Physics and chemistry of the gas-condensed phase interface

Franck RICHARD
University of Poitiers
France

MacFP workshop
IAFSS - Lund
June, 11th 2017

Background

Burning behavior of condensed phase fuels remains a challenge

- Due to complex interactions at interface between gas-phase flame and condensed phase

- This complexity increases as scales increase

Challenge

Explore the dynamic relationship between combustible condensed fuel surface and gas-phase flame

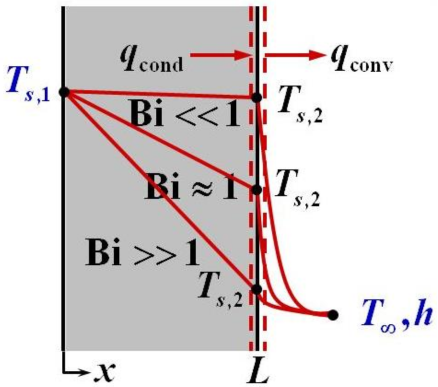
Background

A variety of configurations

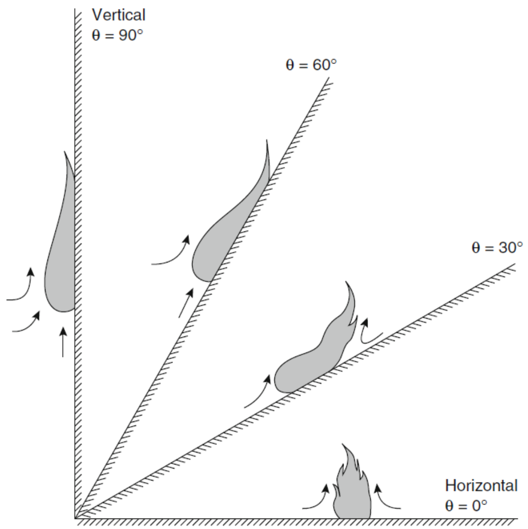
- ***Solid material type***
  - ✓ Chemically inert (e.g concrete)
  - ✓ Flammable (e.g plastic, wood, fabric)

Material properties
Physical, chemical, optical properties

- ***material « thickness »***
  - ✓ Thermally thin
  - ✓ Thermally thick

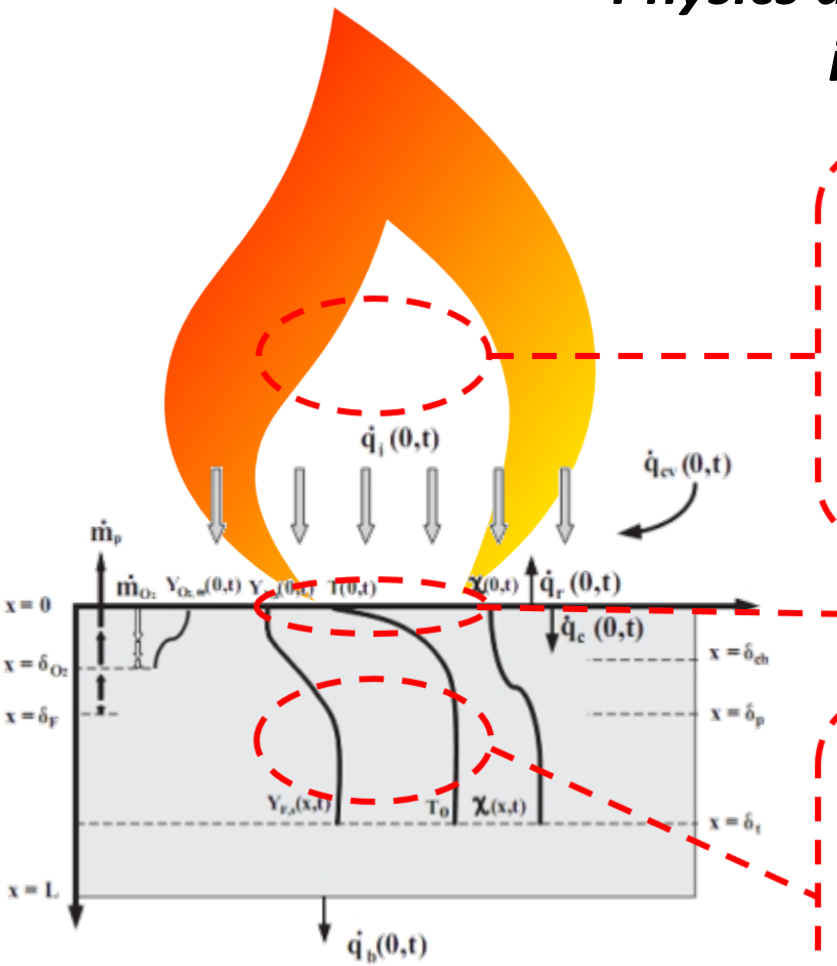


- ***Material orientation***
  - ✓ Floor fire
  - ✓ Ceiling fire
  - ✓ Wall fire



Background

Physics and chemitry processes involved in solid fuel combustion



- **Heat transfer**
  - ✓ *Conduction, convection, radiation*
- **Mixing & Mass transfer**
  - ✓ *Advection, mixing at micro-scale*
- **Chemistry**
  - ✓ *Chemical reactions (finite rate)*

Gas phase

Heat & mass transfer

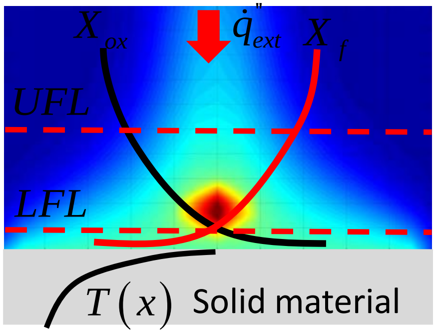
- **Heat & mass transfer**
  - ✓ *Diffusion, heat transfer*
- **Solid chemistry**
- **Structure change**
  - ✓ *Optical & physical properties*

Condensed phase

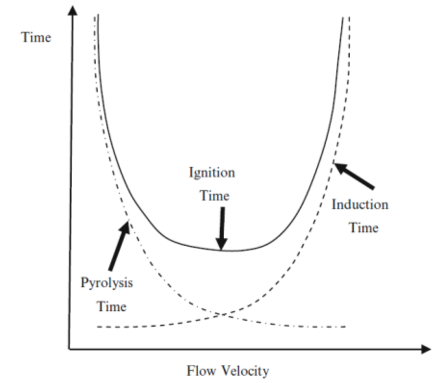
Background

Interface play a role on many processes

- Ignition
- Propagation



Roblin (2017)



Nioka (1981)
Fernandez-Pello (1995)

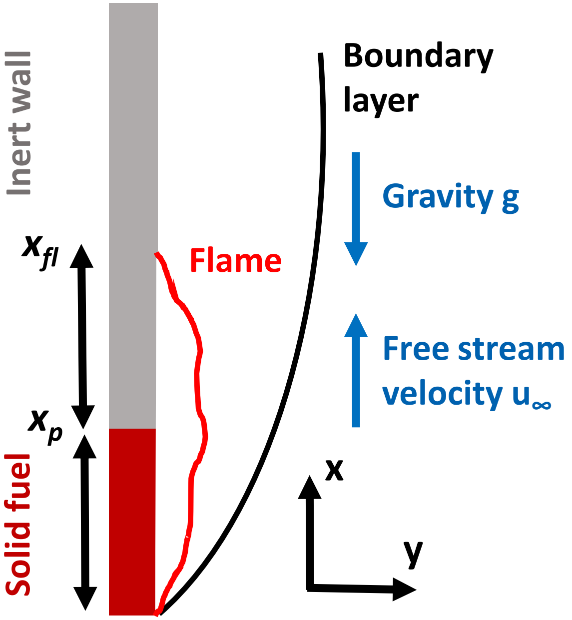
Non-spreading wall flame
Buoyancy-driven (u_∞ small) or momentum-driven (u_∞ large) flow

✓ Pyrolysis region $0 \leq x \leq x_p$

✓ Wall flame region $0 \leq x \leq x_{fl}$

✓ Inert wall region $x_p \leq x$

✓ Wall plume region $x_{fl} \leq x$

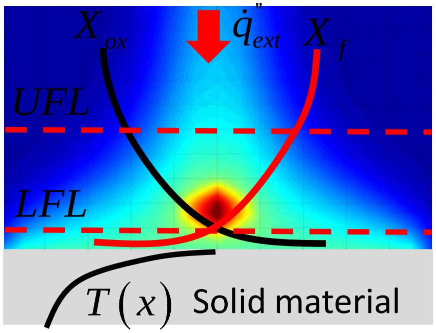


A.Trouvé

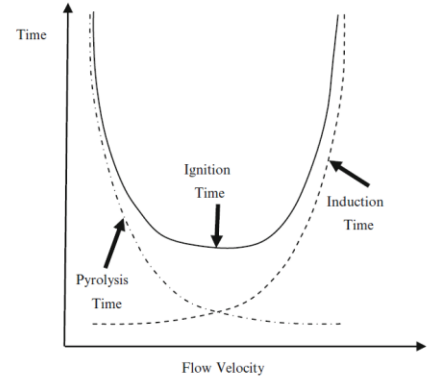
Background

Interface play a role on many processes

- Ignition
- Propagation



Roblin (2017)



Nioka (1981)
Fernandez-Pello (1995)

