



Évaluation des modèles semi-empiriques de suie dans un panache turbulent de fumées provenant d'un feu libre

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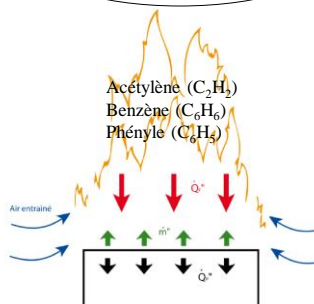
H. Y. Wang



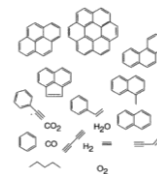
CONTEXTE

Production de suie

Phénomènes physico-chimiques



Précurseur de la nucléation



$C_6H_6, C_6H_5, C_2H_2, H_2, OH$

HAP (Hydrocarbures Aromatiques Polycycliques)

Transfert de chaleur

Débit massique de la pyrolyse :

$$\dot{m}_r = \frac{\rho D}{L} \text{Nu} \ln \left[\frac{1 - Y_{F,r}}{1 - Y_{F,i}} \right]$$

$$Y_{F,i} = \frac{MW_F}{MW_a} \exp \left[- \frac{L_r MW_F}{R_a} \left(\frac{1}{T_{\text{liq},F}} - \frac{1}{T_E} \right) \right]$$

MODELISATION NUMERIQUE

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

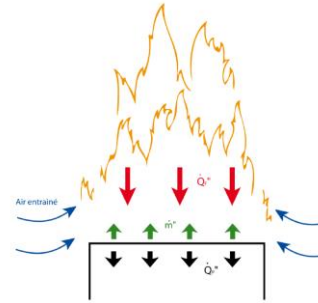
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p - \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{u}) = \nabla \cdot (\rho D \nabla Y_i) + \dot{\omega}_i'''$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \mathbf{u}) = \nabla \cdot (k \nabla T) + \dot{q}''' - \nabla \cdot \mathbf{q}_r$$

$$\bar{\nabla} \cdot \bar{\boldsymbol{\Omega}} \mathbf{I} + \kappa \mathbf{I} = \kappa \frac{\sigma T^4}{\pi}$$

$$-\nabla \cdot \mathbf{q}_r(\mathbf{x}) = \kappa(\mathbf{x}) [U(\mathbf{x}) - 4\pi I_b(\mathbf{x})] \quad \text{avec} \quad U(\mathbf{x}) = \int_{4\pi} \mathbf{I}(\mathbf{x}, \mathbf{s}) d\Omega$$



MODÈLES SEMI-EMPIRIQUES DE SUIE

$$\frac{\partial \rho N}{\partial t} + \frac{\partial [\rho N(u_i + u_i^{th})]}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{\mu}{Sc} \frac{\partial N}{\partial x_j} \right) = \dot{\omega}_{N,inc} + \dot{\omega}_{N,coa}$$

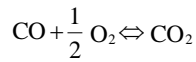
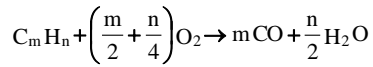
$$\frac{\partial \rho M}{\partial t} + \frac{\partial [\rho M(u_i + u_i^{th})]}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{\mu}{Sc} \frac{\partial M}{\partial x_j} \right) = \dot{\omega}_{M,inc} + \dot{\omega}_{M,gro} + \dot{\omega}_{M,oxi}$$

$$M = \rho Y_s$$

Nucléation / Coagulation / Grossissement / Oxydation

$$\dot{\omega}_M''' = \dot{\omega}_{M,inc}''' + \dot{\omega}_{M,gro}''' + \dot{\omega}_{M,oxi}'''$$

SOOT CONVERSION MODEL (conversion de suie via la consommation du combustible)



$$\dot{\omega}_F = \rho \frac{dY_i}{dt} = \rho \left[\frac{\xi}{\tau_{mix}} (Y_i - Y_i^0) + (1 - \xi) \frac{dY_i}{dt} \right]$$

$$\dot{\omega}_S = \frac{d\rho Y_S}{dt} = y_{soot_yield} \frac{W_F}{W_S} \dot{\omega}_F$$

