$

●  $Y_s$  SOOT MASS FRACT. IN GAS/PARTICLE MIXT.

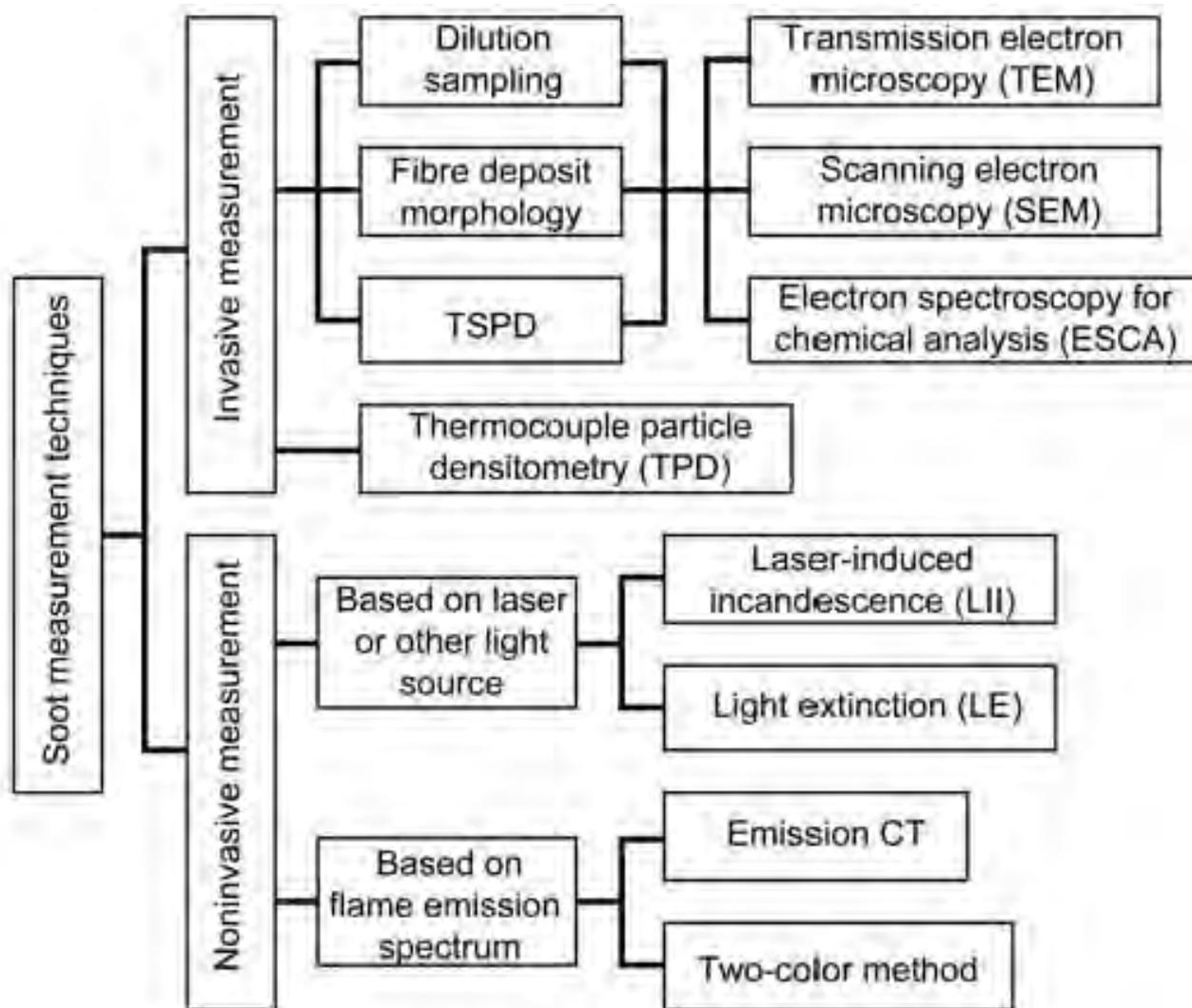
●  $\rho_{mixture} \sim$  a few  $\text{kg}/\text{m}^3$ ,  $\rho_{soot} \sim 1800 - 2000 \text{ kg}/\text{m}^3$