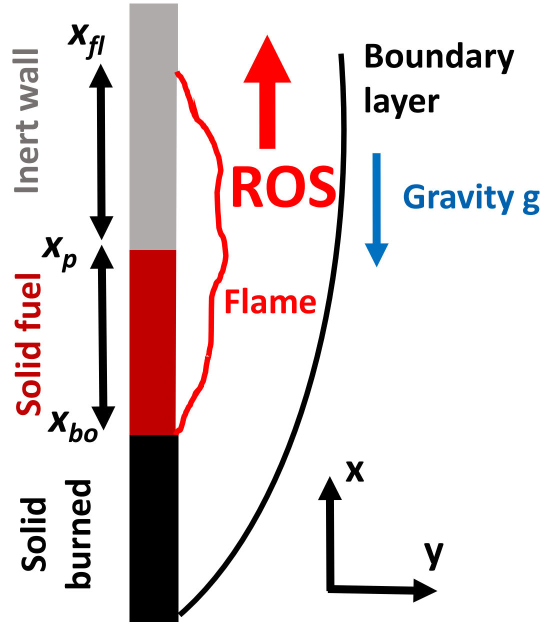
Spreading wall flame with upward spread (flow –aided)

✓ Pyrolysis region
$x_{bo}(t) \leq x \leq x_p(t)$

✓ Wall flame region
$x_{bo}(t) \leq x \leq x_{fl}(t)$

✓ Inert wall region
$x \leq x_{bo}(t)$ *and* $x_p(t) \leq x$

✓ Wall plume region
$x_{fl} \leq x$

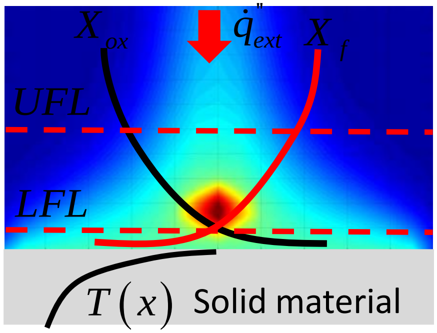


A.Trouvé

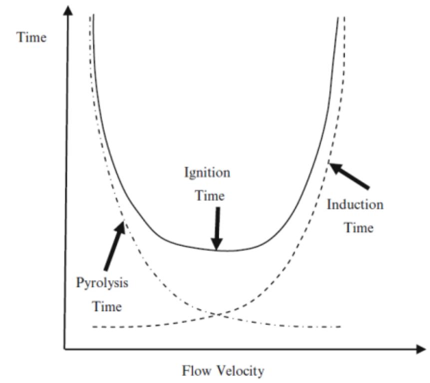
Background

Interface play a role on many processes

- Ignition
- Propagation



Roblin (2017)



Nioka (1981)
Fernandez-Pello (1995)

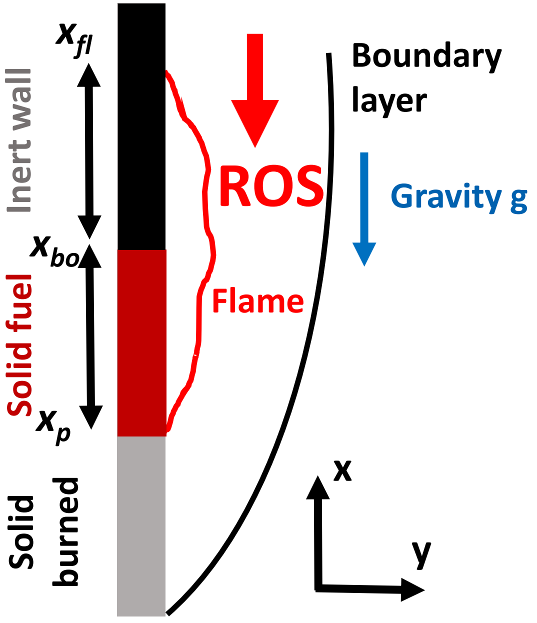
Spreading wall flame with downward spread (flow –opposed spread)

✓ Pyrolysis region
$x_p(t) \leq x \leq x_{bo}(t)$

✓ Wall flame region
$x_p(t) \leq x \leq x_{fl}(t)$

✓ Inert wall region
$x \leq x_p(t)$ and $x_{bo}(t) \leq x$

✓ Wall plume region
$x_{fl} \leq x$

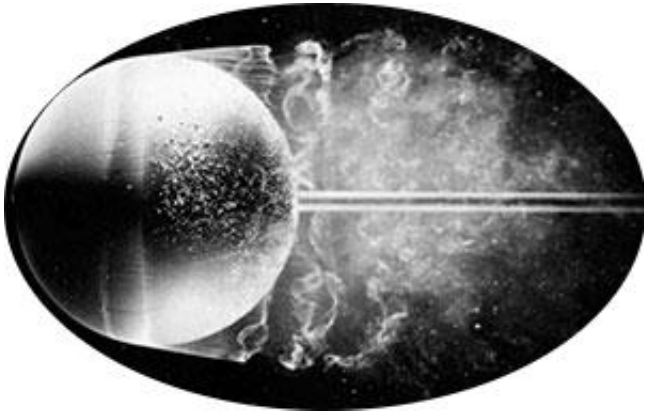


A.Trouvé

Boundary layer

Flow over solid surfaces usually produce a shear layer due to « non-slip » conditions

Boundary Layer :

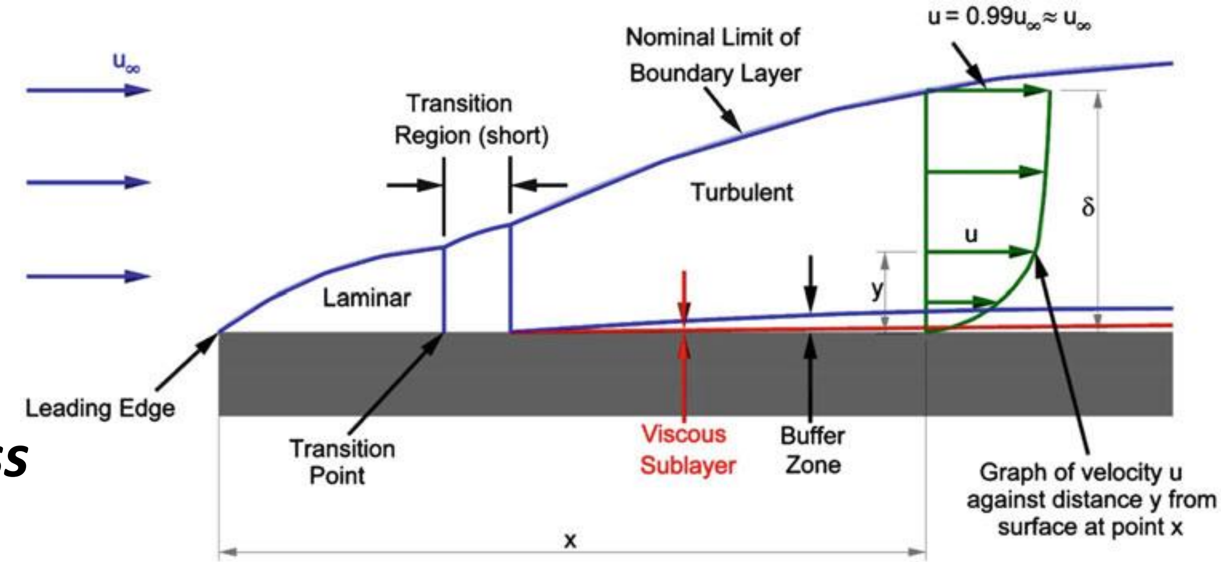


- Predominant direction of flow
- Shear stresses, heat fluxes and mass-diffusion fluxes significant in directions normal to the predominant direction of flow
- Shear layer at fluid-solid interface due to « non-slip » conditions

Boundary layer

- ***At solid boundary***

« no-slip » boundary condition due to viscous forces



B.Merci (SFPE)

- ***Boundary layer thickness***

$$y = \delta,\ v_x = 0.99U_\infty$$

$y < \delta$ | Strong velocity gradients and viscous shear stresses

$y > \delta$ | Negligible velocity gradients and viscous shear stresses

- ***Laminar boundary layer thickness***

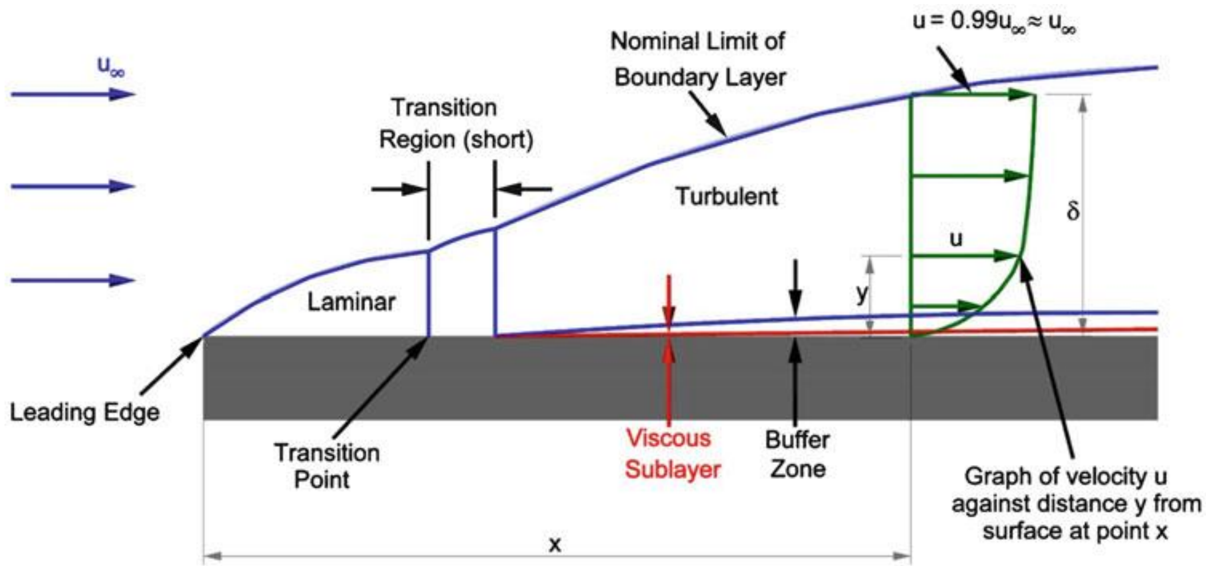
In the assumption that $(\delta \ll x)$, It can be shown that $\delta_{lam} \sim \left(\frac{\mu x}{\rho U_\infty} \right)^{1/2}$

