Combustion and radiation modelling at Faculty of Mechanical Engineering and Naval Architecture

Neven Duić, Mario Baburić, Milan Vujanović, Marko Ban, Daniel R. Schneider, Željko Bogdan

http://powerlab.fsb.hr/avl
NUGEN     ZONAL     FLUENT     FIRE/SWIFT
Heat flux to the furnace walls, 1992
\[
\frac{\partial}{\partial x_j}(\rho v_j) = 0 \\
\frac{\partial}{\partial x_j}(\rho v_j v_i) = \frac{\partial}{\partial x_j} \left[ \mu_{\text{eff}} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \mu_{\text{eff}} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right] - \rho g_i - \frac{\partial p}{\partial x_i} \\
\frac{\partial}{\partial x_j}(\rho v_j Y_\alpha) = \omega_\alpha + \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}}}{\sigma_\alpha} \frac{\partial Y_\alpha}{\partial x_j} \right) \\
\frac{\partial}{\partial x_j}(\rho v_j h) = q^c - q^r - \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}}}{Pr} \frac{\partial h}{\partial x_j} \right)
\]
\[
\omega_\alpha = W_\alpha \sum_{j=1}^{n_j} \left( \nu^{\prime\prime}_{a_j} - \nu^{\prime}_{\alpha_j} \right) k_{f,j} \prod_{k=1}^{n_\alpha} C_k^{\nu_k} \left( 1 - \frac{1}{K_{C,j}} \prod_{k=1}^{n_\alpha} C_k^{\nu_k - \nu_j} \right)
\]

\[
q^{\prime\prime\prime}_C = -\sum_{k=1}^{n_\alpha} \frac{\partial}{\partial t} \left[ C_k (\Delta H_{t,k}^0) T \right]
\]

\[
q^{\prime\prime\prime}_R = \alpha_g \int_V \left\{ \frac{\partial}{\partial x_j} \left[ \varepsilon \sigma T^4 + (1 - \varepsilon) dQ_s^+ \right] \frac{\tau(r)}{\pi r^3} r_j \right\} + \sigma T^4 \frac{\alpha(r)}{\pi r^2} dV - 4 \alpha_g \sigma T^4
\]

\[
k_{f,j} = k_{0,j} T^{\alpha_j} e^{-\frac{E_{a,j}}{RT}}
\]
Bogdan combustion model (Bogdan et al., 1992)

\[ r_B = -\rho \cdot \frac{\partial Y_B}{\partial t} = -\rho \cdot k \cdot Y_B^{v_B} \cdot Y_{O_2}^{v_{O_2}} \]

\[ k = \frac{b_k}{\tau_k} \]

\[ \tau_k = \tau_{ox} + \tau_{ei} + \tau_{cc} \]

\[ \tau_{ox} = \frac{d_o^2}{0.0032 \cdot (T - 273.15) - 1.79} \]

\[ \tau_{ei} = 9.434 \cdot 10^{-7} \cdot \frac{10^5}{e^{RT}} + 0.45695 \cdot d_o^2 \quad d_o = 0.3 \]

\[ \tau_{cc} = \chi \cdot (\tau_{ei} + \tau_{ox}) \quad \chi \approx 0.75 \]
Combustion in oil-fired furnaces

“Bogdan combustion model” - implementation in AVL’s code FIRE™; commercial name of model - “Steady combustion model” (Baburić et al., 2001)

Flame temperature

Temperature [K]

Axial distance [m]
NO\textsubscript{x}? Nitrogen oxides formation mechanisms (Duić, 1998)
Modelling of pollutants formation