→  $f_v \ll Y_s$



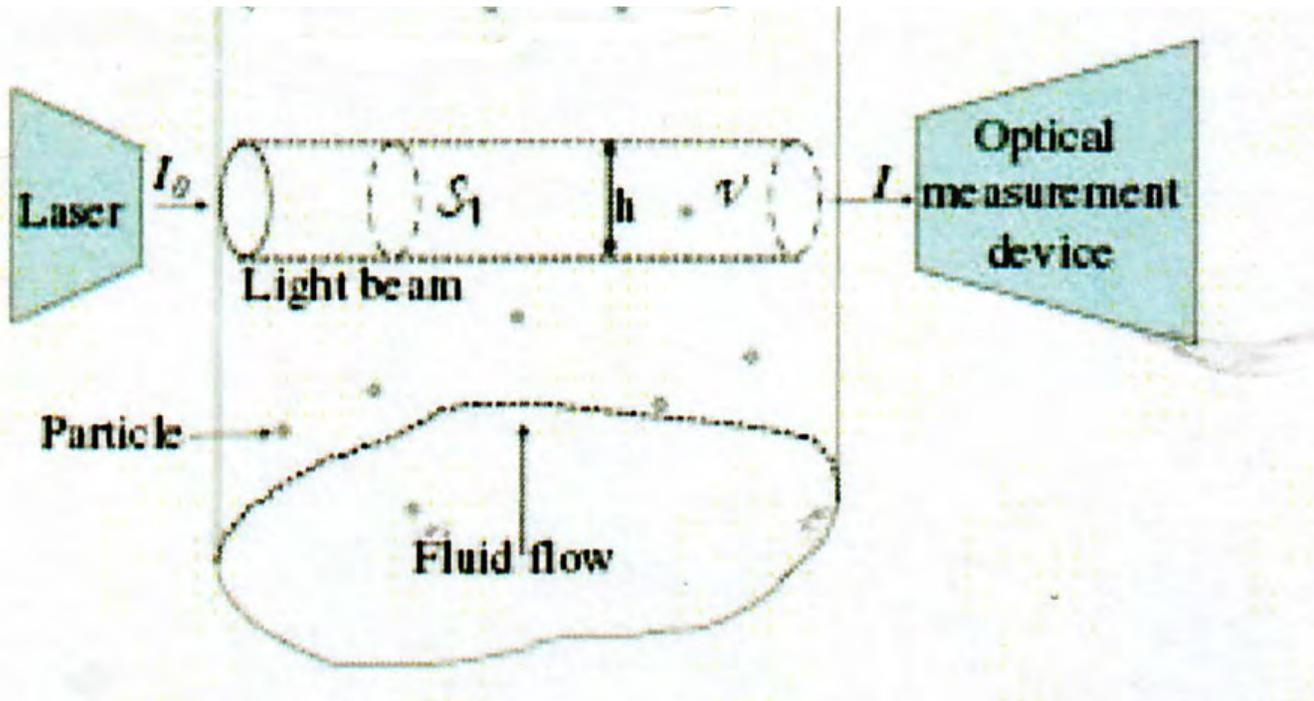
## 7 TECHNIQUES

- INTRUSIVE/NON-INTRUSIVE  
(or Invasive/Non-invasive):



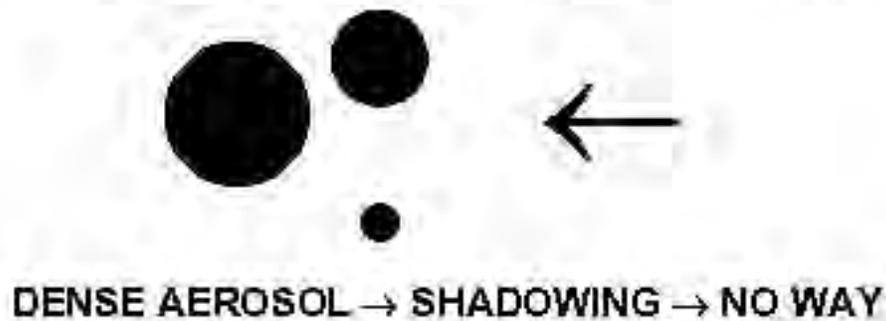
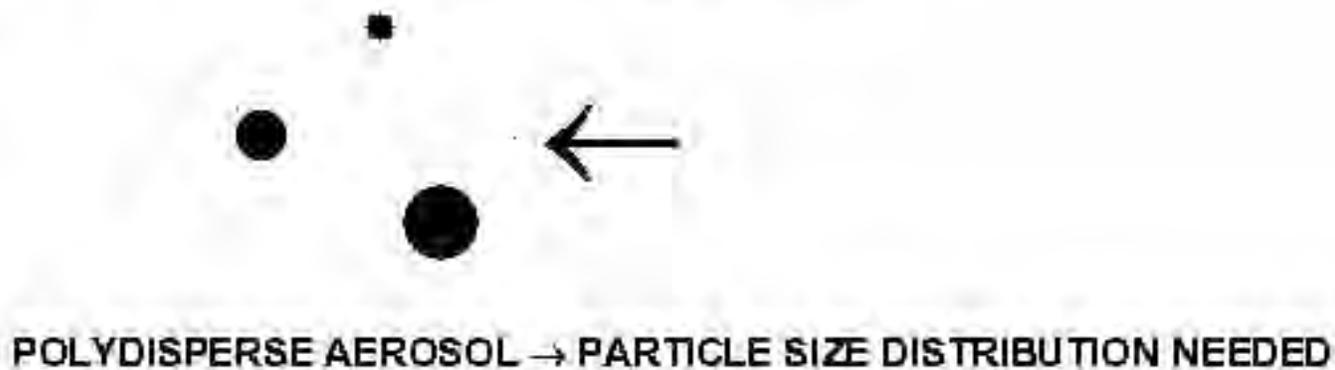
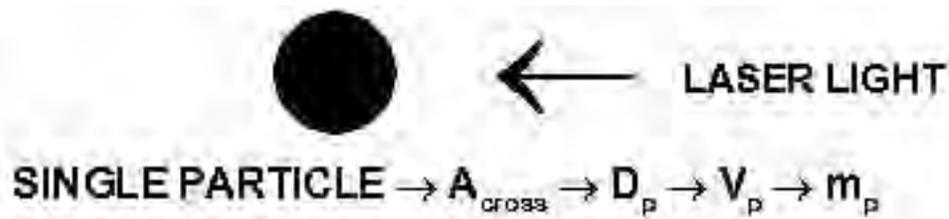
8	LASER EXTINCTION
	LASER INDUCED INCANDESCENCE