Boundary layer

- ***Viscous shear stress (at interface)***

$$\tau_s = \mu \left(\frac{\partial v_x}{\partial y} \right) \bigg|_{y=0}$$

$$\sim \rho \nu \frac{U_\infty}{\delta} \sim \rho U_\infty^2 \left(\frac{U_\infty x}{\nu} \right)^{-1/2}$$



B.Merci (SFPE)

- ***Friction coefficient***

$$C_{f,x} = \frac{\tau_{s,x}}{0.5 \rho U_\infty^2} \sim \left(\frac{U_\infty x}{\nu} \right)^{-1/2} = \mathrm{Re}_x^{-1/2}$$

$$\delta_{turb} = 0.37 x \, \mathrm{Re}_x^{-1/5}$$

$$C_{f,x,turb} = 0.0592 \, \mathrm{Re}_x^{-1/5}$$

- ***Blasius solution yields***

$$\delta_{lam} = 4.92 x \, \mathrm{Re}_x^{-1/2}, \; C_{f,x,\mathrm{lam}} = 0.664 \, \mathrm{Re}_x^{-1/2}$$

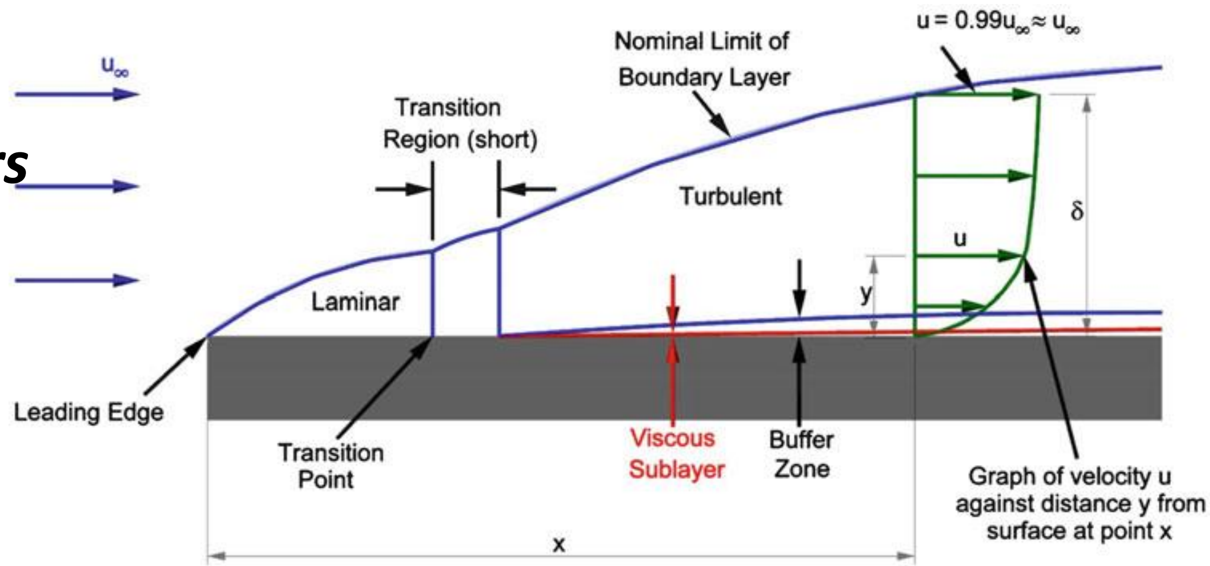
As $x \nearrow$ Turbulence can start

Turbulent b.l grows more rapidly than a laminar b.l

Boundary layer

- ***Introducing non dimentional parameters***
  - ✓ Friction velocity
  - ✓ Distance from solid boundary

$$u^* = \sqrt{\frac{\tau_s}{\rho}} \; ; \; y^+ = \frac{y u^*}{\nu}$$



B.Merci (SFPE)

3 regions can be distinguished (inner boundary layer)

- Viscous sub-layer

$\left(y^+ < 5\right)$

> Turbulence is damped (blocking effects and viscous forces)
>
> Velocity ↗ linearly with the distance from solid

Boundary layer

- Buffer layer

  $\left(5 < y^{+} < 30\right)$

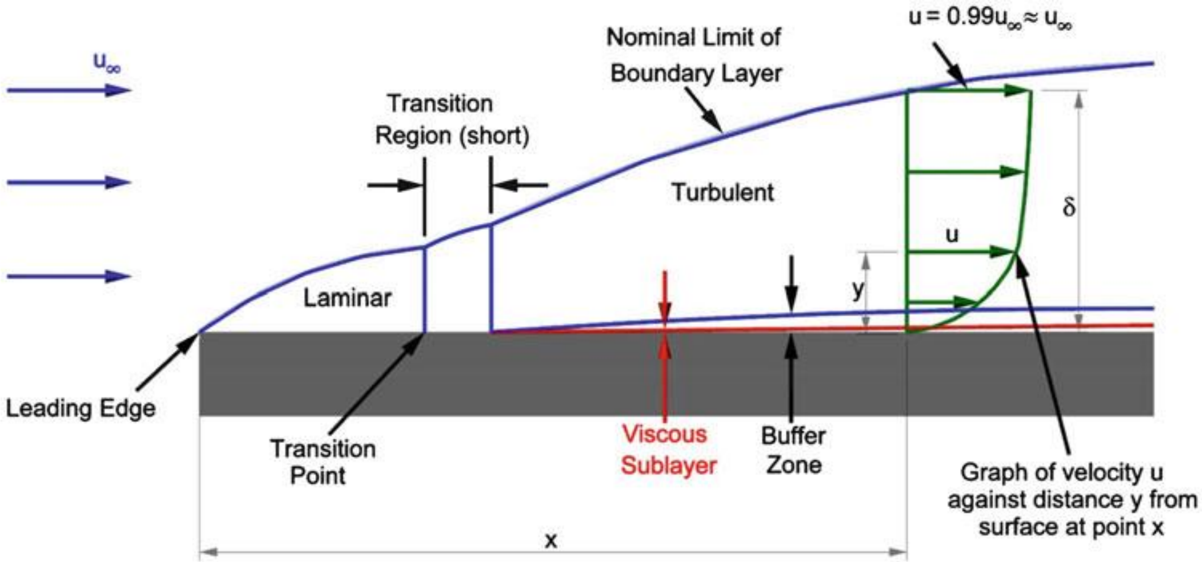
  Transitional region

- Logarithmic layer

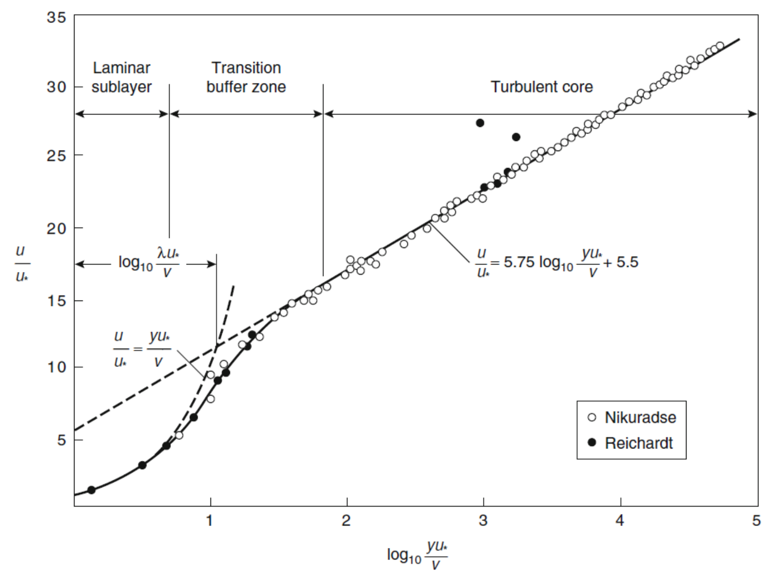
  $\left(30 < y^{+} < 300\right)$

  Turbulent motions

  Log relation between mean velocity and distance from the solid



B.Merci (SFPE)