Hydrogen chemistry

C₂ chain

C₁ chain
Modelling of pollutants formation

<table>
<thead>
<tr>
<th>$j$</th>
<th>Reakcija</th>
<th>$k_0$</th>
<th>$E_a/R$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>$O_2+H \rightarrow O+OH$</td>
<td>1.7000E+13</td>
<td>9.1145E+03</td>
<td>-0.3700</td>
</tr>
<tr>
<td>2.</td>
<td>$H_2+O \rightarrow H+OH$</td>
<td>2.5000E+09</td>
<td>3.8774E+03</td>
<td>0.0000</td>
</tr>
<tr>
<td>3.</td>
<td>$H_2+OH \rightarrow H_2O+H$</td>
<td>6.3000E+10</td>
<td>2.9710E+03</td>
<td>0.0000</td>
</tr>
<tr>
<td>4.</td>
<td>$OH+OH \rightarrow H_2O+O$</td>
<td>7.6000E+09</td>
<td>5.0356E+03</td>
<td>0.0000</td>
</tr>
<tr>
<td>5.</td>
<td>$H_2+O_2 \rightarrow OH+OH$</td>
<td>1.7000E+10</td>
<td>2.4060E+04</td>
<td>0.0000</td>
</tr>
<tr>
<td>6.</td>
<td>$H+H+M \rightarrow H_2+M$</td>
<td>7.0000E+10</td>
<td>0.0000E+00</td>
<td>-0.5000</td>
</tr>
<tr>
<td>7.</td>
<td>$H+OH+M \rightarrow H_2O+M$</td>
<td>3.0000E+13</td>
<td>0.0000E+00</td>
<td>-1.0000</td>
</tr>
<tr>
<td>8.</td>
<td>$O+O+M \rightarrow O_2+M$</td>
<td>2.0000E+13</td>
<td>0.0000E+00</td>
<td>-1.5000</td>
</tr>
</tbody>
</table>

$$k_{f,j} = k_{0,j} T^{\alpha_j} e^{\frac{E_{a,j}}{RT}}$$
Modelling of pollutants formation

- Temperature $x_y > iz = 1$
- Temperature $x_z > iz = 7$

- Graph showing temperature changes with $x$ [m]
**SO₃ model** (Schneider, 2002)

- **SO₃ reactions** (homogenous gas-phase reactions only):

  \[
  \begin{align*}
  &\text{SO}_2 + O + M \xleftrightarrow[k_{3b}]{k_{3f}} \text{SO}_3 + M \\
  &\text{SO}_3 + O \xleftrightarrow[k_{4b}]{k_{4f}} \text{SO}_2 + O_2
  \end{align*}
  \]
  
  third body reactants M:
  \[
  \text{N}_2/1.3/, \text{SO}_2/10.0/, \text{H}_2\text{O}/10.0/
  \]

- **Rate of change of SO₃ concentration**:

  \[
  \frac{dc_{SO_3}}{dt} = k_{3f} c_{SO_2} c_O c_M + k_{4b} c_{SO_2} c_{O_2} - k_{3b} c_{SO_3} c_M - k_{4f} c_{SO_3} c_O
  \]

  \[
  k_{3f} = 9.2 \cdot 10^{10} \exp\left(\frac{-1200.38}{RT}\right) \left[\frac{\text{cm}^3}{\text{mol}}\right]^2 \frac{1}{\text{s}}, \quad k_{3b} = \frac{k_{3f}}{K_{c,3}}
  \]

  \[
  k_{4f} = 2 \cdot 10^{12} \exp\left(\frac{-10064.95}{RT}\right) \left[\frac{\text{cm}^3}{\text{mol s}}\right], \quad k_{4b} = \frac{k_{4f}}{K_{c,4}}
  \]
SO₃ transport equation:

\[
\frac{\partial (\rho Y_{SO₃} u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_{eff}}{\sigma} \frac{\partial Y_{SO₃}}{\partial x_i} \right) + S_{SO₃}
\]

Schmidt-Prandtl number \( \sigma = 0.7 \)

source term:

\[
S_{SO₃} = M_{SO₃} \frac{dc_{SO₃}}{dt} = M_{SO₃} \left( k_{3f} c_{SO₂} c MCC + k_{4b} c_{SO₂} c_{O₂} - k_{3b} c_{SO₃} c_{M} - k_{4f} c_{SO₃} c_{O} \right)
\]
Results

a) SO$_3$, CO$_2$, H$_2$O, SO$_2$ mole fractions (SO$_2$ is normalized by factor 1.3e2 for comparing with CO$_2$ and H$_2$O, *refers to measured data), b) CO, H$_2$, SO mole fractions, c) average gas temperature, wall net heat flux, and d) NO mole fraction and soot mass fraction at the furnace exit vs. air excess ratio.
Flamelet (SLFM) concept:
- Non-premixed flame – stretched laminar flamelets attached to the instantaneous position of the flame surface
- Flamelets are smaller compared in size with Kolmogorov eddies
- Flame surface is presumed to coincide with stoichiometric iso-surface $Z=Z_{st}$
- Gradients of reactive scalars are negligible in tangential directions to mixture fraction iso-surface