SMOKE-POINT (Delichatsios)

$$\dot{\omega}_{M,inc}'' = A_f \rho^2 T^{2.25} \frac{f - f_{st}}{1 - f_{st}} \exp(-2000/T)$$

$$f = Y_F + \frac{1 + Y_P}{s}$$

$$\frac{A_{f,Fuel}}{A_{f,C_2H_4}} = \frac{L_{C_2H_4}}{L_{Fuel}}$$

$$\dot{\omega}_{M,gro}'' = C_\gamma \rho T^{1/2} X_F \exp(-T_\gamma/T) N^{1/3} (\rho Y_S)^{2/3}$$

$$d_p = \frac{6}{\rho_s A_s}$$

$$N = \frac{6 Y_S}{\pi d_p^3 \rho_s}$$

FUEL INCEPTION MODEL (Moss)

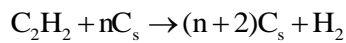
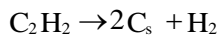
$$\dot{\omega}_{N,inc} = C_{\alpha} N_A \rho^2 T^{1/2} X_F e^{-T_{\alpha}/T}$$

$$\dot{\omega}_{N,coa} = -\frac{C_{\beta}}{N_A} T^{1/2} N^2$$

$$\dot{\omega}_{M,inc} = \frac{C_{\delta}}{N_A} \dot{\omega}_{N,inc}$$

$$\dot{\omega}_{M,gro} = C_{\gamma} \rho T^{1/2} X_F e^{-T_{\gamma}/T} N^{1/3} M^{2/3}$$

ACETYLENE INCEPTION MODEL (Leung)



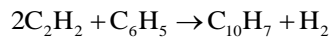
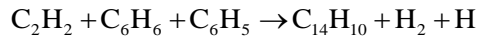
$$\dot{\omega}_{N,inc} = c_1 N_A \left[\rho \frac{Y_{C_2H_2}}{W_{C_2H_2}} \right] e^{-\frac{21100}{T}}$$

$$\dot{\omega}_{N,coa} = -\left(\frac{24R}{\rho_{soot} N_A} \right)^{1/2} \left(\frac{6}{\pi \rho_{soot}} \right)^{1/6} T^{1/2} M^{1/6} N^{11/6}$$

$$\dot{\omega}_{M,inc} = \frac{M_p}{N_A} \dot{\omega}_{N,inc}$$

$$\dot{\omega}_{M,gro} = c_4 \left(\rho \frac{Y_{C_2H_2}}{W_{C_2H_2}} \right) e^{-\frac{12100}{T}} \left[(\pi N)^{1/3} \left(\frac{6M}{\rho_{soot}} \right)^{2/3} \right]$$

PAH (Poly-Aromatics Hydrocarbons) INCEPTION MODEL (Hall)

Acétylène C_2H_2 Benzène C_6H_6 Phényle C_6H_5 

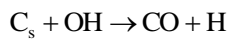
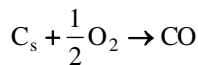
$$\dot{\omega}_{N,inc} = \frac{8N_A}{M_p} \left\{ c_2 \left[\left(\frac{\rho Y_{C_2H_2}}{W_{C_2H_2}} \right)^2 \frac{Y_{C_6H_6} W_{H_2}}{W_{C_6H_6} Y_{H_2}} \right] e^{-\frac{4378}{T}} + c_3 \left[\frac{\rho^2 Y_{C_2H_2} Y_{C_6H_6} Y_{C_6H_5} W_{H_2}}{W_{C_2H_2} W_{C_6H_6} W_{C_6H_5} Y_{H_2}} \right] e^{-\frac{6390}{T}} \right\}$$

$$\dot{\omega}_{N,coa} = - \left(\frac{24R}{\rho_{soot} N_A} \right)^{1/2} \left(\frac{6}{\pi \rho_{soot}} \right)^{1/6} T^{1/2} M^{1/6} N^{11/6}$$

$$\dot{\omega}_{M,inc} = \frac{M_p}{N_A} \dot{\omega}_{N,inc}$$

$$\dot{\omega}_{M,gro} = c_4 \left(\rho \frac{Y_{C_2H_2}}{W_{C_2H_2}} \right) e^{-\frac{12100}{T}} \left[(\pi N)^{1/3} \left(\frac{6M}{\rho_{soot}} \right)^{2/3} \right]$$