Thermal boundary layer

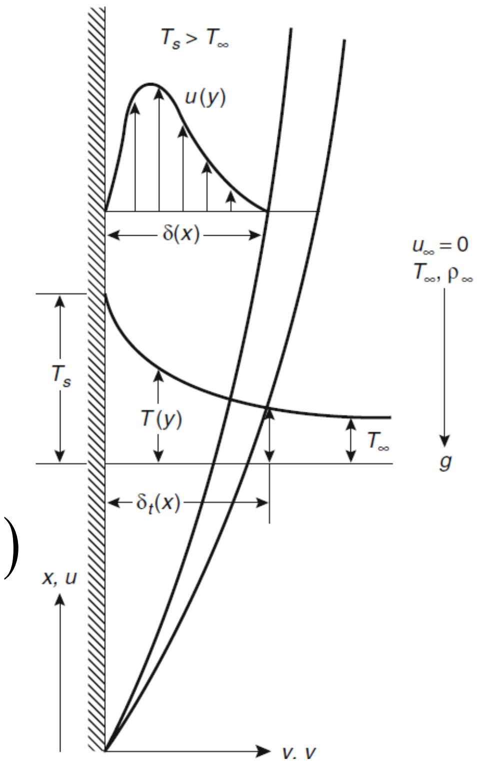
Similar to boundary layers at level of velocities, thermal boundary layer can be defined

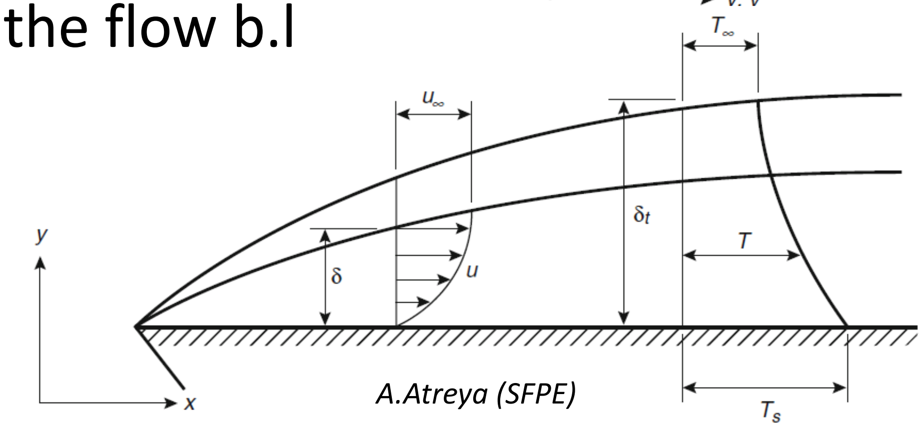
- Thermal diffusivity plays the same role for heat transfer as the kinetic viscosity does for momentum transfer

Boundary layer thickness : $y=\delta_T : T-T_S = 0.99\left(T_\infty - T_S\right)$

- Prandtl number determines whether the thermal b.l is thicker or not than the flow b.l

$$\mathrm{Pr}=1: \delta=\delta_T$$
$$\mathrm{Pr}<1: \delta<\delta_T$$
$$\mathrm{Pr}>1: \delta>\delta_T$$





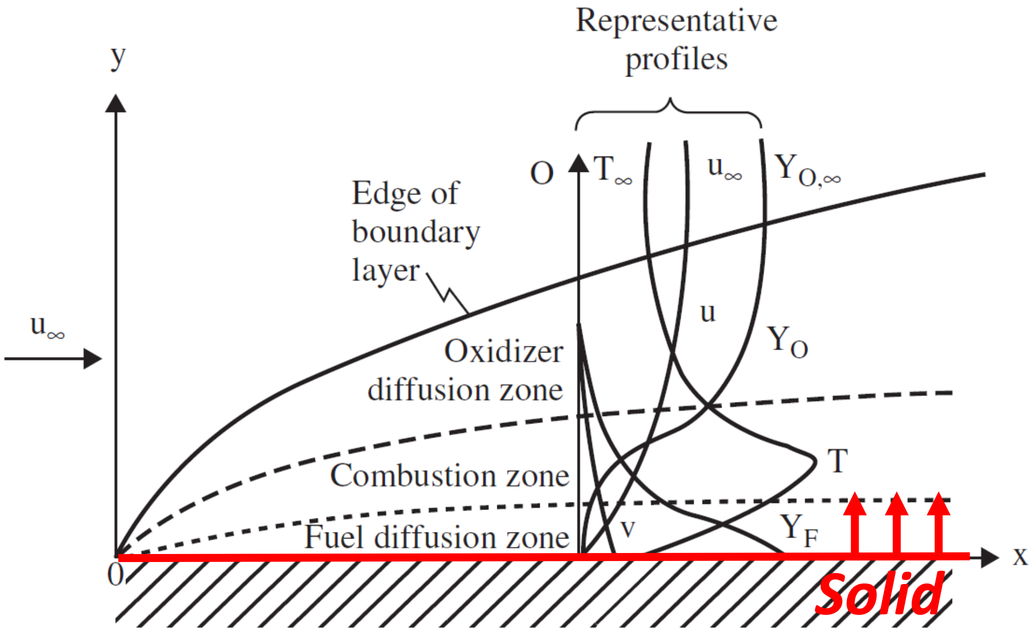
A.Atreya (SFPE)

Reacting boundary layer

Introduced & developped by many authors

- ***Emmons (1956)***

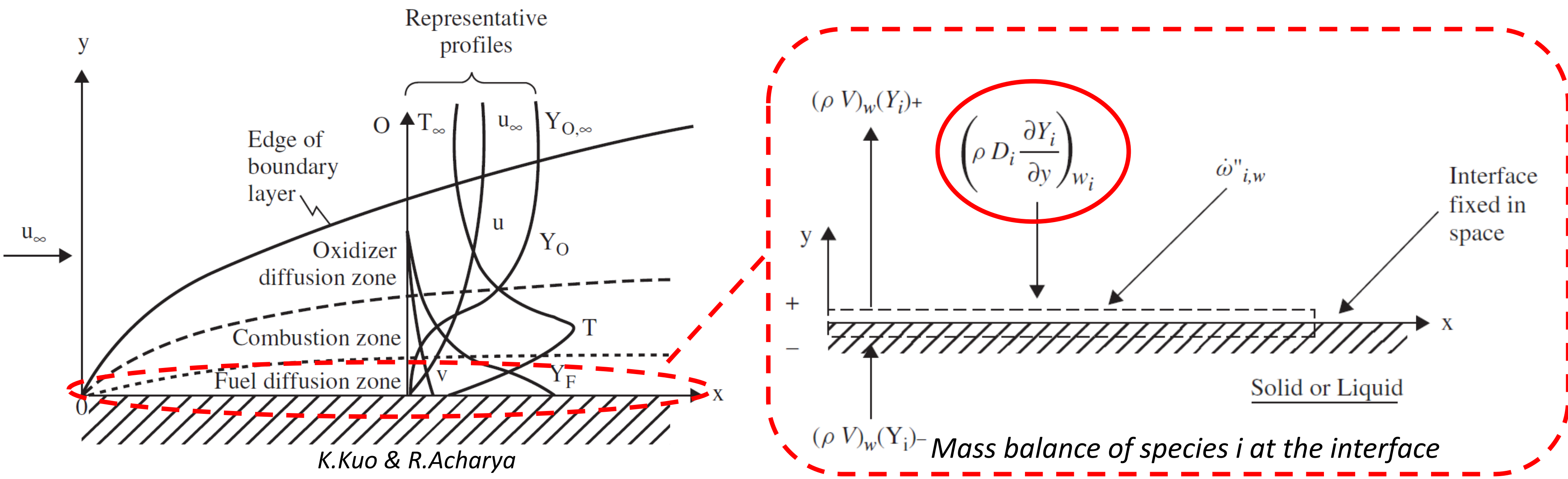
Studied the burning of condensed fuel (flat plate) in an oxidizer streem



Parameter	Types
Magnitude of reaction rate	Equilibrium or nonequilibrium
Site of chemical reaction	Gas phase, heterogeneous, or both
Turbulence level	Laminar or turbulent
Geometric contour	Planar (two-dimensional), axisymmetric, or three-dimensional
Steadiness of boundary-layer flow	Steady or unsteady
Presence of particles	Single-phase or multiphase
Free-stream Mach number	Subsonic, transonic, supersonic, or hypersonic
Exothermicity of reaction	Exothermic or endothermic
Mixing condition of reactants	Premixed or non-premixed (diffusion)

K.Kuo & R.Acharya (2012)

Reacting boundary layer



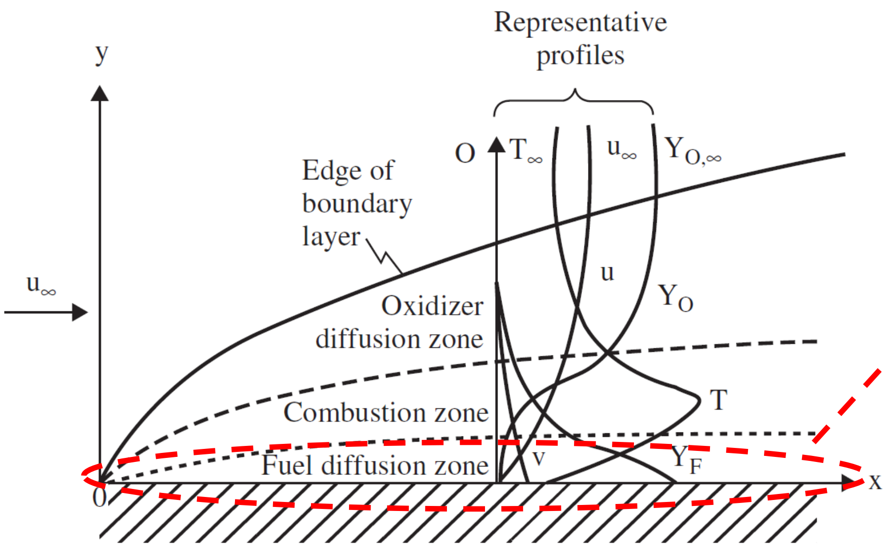
K.Kuo & R.Acharya (2012)