- LE: ATTENUATION  $I/I_0$  OF LASER LIGHT INTENSITY DUE TO OPAQUE PARTICLES



- LII: PARTICLES BROUGHT TO HIGH  $T$  BY LASER PULSE, EMITTED RADIATION MEASURED

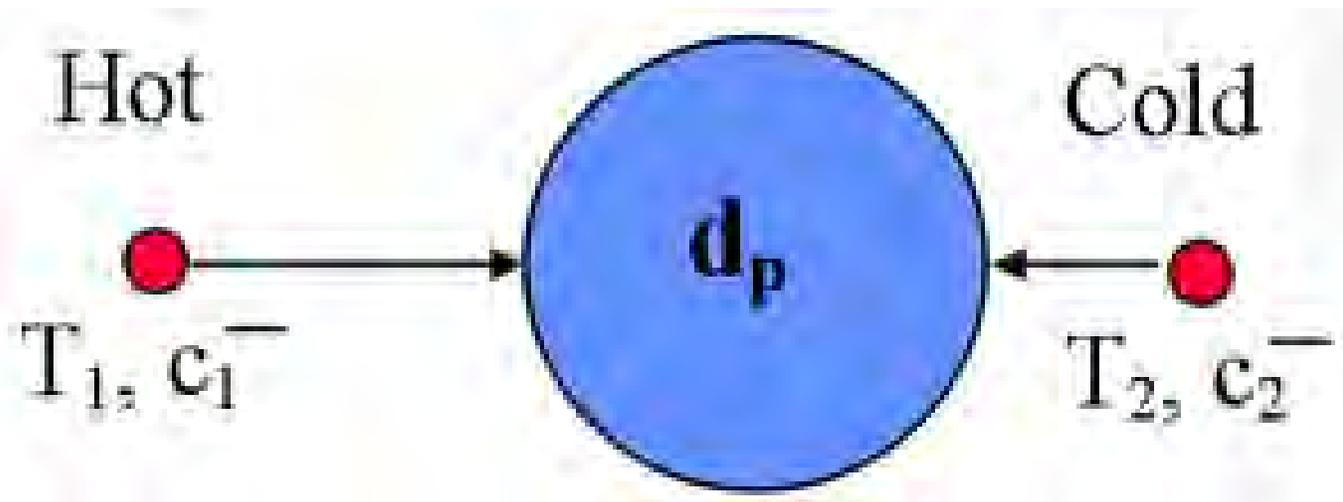
## 9 LIMITS OF LASER EXTINCTION TECHNIQUE



- FURTHER, CANNOT DETECT TRANSLUCENT PARTICLES
- NOT APPLICABLE IN CLOSED CHAMBERS

## 10 THERMOPHORESIS

- PARTICLES DRIFTED IN DIRECTION OF LOWER TEMPERATURE



- IF A (COLD) WIRE OR PLATE IS PUT INTO THE FLAME, SOOT WILL DEPOSIT ON IT
- EFFECTIVE ONLY ON VERY SMALL PARTICLES,  $< 1 \mu m$
- (THE SAME HOLDS FOR GAS MOLECULES):

$$\frac{\partial}{\partial t} (\rho Y_i) + \frac{\partial}{\partial x_k} (\rho u_k Y_i) = \left[ \begin{array}{c} \text{DIFFUSION} \\ \propto \partial Y_i / \partial x_k \end{array} \right] + \left[ \begin{array}{c} \text{SORET} \\ \propto \partial T / \partial x_k \end{array} \right] + w_i$$

$$\frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_k} (\rho u_k h) = \left[ \begin{array}{c} \text{DIFFUSION} \\ \propto \partial T / \partial x_k \end{array} \right] + \left[ \begin{array}{c} \text{DUFOUR} \\ \propto \partial Y_i / \partial x_k \end{array} \right] + \text{RADTN}$$