SOOT PARTICLES OXIDATION

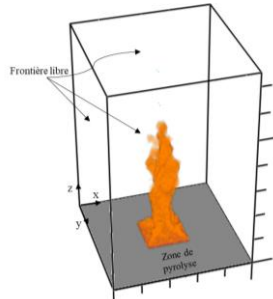


$$\dot{\omega}_{M,oxi} = -c_5 \tau \rho \frac{Y_{OH}}{W_{OH}} T^{1/2} (\pi N)^{1/3} \left(\frac{6M}{\rho_{soot}} \right)^{2/3} - c_6 \rho \frac{Y_{O_2}}{W_{O_2}} T^{1/2} (\pi N)^{1/3} \left(\frac{6M}{\rho_{soot}} \right)^{2/3} e^{-\frac{19778}{T}}$$

$$\dot{\omega}_{M,oxi}''' = -4.7 \times 10^{10} [Y_s [Y_o]] \exp(-211000 / RT)$$

$$\dot{\omega}_{M,oxi} = \rho \frac{dY_s}{dt} = \rho \left[\frac{\xi}{\tau_{nix}} (Y_s - Y_s^0) + (1 - \xi) \frac{dY_s}{dt} \right]$$

FEUX DE NAPPE EN MILIEU OUVERT



Configuration numérique

Domaine de calcul : $L = W = 1 - 2$ m, $H = 0.6 - 1.5$ m

Diamètre du foyer : $D = 7 - 30$ cm

Taille du maillage : $0.5 - 1$ cm

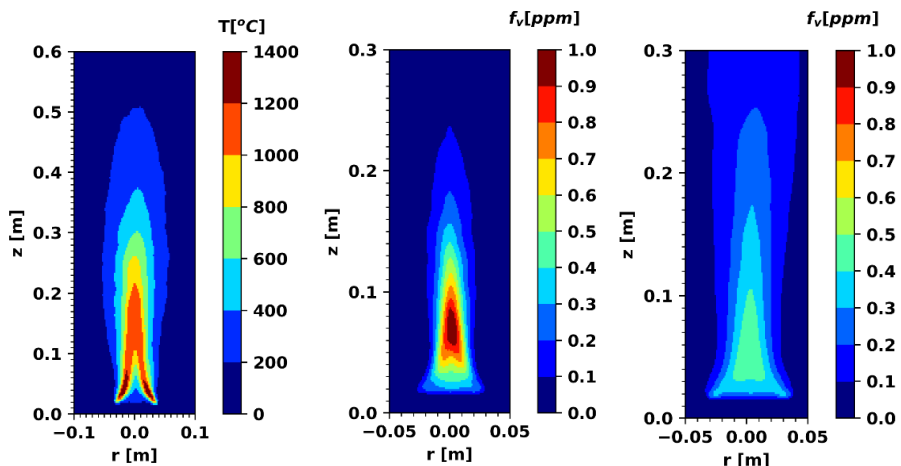
Combustible liquide : Heptane (98°C)

Combustible gazeux : Ethylène

Temps physique : 30 s

Temps CPU: 48 - 72 h

FEUX DE NAPPE D'ETHYLENE (D=7 cm)