- Rate of diffusion of species transported from the gas to the solid

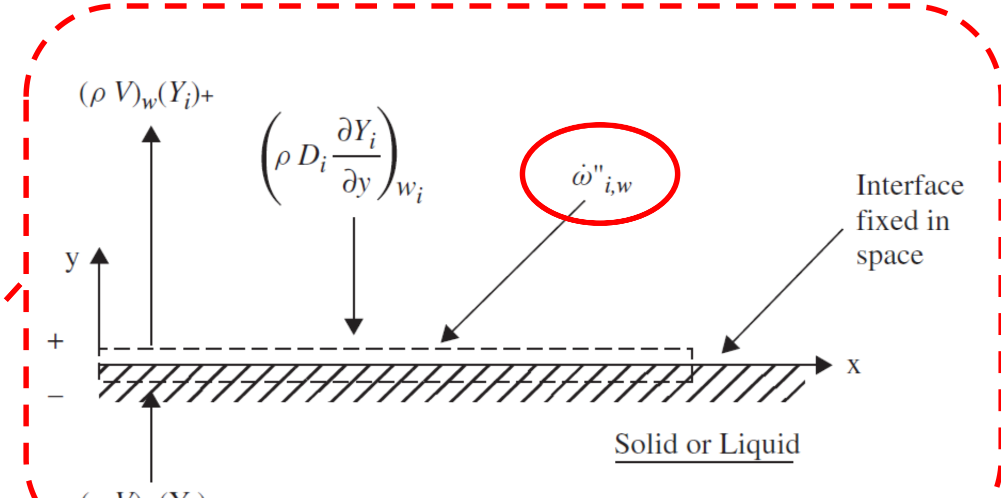
- Net rate of species production

- Rate of species transported away from the interface by the normal bulk motion of the fluid in the gas phase and toward the interface in the solid (may be porous)

Reacting boundary layer



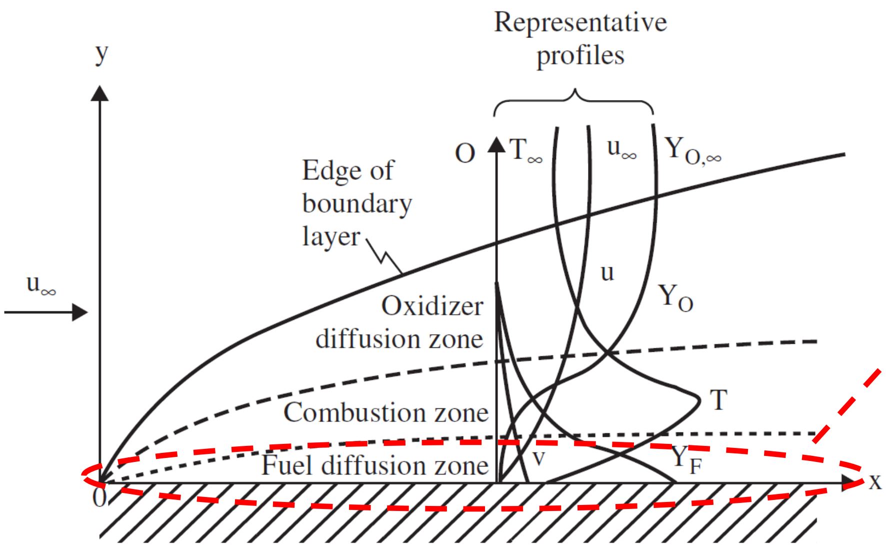
K.Kuo & R.Acharya (2012)



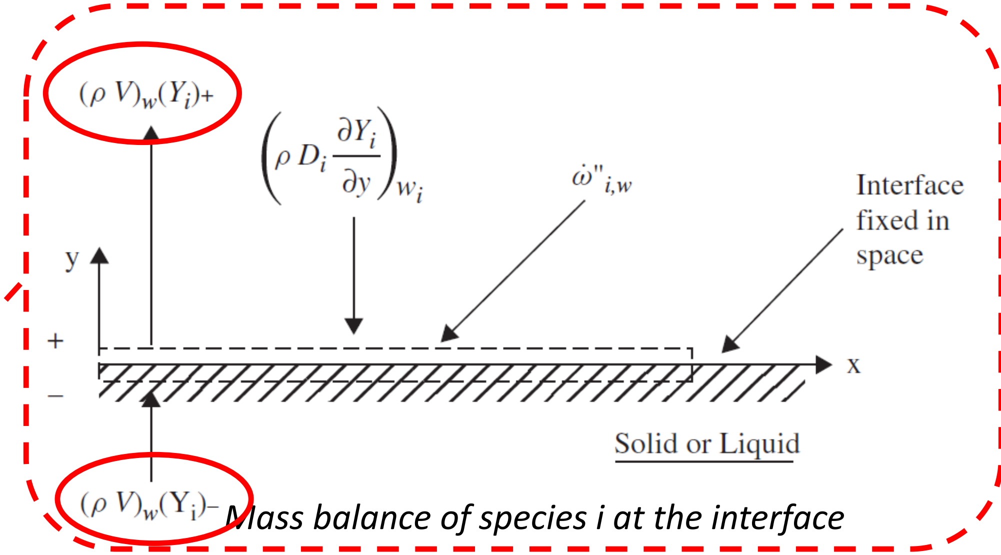
Mass balance of species i at the interface

- Rate of diffusion of species transported from the gas to the solid
- Net rate of species production
- Rate of species transported away from the interface by the normal bulk motion of the fluid in the gas phase and toward the interface in the solid (may be porous)

Reacting boundary layer



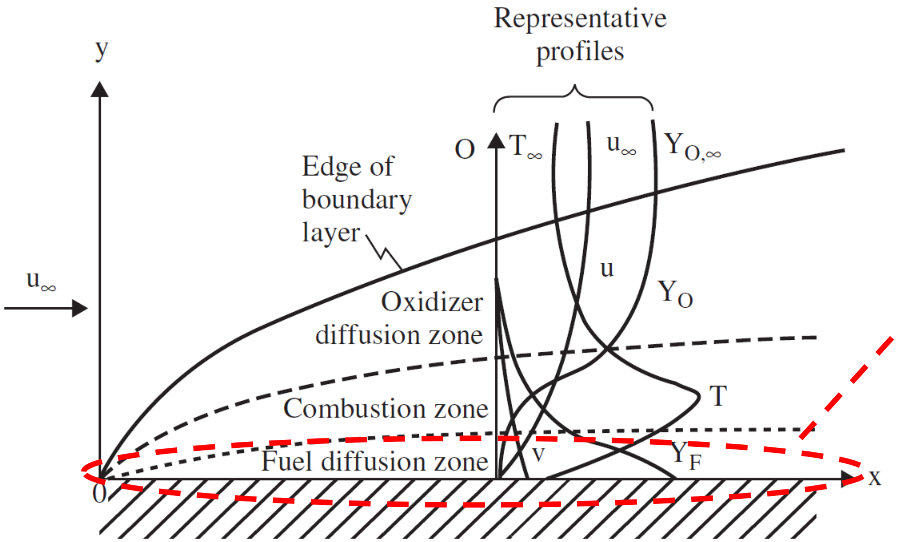
K.Kuo & R.Acharya (2012)



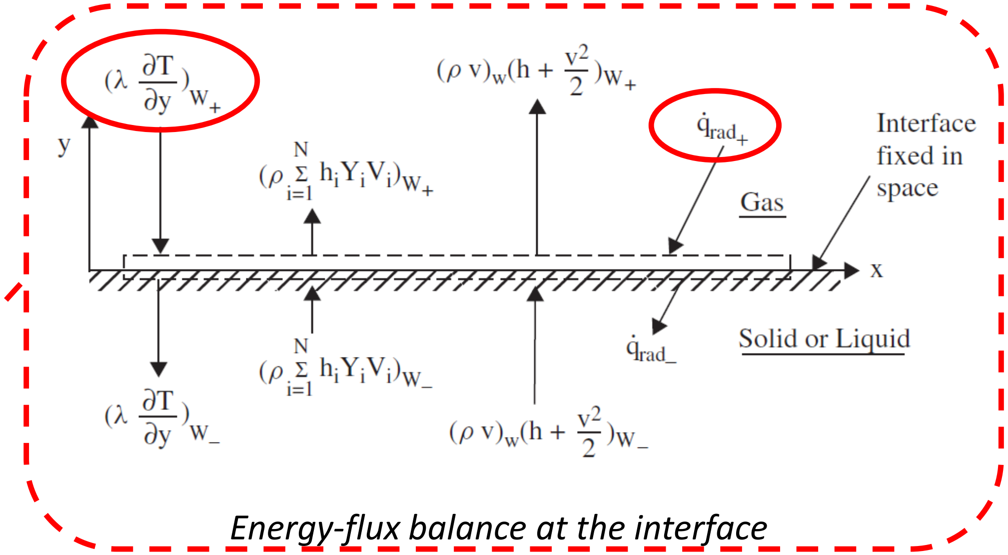
Mass balance of species i at the interface

- Rate of diffusion of species transported from the gas to the solid
- Net rate of species production
- Rate of species transported away from the interface by the normal bulk motion of the fluid in the gas phase and toward the interface in the solid (may be porous)