$flamelet$ equations
Flamelet equations

\[
\rho \frac{\partial Y_i}{\partial \tau} - \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} - \dot{\omega}_i = 0
\]

\[
\rho \frac{\partial T}{\partial \tau} - \rho \chi \frac{\partial^2 T}{\partial Z^2} - \rho \chi \frac{\partial T}{\partial Z} \frac{\partial c_p}{\partial Z} - \sum_{i=1}^{N_{\text{spec}}} \rho \chi \frac{c_{pi}}{2c_p} \frac{\partial Y_i}{\partial Z} \frac{\partial T}{\partial Z} \frac{1}{c_p} \sum_{i=1}^{N_{\text{spec}}} h_i \dot{\omega}_i - \frac{q_R}{c_p} = 0
\]

→ stiff ODE system; stationary solutions are searched for

\[
Y_i = Y_i(Z, \chi_{st}) \quad T = T(Z, \chi_{st})
\]

Scalar dissipation rate

→ The combustion/turbulence interaction → accomplished via presumed β probability density function
Flamelet (Baburić et al., 2003)

- Flamelet pre-processor: CSC solver (http://powerlab.fsb.hr/mbaburic/CSC.htm)
Flamelet (Baburić et al., 2003)

- CSC solver – Graphical User Interface (GUI) (MATLAB):
Flamelet (Baburić et al., 2003)

Sandia piloted jet diffusion flame D

- **Dimensions:** Nozzle diameter = 7.2mm; Pilot diameter = 18.2mm
- **Main jet:** 25% CH₄, 75% air; F_stolc = 0.351, L_visc ~ 67d
- **Reynolds numbers:** C-13400, D-22400, E-33600, F-44800
- **Pilot:** The pilot flame burns a premixture of C₂H₂, H₂, air, CO₂, and N₂ having nominally the same equilibrium composition and enthalpy as CH₄/air. The pilot is operated lean, phi ~ 0.77, and the flow rate is scaled in the four turbulent flames to maintain the pilot at ~5% of the power of the main flame.
- **Scalar Measurements:** Raman/Reynleigh/LIF measurements of F, T, N₂, O₂, CH₄, CO₂, H₂O, H₂, CO, OH, and NO were obtained with a spatial resolution of 0.75 mm. Results include axial profiles in each flame (r/d = 5, 10, 15, ..., 80), radial profiles (r/d = 1, 2, 3, 7.5, 15, 30, 45, 60, 75). Averaged results (both Farre and Reynolds averages) and single-shot data are included in the archive.
- **Velocity Measurements:** Two-component LDV measurements were carried out at the Technical University of Darmstadt.

http://www.ca.sandia.gov/TNF/DataArch/FlameD.html

Velocity profiles at inlets
Flamelet (Baburić et al., 2003)

- Computational mesh (28 000 control volumes):

0-720 mm in axial direction; 0-150 mm in radial direction

Chemistry:
- Stationary laminar flamelet model
- GRI-Mech 3.0 mechanism (53 species and 325 reactions)

Turbulence:
- k-ε
- AVL’s hybrid turbulence models (HTM1, HTM2)

Turbulence/chemistry coupling:
- Presumed β-PDF
Flamelet (Baburić et al., 2003)

- Results: Mean mixture fraction, mean temperature (axial, centreline profiles)
Flamelet (Baburić et al., 2003)

- Results: Mean mass fractions – CH₄, O₂, H₂, CO₂
Three different NO mechanisms:

**Thermal NO** – formed from oxidation of atmospheric nitrogen at high temperatures
- Strong temperature-dependence
  - $T < 1000 \text{ K}$ – insignificant
- Atomic oxygen dependence
- Produces the majority of NO in the combustion of Gases and Light Oils

**Prompt NO** – formed by the reaction of atmospheric nitrogen with hydrocarbon radicals in fuel-rich regions of flame

**Fuel NO** – formed from nitrogen chemically bound in the fuel
- This mechanism is not highly sensitive to temperature changes, but is more sensitive to Air/Fuel Ratio
- This mechanism is important when using Heavy Fuel Oils, which contain 0.5-2% fuel nitrogen by weight
Thermal NO is described by extended Zeldovich mechanism:

\[
\begin{align*}
N_2 + O & \xrightleftharpoons[k_{1b}]{k_{1f}} NO + N \\
N + O_2 & \xrightleftharpoons[k_{2b}]{k_{2f}} NO + O \\
N + OH & \xrightleftharpoons[k_{3b}]{k_{3f}} NO + H
\end{align*}
\]

\[
k_{1f} = 1.8 \times 10^8 \exp \left( -\frac{38370}{T} \right)
\]

\[
k_{3b} = 1.7 \times 10^8 \exp \left( -\frac{24560}{T} \right)
\]