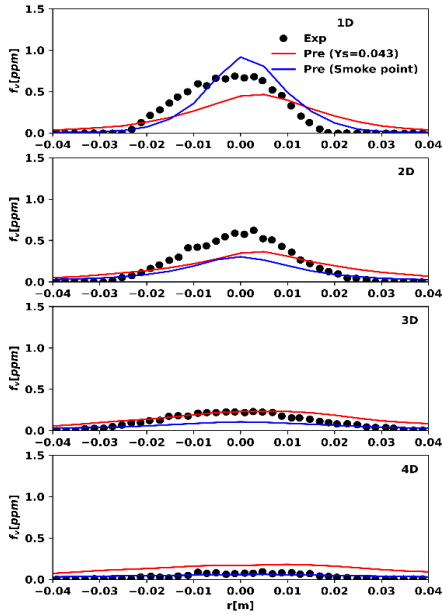


Smoke-Point

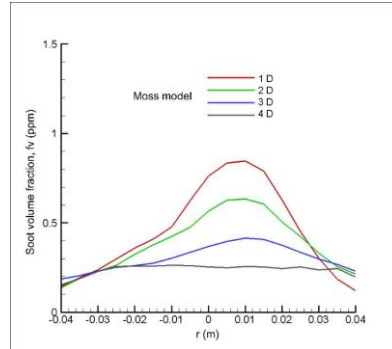
Soot-yield=0.043

COMPARAISON DE LA FRACTION VOLUMIQUE DE SUIE (ETHYLENE)

Smoke-point, Soot-yield

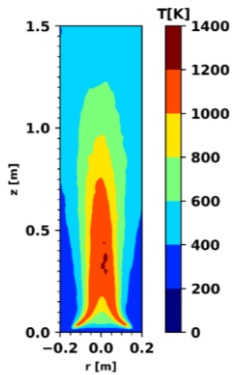
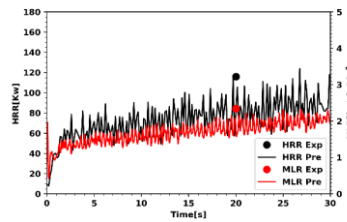


Fuel inception model

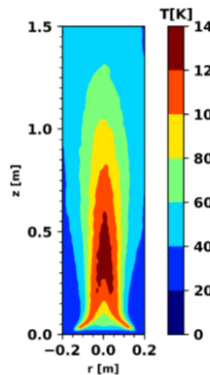


FEU DE NAPPE D'HEPTANE (D=30 cm)