Reacting boundary layer



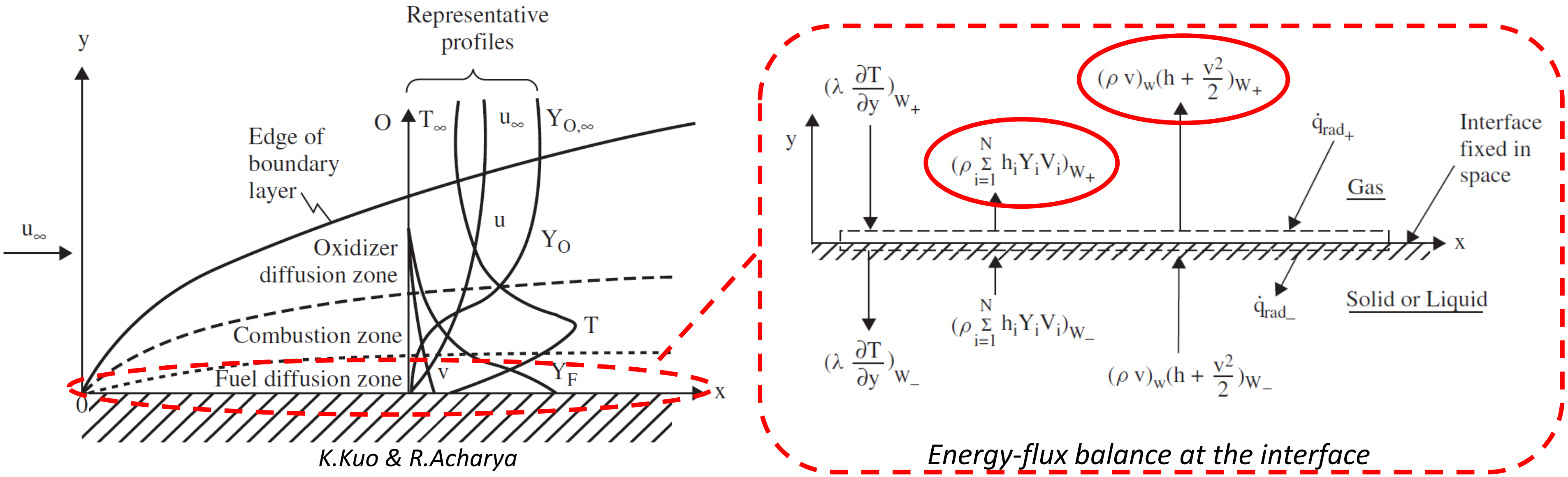
K.Kuo & R.Acharya (2012)



Energy-flux balance at the interface

- Energy fluxes from boundary layer to solid by conduction and radiation
- Energy transported away from the interface by mass diffusion and upward bulk motion of the gas
- Energy transferred away from interface by conduction and radiation
- Energy flux transported to the interface (in case of surface regression)
- Energy flux transported to the interface (If mass diffusion is present below the interface)

Reacting boundary layer

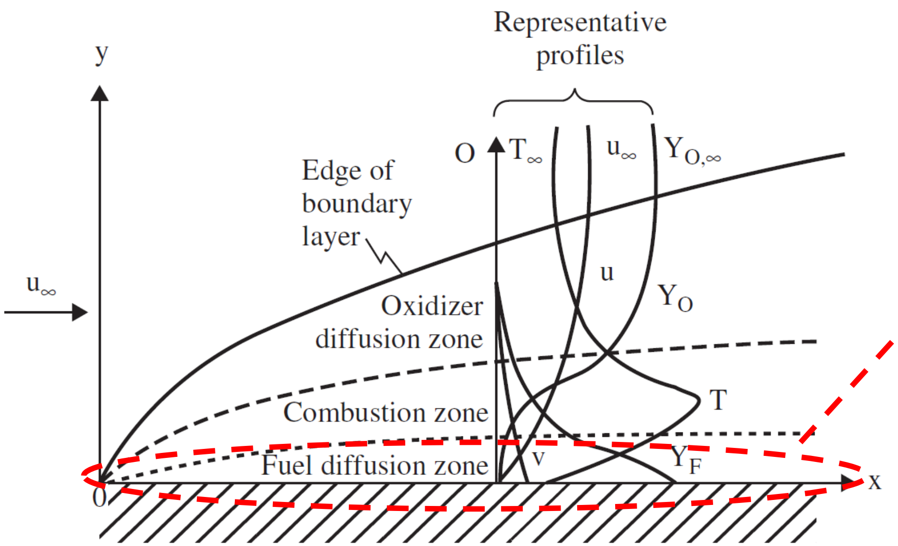


K.Kuo & R.Acharya (2012)

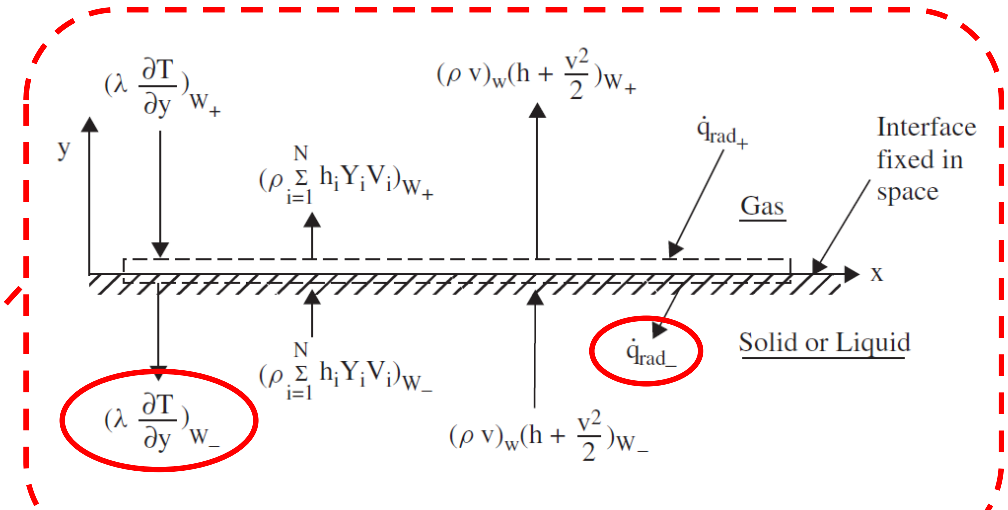
Energy-flux balance at the interface

- Energy fluxes from boundary layer to solid by conduction and radiation
- Energy transported away from the interface by mass diffusion and upward bulk motion of the gas
- Energy transferred away from interface by conduction and radiation
- Energy flux transported to the interface (in case of surface regression)
- Energy flux transported to the interface (If mass diffusion is present below the interface)

Reacting boundary layer



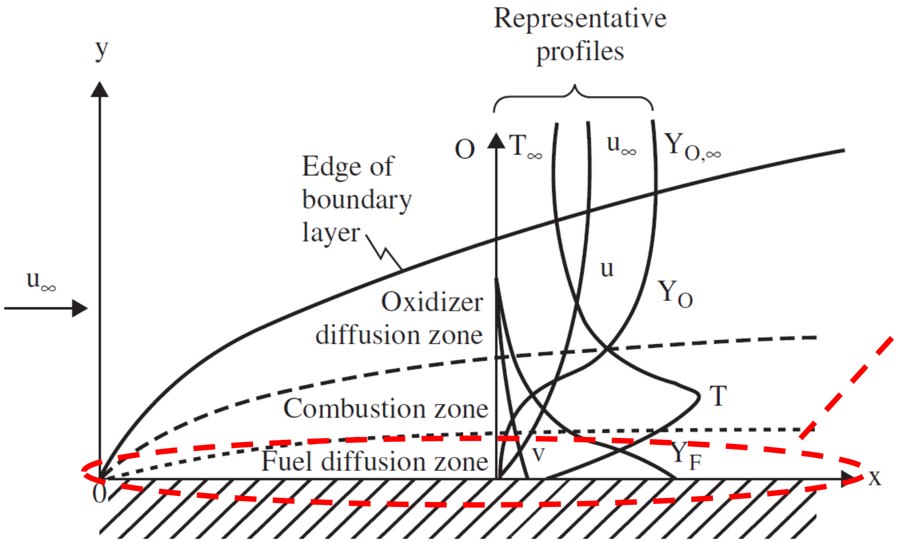
K.Kuo & R.Acharya (2012)



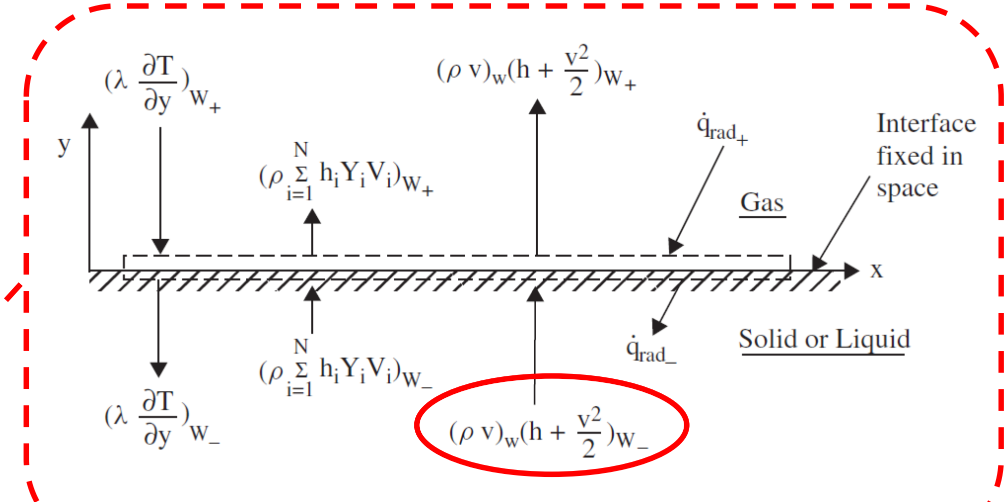
Energy-flux balance at the interface

- Energy fluxes from boundary layer to solid by conduction and radiation
- Energy transported away from the interface by mass diffusion and upward bulk motion of the gas
- Energy transferred away from interface by conduction and radiation
- Energy flux transported to the interface (in case of surface regression)
- Energy flux transported to the interface (If mass diffusion is present below the interface)