## 11 TPD (1)

### THERMOCOUPLE PARTICLE DENSITOMETRY

- INDICES:  $T$  THERMOPH.,  $g$  GAS,  $p$  PARTICLE,  $s$  SOOT,  $w$  WALL/WIRE, " PER UNIT AREA
- THERMOPHORETIC VELOCITY  $v_T = -\mathcal{D}_T \frac{\nabla T_g}{T_g}$
- IF DIAMETER  $D_p \ll$  MEAN FREE PATH  $\lambda$   
 $\rightarrow \mathcal{D}_T \simeq 0,54 \nu_g$  (OTHERWISE, MORE COMPLEX EXPRESSION)

- $\lambda = 2 \nu_g / \sqrt{8RT/\pi} =$ 

(FOR AIR)	1000 K	2000 K
1 atm	275 nm	580 nm
10 atm	27.5 nm	58 nm

- MASS FLUX DUE TO THERMOPHORESIS  
 $(k_g$  CONDUCTIVITY,  $\dot{q}''$  HEAT FLUX):

$$\dot{m}'' = \rho_s f_v v_T = \rho_s f_v \left[ -\frac{\mathcal{D}_T}{T_g} \frac{\partial T_g}{\partial n} \right]_w = \rho_s f_v \frac{\mathcal{D}_T}{k_g T_g} \dot{q}''$$

$$\dot{q}'' = h_c (T_g - T_w) = \frac{Nu k_g}{D_w} (T_g - T_w)$$

- BUT  $k_g = k_g(T) \simeq k_{g0} T \rightarrow$  MORE CORRECTLY  $\rightarrow$

12 TPD (2)

$$\dot{q}'' \simeq \frac{Nu k_{g0}}{D_w} \int_{T_w}^{T_g} T dT = \frac{Nu k_{g0}}{2 D_w} (T_g^2 - T_w^2) = \frac{Nu k_g T_g}{2 D_w} \left[ 1 - \left( \frac{T_w}{T_g} \right)^2 \right]$$

$$\dot{m}'' = \rho_s f_v \mathcal{D}_T \frac{Nu}{2 D_w} \left[ 1 - \left( \frac{T_w}{T_g} \right)^2 \right] \quad (1)$$

- INDICES:  $d$  DEPOSIT,  $j$  JUNCTION (THERMOC.)
- $\rho_d \simeq 170 \text{ kg/m}^3 \ll \rho_s \quad (1800 \text{ kg/m}^3)$

$$\dot{m}'' = \frac{\rho_d}{2} \frac{dD_j}{dt}$$

- HPs:

1. NO RADIATIVE HEAT TRANSFER TO JUNCTN
2. NO CHEMICAL HEAT RELEASE AT SURFACE
3. NO HEAT CONDUCTION ALONG WIRE
4. NEGLIGIBLE JUNCTION THERMAL INERTIA

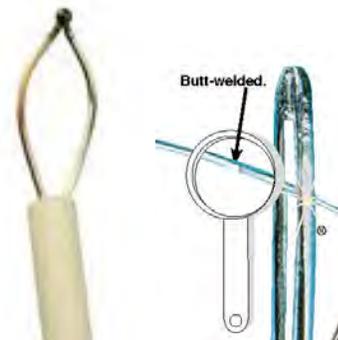


Figure 1: Thermocouple junctions: (left) standard, (right) butt-welded.

## 13 TPD (3)

- RADIATION = CONVECTION

$$\epsilon_j \sigma T_j^4 = \frac{Nu k_{g0}}{2 D_j} (T_g^2 - T_j^2) \quad \rightarrow$$

$$D_j = \frac{Nu k_{g0}}{2 \epsilon_j \sigma} \left( \frac{T_g^2}{T_j^4} - \frac{1}{T_j^2} \right) \quad \rightarrow \quad (2)$$

$$\frac{dD_j}{dt} = \frac{Nu k_{g0}}{\epsilon_j \sigma} \left( \frac{1}{T_j^3} - 2 \frac{T_g^2}{T_j^4} \right) \frac{dT_j}{dt}$$

$$\rho_s f_v \frac{Nu \mathcal{D}_T}{2 D_j} \left[ 1 - \left( \frac{T_j}{T_g} \right)^2 \right] = \frac{\rho_d}{2} \frac{Nu k_{g0}}{\epsilon_j \sigma} \left( \frac{1}{T_j^3} - 2 \frac{T_g^2}{T_j^4} \right) \frac{dT_j}{dt}$$

- USING (2) FOR  $D_j \rightarrow$  DIFFERENTIAL EQ. IN  $T_j$ ;  
SOLUTION:

$$G = \beta f_v t + G_0 \quad \left\{ \begin{array}{l} G = 1/4 \cdot (T_g/T_j)^8 - 1/6 \cdot (T_g/T_j)^6 \\ \beta = 2 \mathcal{D}_T (\epsilon_j \sigma)^2 T_g^4 / (\rho_d k_{g0} Nu / \rho_s) \end{array} \right.$$