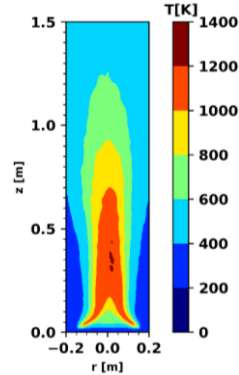
Puissance et Perte de masse



Smoke-Point

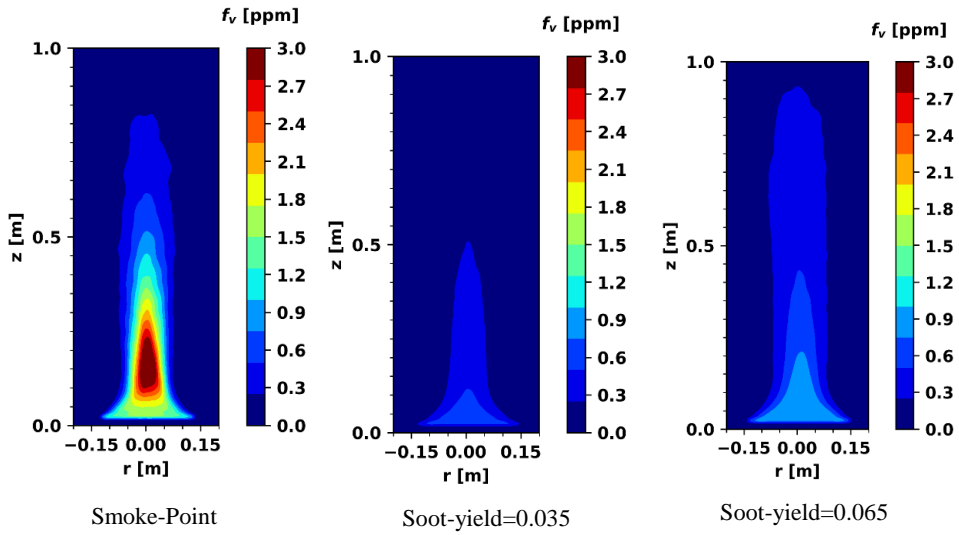


Soot-yield=0.035

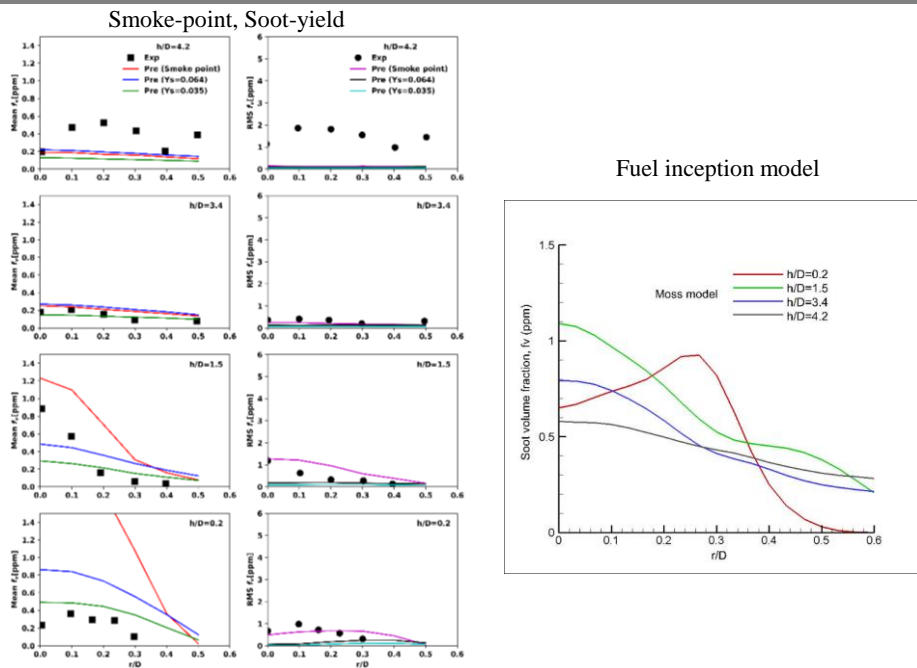


Soot-yield=0.065

CHAMPS DE LA FRACTION VOLUMIQUE DE SUIE

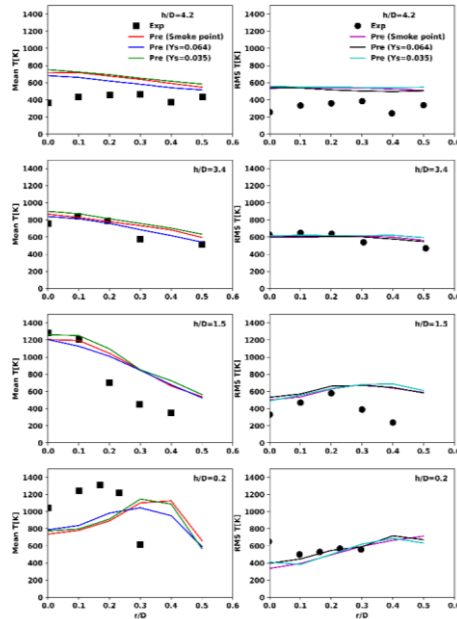


COMPARAISON DE LA FRACTION VOLUMIQUE DE SUIE (moyenne et fluctuation)



COMPARAISON DE LA TEMPÉRATURE (moyenne et fluctuation)

Smoke-point, Soot-yield



CONCLUSIONS ET PERSPECTIVES

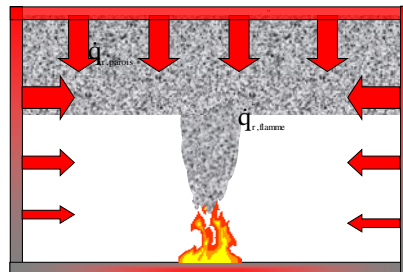
Soot-yield \Rightarrow Richesse globale : $\phi = \dot{m}_s S / \dot{m}_A$

Prédictions satisfaisantes et acceptables
avec un modèle de combustion simple (EDC)

Smoke-point model

Fuel inception model

Feux dans un milieu confiné sous-ventilé



Améliorations avec une cinétique chimique complexe

Acetylene inception model

PAH (Poly-Aromatics Hydrocarbons) inception model