Reacting boundary layer



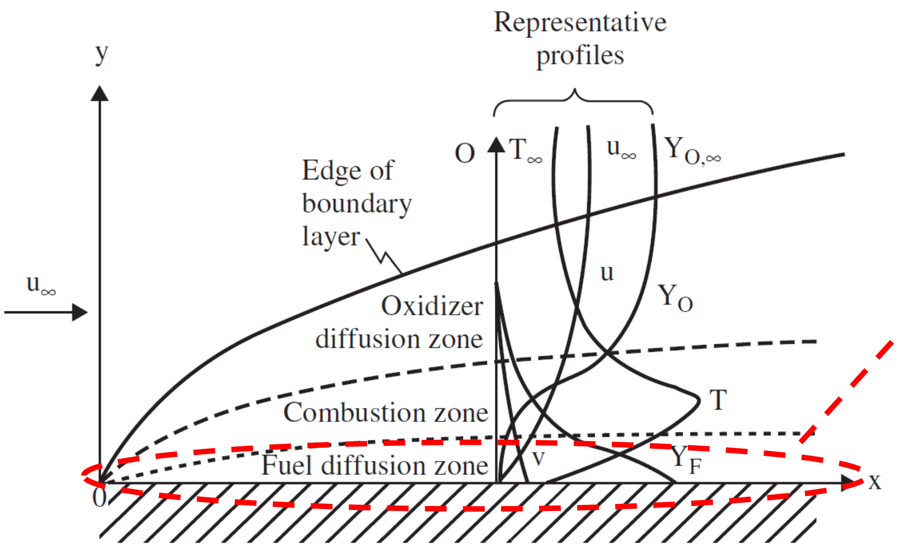
K.Kuo & R.Acharya (2012)



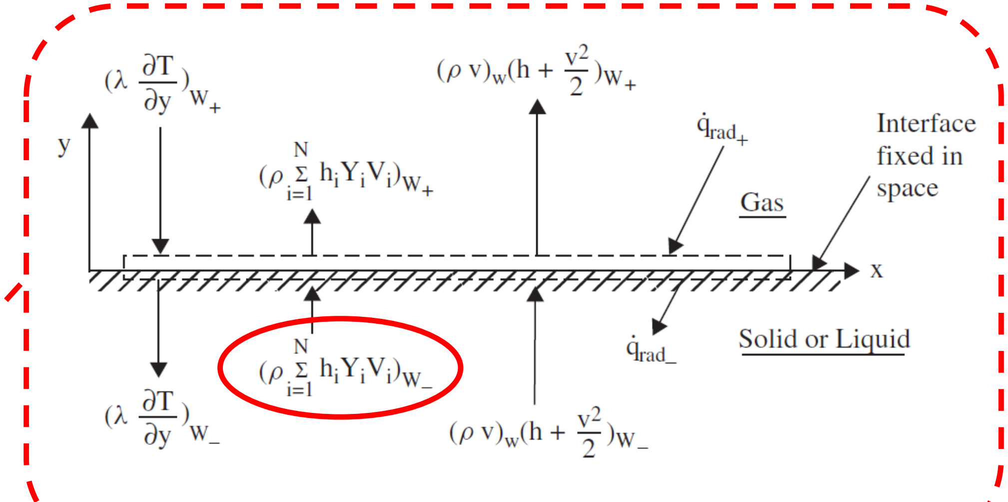
Energy-flux balance at the interface

- Energy fluxes from boundary layer to solid by conduction and radiation
- Energy transported away from the interface by mass diffusion and upward bulk motion of the gas
- Energy transferred away from interface by conduction and radiation
- Energy flux transported to the interface (in case of surface regression)
- Energy flux transported to the interface (If mass diffusion is present below the interface)

Reacting boundary layer



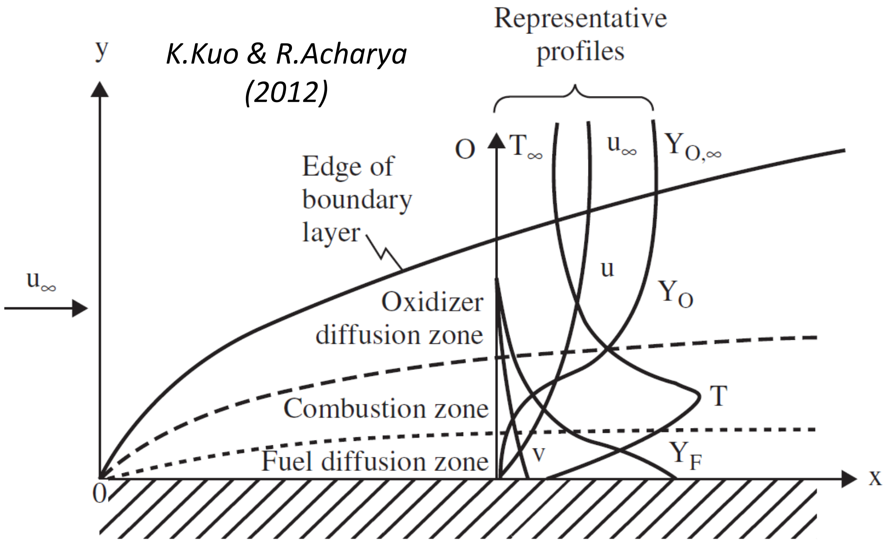
K.Kuo & R.Acharya (2012)



Energy-flux balance at the interface

- Energy fluxes from boundary layer to solid by conduction and radiation
- Energy transported away from the interface by mass diffusion and upward bulk motion of the gas
- Energy transferred away from interface by conduction and radiation
- Energy flux transported to the interface (in case of surface regression)
- Energy flux transported to the interface (If mass diffusion is present below the interface)

Reacting boundary layer



As in gas-phase 2 regimes are identified

- Damkohler number for surface reaction

$$Da_i = \left(\frac{\tau_{diff}}{\tau_{ch}} \right)_i$$

- 2 extreme cases : « frozen » and equilibrium chemistry at the surface

$Da_i \to 0$ | No effect of surface reaction on species boundary layer, reaction rate is much smaller than the diffusion rate

$Da_i \to \infty$ | Reaction rate is much greater than the diffusion rate, chemistry is at equilibrium

- Intermediate cases

$Finite\ Da_i$ | Gas layer at the surface is in a state of chemical non-equilibrium

Reacting boundary layer (solid)

Emmons problem (1956)

Non spreading laminar wall flame with forced convection (external flow)

- ***Assumptions***

✓ Constant and uniform free streem conditions
✓ No gravity
✓ Boundary layer approximation
✓ Constant wall temperature
✓ Infinitely fast chemistry (single step)
✓ No thermal radiation

- ***The Spalding B number is defined***

Ratio of heat released by unit mass of oxidizer divided by heat required to gasify unit mass of fuel

$$B = \frac{c_p \left(T_\infty - T_w\right) Y_{O_2,\infty} \Delta H_{comb}}{\Delta H_{pyr}}$$

Reacting boundary layer (solid)

Université de Poitiers

- ***By introducing a modified stream function and look for a similarity solution***

  ✓ Fuel mass loss rate (with treatment of buoyancy)

$$\dot{m}_w = \frac{3\rho_w \nu_w \left(Gr_x\right)^{1/4}}{\sqrt{2}x}; \; Gr_x = \frac{g\left(T_w - T_\infty\right)x^3}{\left(\nu_w\right)^2 T_\infty}$$

Scaling $x \sim 1/x^{1/4}$

- ***Limitation of Emmons theory***

  ✓ Neglects role of thermal radiation

$$\dot{m}_w^{"}\Delta H_{pyro} = \lambda_w \left(\frac{\partial T}{\partial y}\right)_w \rightarrow \dot{m}_w^{"}\Delta H_{pyro} = \lambda_w \left(\frac{\partial T}{\partial y}\right)_w + \dot{q}_{w,rad}^{"}$$

$$\Delta H_{comb} \rightarrow \left(1 - \chi_{rad}\right)\Delta H_{comb}$$

Reacting boundary layer (solid)

- ✓ Neglects role of pyrolysis process occuring inside condensed phase & assume thermally thin solid (in-depth processes rather than surface processes)

$$T_w = \frac{T_\infty + \left(Y_{O_2,\infty}\right)\Delta H_{comb} - B\Delta H_{pyro}}{c_p} \rightarrow T_w \neq cste$$

$$\dot{m}_w^{"}\Delta H_{pyro} = \lambda_w \left(\frac{\partial T}{\partial y}\right)_w \rightarrow \dot{m}_w^{"}\Delta H_{pyro} + \lambda_{s,w}\left(\frac{\partial T_s}{\partial y}\right)_w = \lambda_w \left(\frac{\partial T}{\partial y}\right)_w + \dot{q}_{w,rad}^{"}$$

$$\rightarrow \dot{m}_w^{"} = \int_{-\Delta}^{0} \dot{w}_g^{'''}\left(x,t\right)dx$$