- $T_j$  AND  $T_g$  NEED TO BE MEASURED

14 TPD (4)
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- THREE PHASES; DIFFERENT  $\epsilon_j$ 's

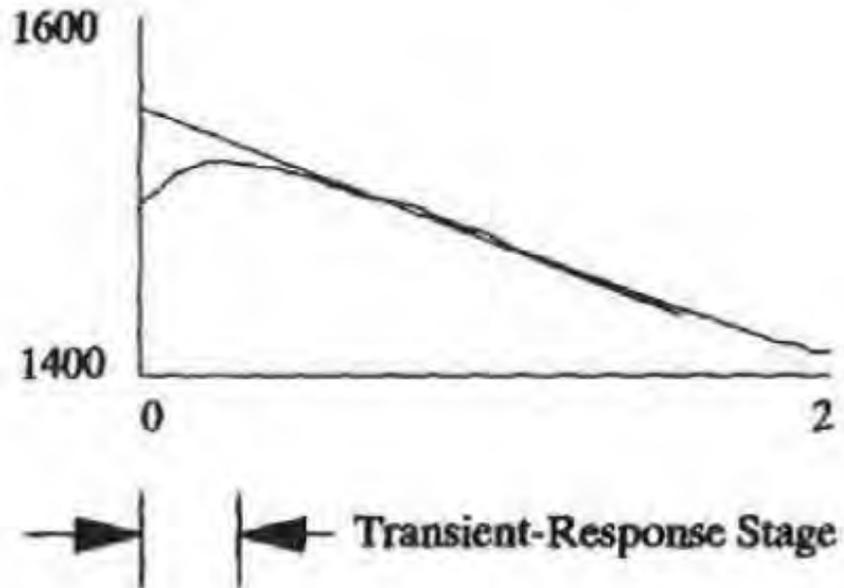


Figure 2: Thermocouple junction temperature *vs.* time, and extrapolated gas temperature.

**15 SCED**  
**SOOT CONCENTRATION ESTIMATE**  
**via DEPOSITION**

- **TECHNIQUE UNDER DEVELOPMENT, AIMING AT MEASUREMENTS INSIDE A COMB. CHAMBER**
- **TUNGSTEN (W) WIRE USED FOR HIGHER  $T$  (BUT RISK BURNING)**
- **HPs:**
  1. **NO RADIATIVE HEAT TRANSFER TO JUNCTN**
  2. **NO CHEMICAL HEAT RELEASE AT SURFACE**
  3.  **$T_w$  GRADIENT  $\sim$  CONST ALONG WIRE**
  4.  **$T_w/T_g \sim$  CONST ALONG WIRE**
  5. ~~**NO HEAT CONDUCTION ALONG WIRE**~~
  6. ~~**NEGLIGB JUNCTN THERMAL INERTIA**~~
- **TUNGSTEN WIRE HEAT BALANCE:**

$$c_w m_w \frac{dT_w}{dt} = \dot{q}_{in} - \dot{q}_{out}$$

- **WIRE MASS  $m_w = \rho_w \frac{\pi D_w^2}{4} l$**

## 16 SCED (2)

- CONVECTIVE HEAT IN  $\dot{q}_{in} = h_c \pi D_w l (T_g - T_w)$
- RADIATIVE/CONDUCTIVE HEAT OUT

$$\dot{q}_{out} = \epsilon \sigma T_w^4 \pi D_w l + 2 \lambda_W \frac{\pi D_w^2}{4} \frac{dT_w}{dx}$$

- ROUGH GUESS  $T$  GRADIENT AT BOTH ENDS

$$\frac{dT_w}{dx} = \frac{T_w - T_{amb}}{l/4}$$

$$c_W \rho_W \frac{\pi D_w^2}{4} l \frac{dT_w}{dt} =$$

$$= h_c \pi D_w l (T_g - T_w) - \epsilon \sigma T_w^4 \pi D_w l - 2 \lambda_W \frac{\pi D_w^2}{4} \frac{T_w - T_{amb}}{l/4}$$

- BY DIVIDING THROUGH BY  $\pi D_w l$ :

$$c_W \rho_W \frac{D_w}{4} \frac{dT_w}{dt} = h_c (T_g - T_w) - \epsilon \sigma T_w^4 - 2 \lambda_W D_w \frac{T_w - T_{amb}}{l^2}$$

- ESTIMATE  $T_g$  (AVERAGED ALONG WIRE):

$$T_g = \frac{\epsilon \sigma T_w^4}{h_c} + \left( 1 + \frac{2 \lambda_W D_w}{h_c l^2} \right) T_w + \frac{c_W \rho_W D_w}{4 h_c} \frac{dT_w}{dt} - \frac{2 \lambda_W D_w}{h_c l^2} T_{amb}$$

**17 SCED (3)**

- $T_w$  MEASURED AFTER ELECTRIC RESISTANCE

$$R = \rho_{\Omega} l / (\pi D_w^2 / 4)$$

$$\rho_{\Omega} = \rho_{\Omega}^0 + \alpha(T_w - T_0)$$

→ ESTIMATE  $T_w$  (AVERAGED ALONG WIRE)

⇒ ESTIMATE  $T_w/T_g$  (AVERAGED ALONG WIRE)

- MASS RATE OF DEPOSIT PER UNIT AREA

$$\dot{m}'' = \frac{\rho_s V_s}{A \Delta t} = \frac{\rho_d V_d}{A \Delta t}$$

- BY EQUATING TO (1):

$$f_v = \frac{2 D_w}{Nu \mathcal{D}_T} \left[ 1 - \left( \frac{T_w}{T_g} \right)^2 \right]^{-1} \frac{\rho_d / \rho_d V_d}{A \Delta t}$$

- $V_d$  DETERMINED BY ELECTRON MICROSCOPE OR OTHER MEASURING DEVICE

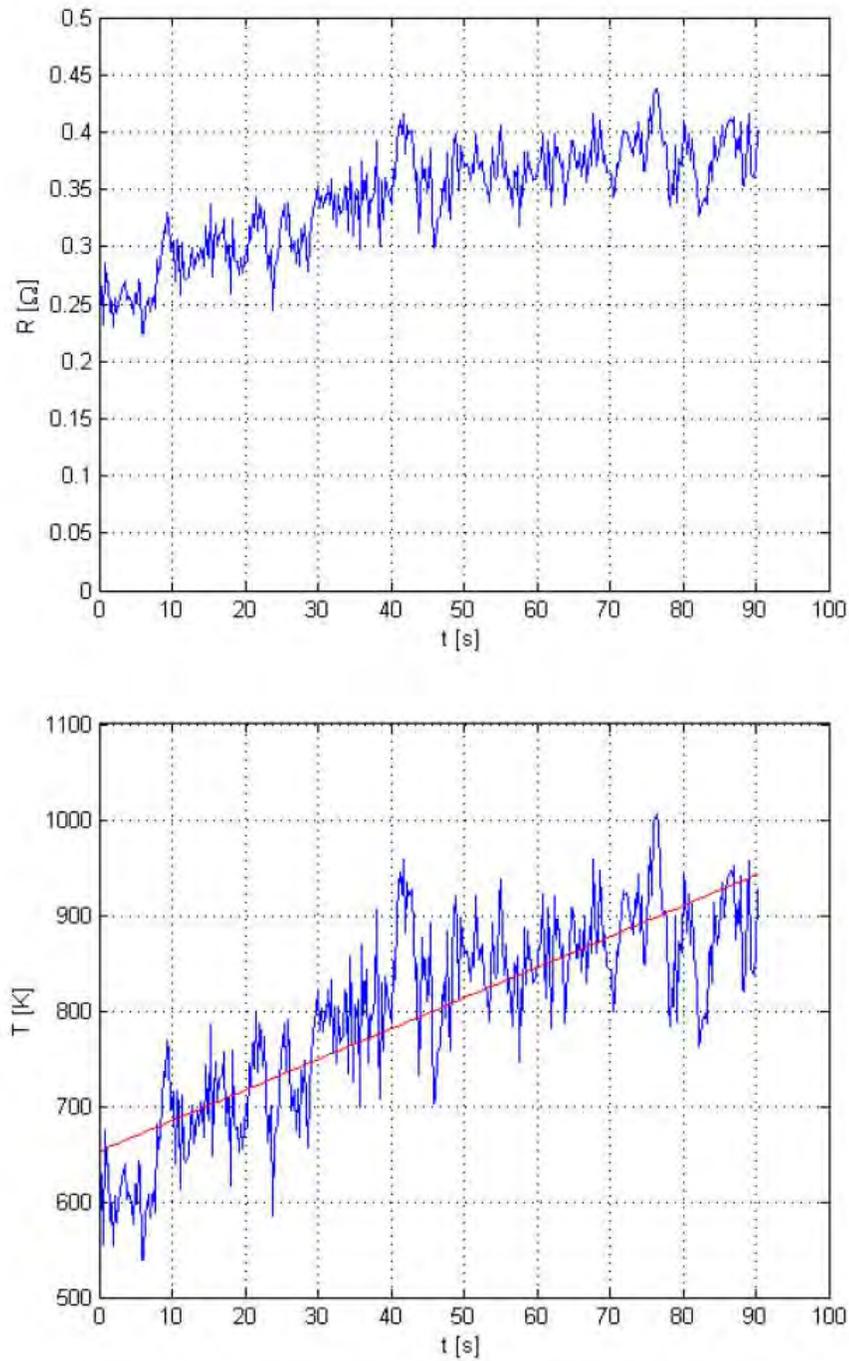
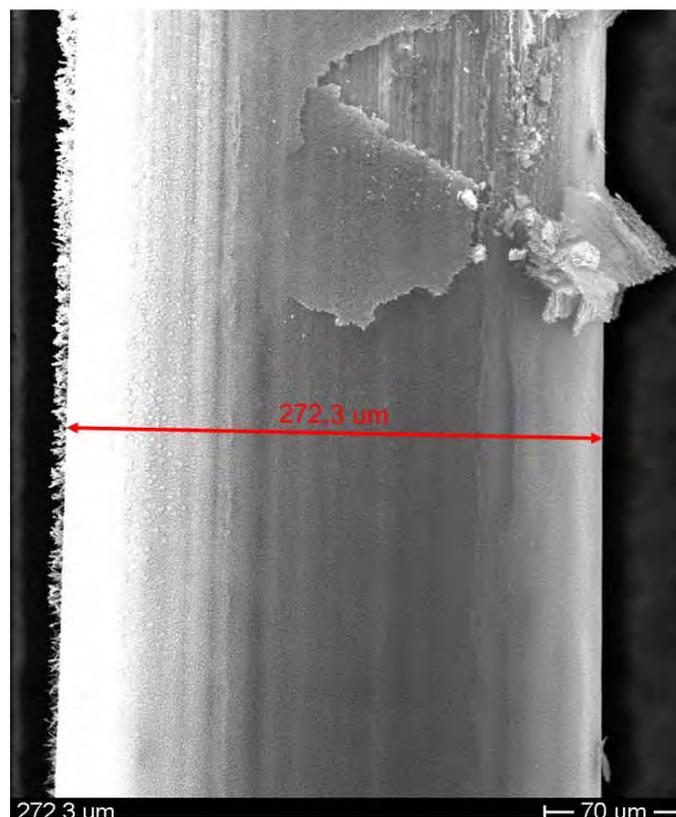
**18 SCED (4)**