- ✓ Assume laminar flow

Turbulent reacting boundary layer

Wall fire combines plume behavior & wall boundary layer effects

- ***4 regions can be distinguished***

✓ ***Regions 1* : pyrolysis zone**

Thermal degradation of solid fuel

✓ ***Regions 2* : combusting plume**

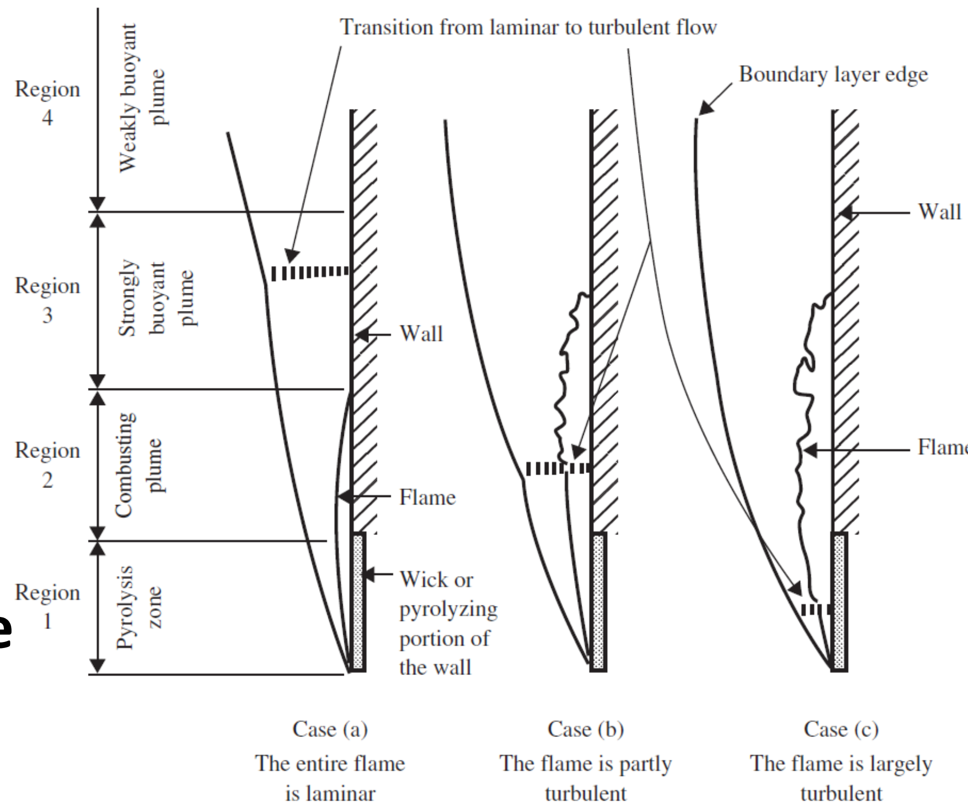
Oxidation of pyrolysis gas

✓ ***Regions 3* : strongly buyant plume**

No additional combustion occurs

✓ ***Regions 4* : weakly buyant plume**

Entrainment of ambiant gas has cooled the plume



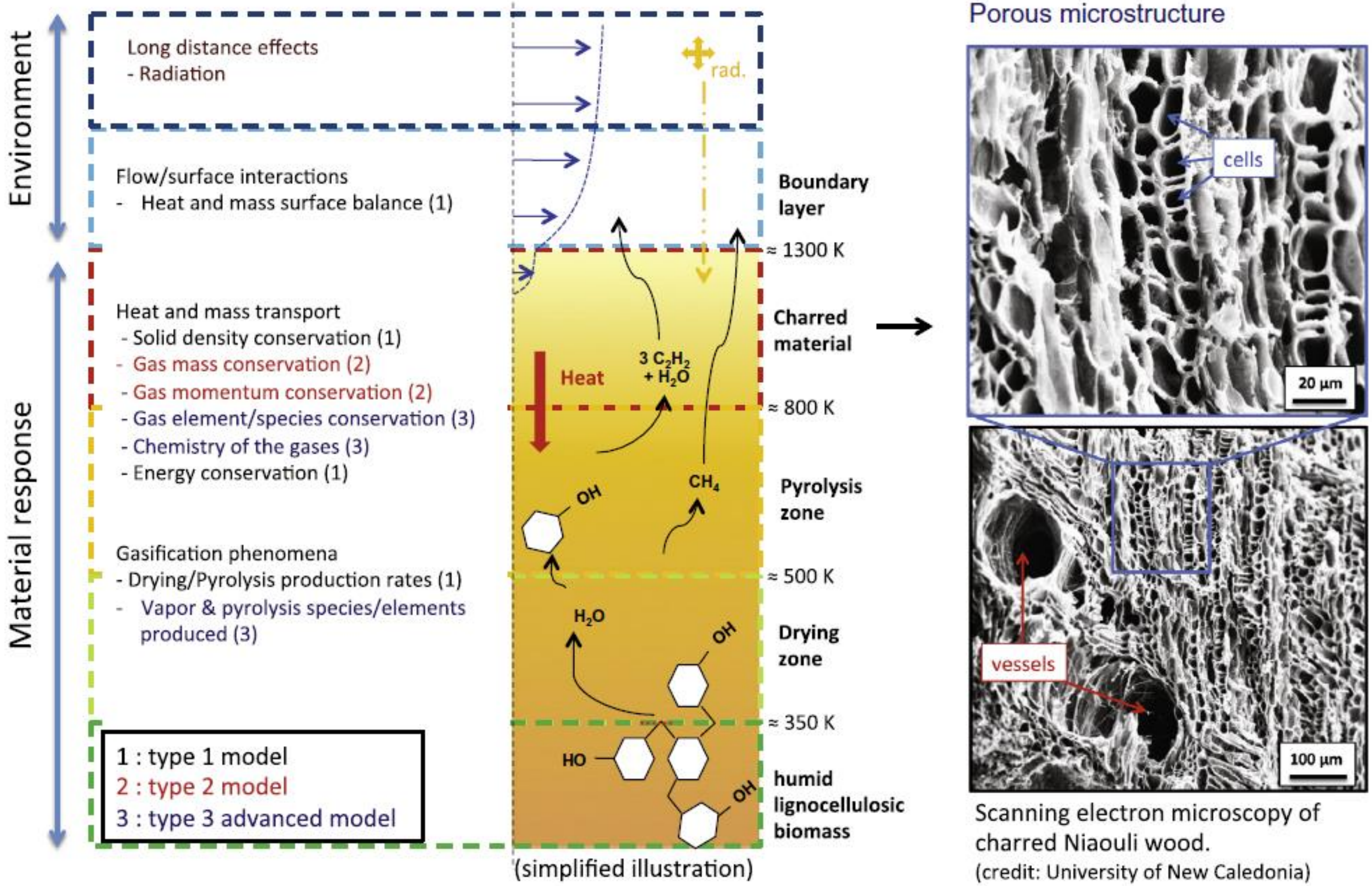
K.Kuo & R.Acharya (2012)

Turbulent reacting boundary layer

Ahmad and Faeth developped an analitical model for turbulent boundary layer (1979)

- ***Assumptions***
  - ✓ 2D, steady state, compressible and turbulent in boundary layer
  - ✓ Ambiant conditions are constant
  - ✓ Molecular physical properties approximate a Howarth-Dorodnitzyn gas $\left(\rho\mu, \rho\lambda, \mathrm{Pr}\ \text{are constant}\right)$
  - ✓ ***Surface conditions*** and the energy of gasification are constant in the pyrolysis zone and the wall heat flux from the flame provides the energy of gasification of the fuel (no external heat flux source)
  - ✓ Wall temperature in the plume region is constant and equal to the ambiant temperature
  - ✓ ***No radiation***
  - ✓ ***1 step global reaction***

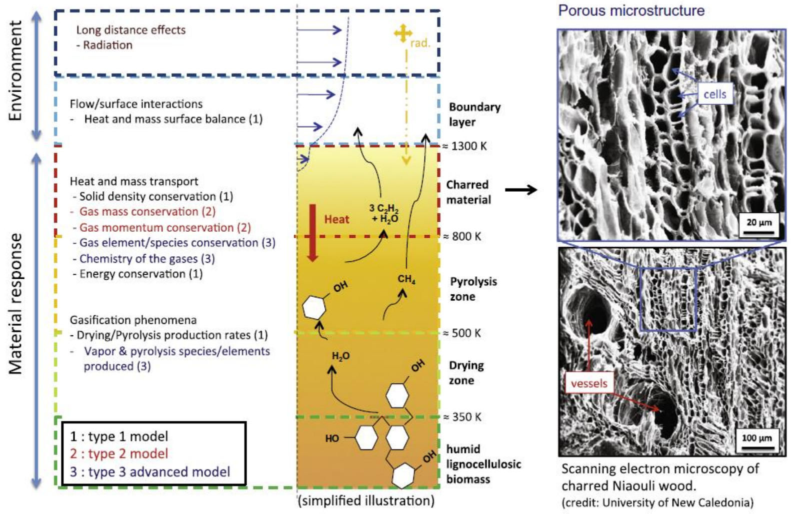
Processes in condensed phase



Scanning electron microscopy of charred Niaouli wood.
(credit: University of New Caledonia)

Lachaud (2017)

Conclusion



Lachaud (2017)

- Turbulent parameters and combustion needs correct near wall treatment $\left(k_{sgs}, \dot{w}_k\right)$ in case of LES simulation
- Pyrolysis gas flow rate governs « blowing effect » that has a strong influence on heat transfer in pyrolysis region (convection)
- Chemistry could affects boundary layer (finite chemistry at interface)
- Ignition of solid fuels is a key process to capture the spread rate of the flame