Figure 3: Electric resistance and temperature as a function of time, methane/air flame, 150 mm height.

# 19 SCED (5)



Full scale counts: 1276

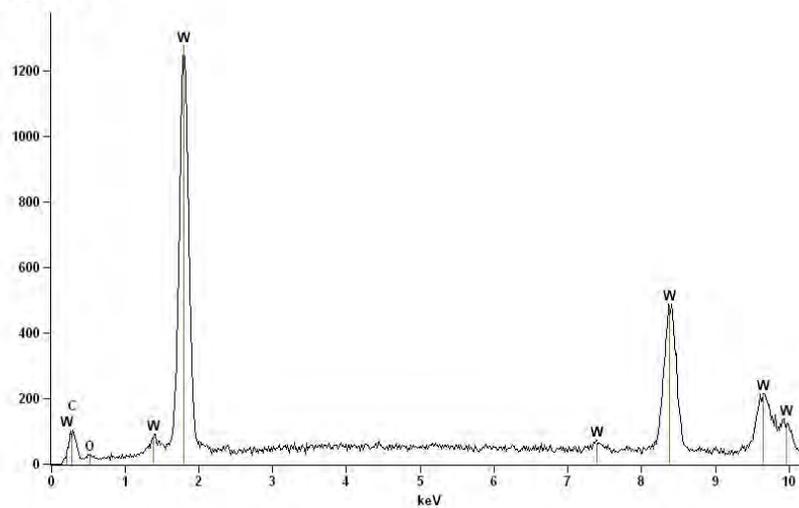


Figure 4: (top) Scanning Electron Microscope image, (bottom) EDS (Energy Dispersive X-ray Spectroscopy) analysis.

## 20 SCED *vs.* TPD

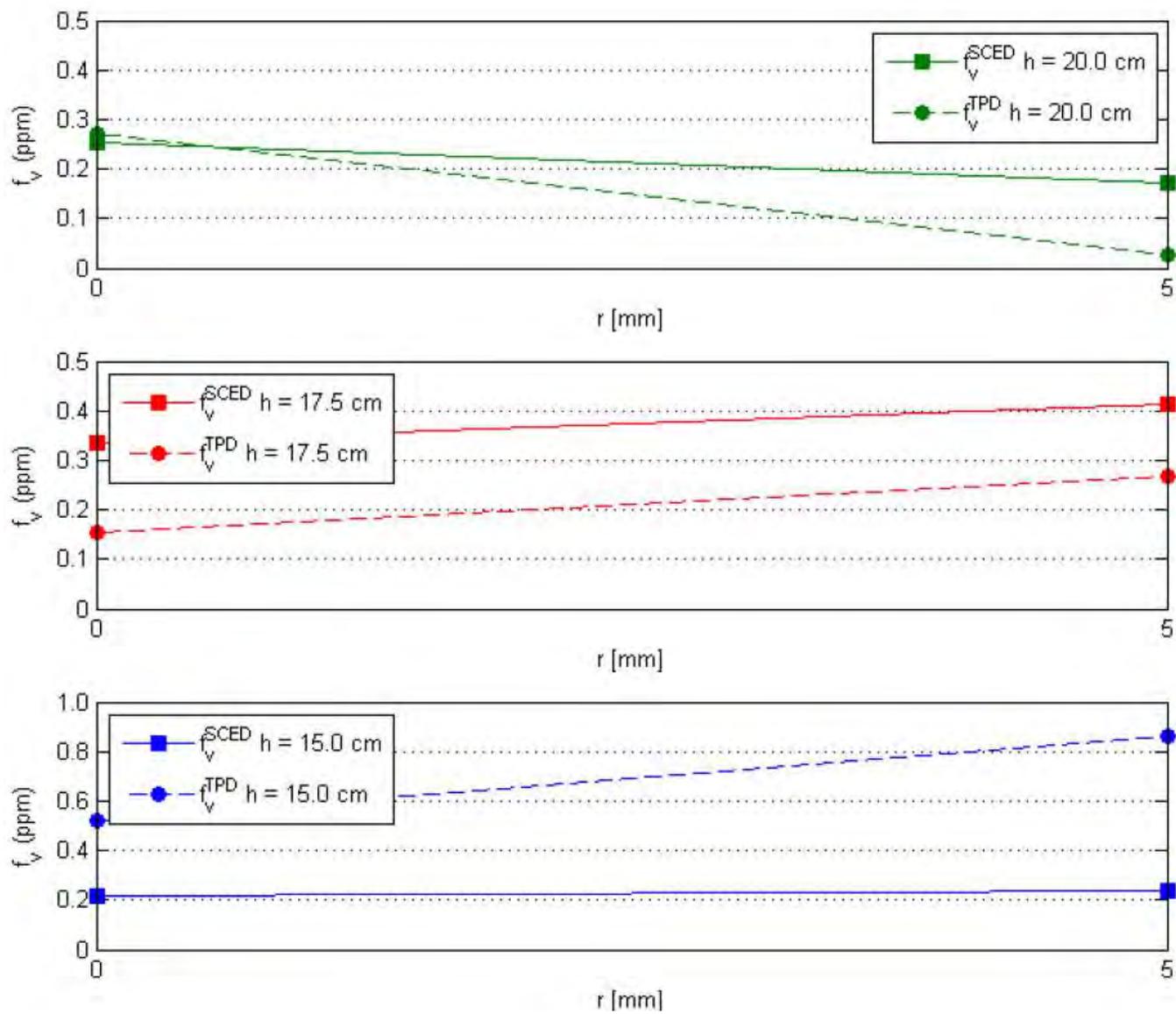


Figure 5: Comparison of SCED and TPD results.

<b>21 PROS AND CONS OF THE DIFFERENT TECHNIQUES</b>
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### LE, LASER EXTINCTION

PROS	CONS
NON-INTRUSIVE ~ ACCURATE POINTWISE	CANNOT DETECT TRANSLUCENT SOOT SOOT SIZE DISTRIBUTION NEEDED CANNOT MEASURE INSIDE CHAMBER

### TPD, THERMOCOUPLE PARTICLE DENSITOMETRY

PROS	CONS
OPAQUE & TRANSLUCENT SOOT POINTWISE	INTRUSIVE UNSUITED $> 2000$ K UNSUITED FOR HIGH $X_{\text{oxidizer}}$ LOTS OF MEASUREMENTS ~ 50% UNCERTAINTY (SURFACE CATALYSIS)

### SCED, SOOT CONCENTRN ESTIMATE via DEPOSITN

PROS	CONS
OPAQUE & TRANSLUCENT SOOT POSSIBLY SUITED TO CHAMBERS MEASURES ALONG WHOLE TRANSVERSE	INTRUSIVE UNSUITED FOR HIGH $X_{\text{oxidizer}}$ REQUIRES PERFORATIONS NOT EXACTLY POINTWISE

**22 SOOT MODELS**

- $n$  NUCLEATION,  $g$  SURFACE GROWTH,  $ox$  OXIDATION,  $a$  AGGLOMERATION
- $Y_s$  SOOT MASS FRACTION
- $N_s$  NUMBER DENSITY (NO. PARTICLES PER UNIT MIXTURE MASS)

$$\frac{\partial}{\partial x_k} (\bar{\rho} \tilde{u}_k \tilde{Y}_s) = 0.55 \frac{\partial}{\partial x_k} \left( \frac{\mu}{\bar{T}} \frac{\partial \bar{T}}{\partial x_k} \tilde{Y}_s \right) + w_{Y_s}$$

$$\frac{\partial}{\partial x_k} (\bar{\rho} \tilde{u}_k \tilde{N}_s) = 0.55 \frac{\partial}{\partial x_k} \left( \frac{\mu}{\bar{T}} \frac{\partial \bar{T}}{\partial x_k} \tilde{N}_s \right) + w_{N_s}$$

- TYPICAL FORM OF SOURCE (PRODUCTION/DESTRUCTION) TERM:

$$w_{Y_s} = r'_n + r_g - r_{ox}$$

$$w_{N_s} = r''_n - r_a$$

- QUITE CRUDE! (ONLY 2 EQS. TO DESCRIBE ALL CHEMICAL AND PHYSICAL PROCESSES)