The overall rate for the three reversible thermal NO reactions:

\[
S_{NO} = 2M_{NO}c_O \left( \frac{k_{1f} c_{N_2} - k_{1b} k_{2b} c_{NO}^2}{k_{2f} c_{O_2}} \right)
\]

\[
1 + \frac{k_{1b} c_{NO}}{k_{2f} c_{O_2} + k_{3f} c_{OH}}
\]
Prompt NO:

\[ \text{CH}_x + \text{N}_2 \leftrightarrow \text{HCN} + \text{N}^{+} \ldots \]

The prompt NO source term:

\[ S_{NO, pr} = M_{NO pr} k c_{O_2}^{b} c_{N_2} c_{fuel} \phi \exp \left( -\frac{E}{RT} \right) \]

\[ f = 4.75 + 0.0819n - 23.2\phi + 32\phi^2 - 12.2\phi^3 \]
Fuel NO:

HCN production and depletion:

\[ S_{\text{HCN}} = S_{\text{HCN,p}} + S_{\text{HCN,1b}} + S_{\text{HCN,2b}} \]

\[ S_{\text{HCN,p}} = R_{\text{fuel}} Y_{\text{C_HCN}} \frac{M_{\text{HCN}}}{M_{\text{H}}} \Delta \text{V} \]

\[ S_{\text{HCN,1b}} = -A_1 X_{\text{HCN}} X_{\text{O}_2} \exp \left( -\frac{E_1}{RT} \right) \frac{M_{\text{HCN}} P}{RT} \]

\[ S_{\text{HCN,2b}} = -A_2 X_{\text{HCN}} X_{\text{NO}} \exp \left( -\frac{E_2}{RT} \right) \frac{M_{\text{HCN}} P}{RT} \]

NO production and depletion:

\[ S_{\text{NO}} = S_{\text{NO,1b}} + S_{\text{NO,2b}} \]

\[ S_{\text{NO,1b}} = A_1 X_{\text{HCN}} X_{\text{O}_2} \exp \left( -\frac{E_1}{RT} \right) \frac{M_{\text{NO}} P}{RT} \]

\[ S_{\text{NO,2b}} = -A_2 X_{\text{HCN}} X_{\text{NO}} \exp \left( -\frac{E_2}{RT} \right) \frac{M_{\text{NO}} P}{RT} \]
\[ S_{\text{NO}} = \int_{0}^{1} P(T) S_{\text{NO}}(T) \, dT \]
\[ S_{\text{HCN}} = \int_{0}^{1} P(T) S_{\text{HCN}}(T) \, dT \]

where:
\[
P(T) = \frac{1}{B(\alpha, \beta)} T^{\alpha-1} (1-T)^{\beta-1}
\]
\[
B(\alpha, \beta) = \int_{0}^{1} T^{\alpha-1} (1-T)^{\beta-1} \, dT = \frac{\Gamma(\alpha) \Gamma(\beta)}{\Gamma(\alpha + \beta)}
\]

\[
\alpha = \bar{T} \left[ \frac{\bar{T} (1-\bar{T})}{\bar{\sigma}^2} - 1 \right] \geq 0;
\]
\[
\beta = (1-\bar{T}) \left[ \frac{\bar{T} (1-\bar{T})}{\bar{\sigma}^2} - 1 \right] \geq 0
\]
\[ \frac{\partial (\rho \bar{Y}_{NO})}{\partial t} + \frac{\partial (\bar{u}_i \rho \bar{Y}_{NO})}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_t \frac{\partial \bar{Y}_{NO}}{\partial x_i} \right) + \tilde{S}_{NO} \]

\[ \frac{\partial (\rho \bar{Y}_{HCN})}{\partial t} + \frac{\partial (\bar{u}_i \rho \bar{Y}_{HCN})}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_t \frac{\partial \bar{Y}_{HCN}}{\partial x_i} \right) + \tilde{S}_{HCN} + \]

\[ \frac{\partial}{\partial t} \left( \rho \sigma^{n^2} \right) + \frac{\partial}{\partial x_i} \left( \rho \bar{u}_i \sigma^{n^2} \right) = \frac{\partial}{\partial x_i} \left( \mu_i \left( \frac{\partial \sigma^{n^2}}{\partial x_i} \right) \right) + C_g \mu_i \left( \frac{\partial \bar{T}}{\partial x_i} \right)^2 - C_d \rho \frac{\varepsilon}{k} \sigma^{n^2} \]
NO$_x$ (Vujanović et al., 2004)

**Results:**
Results - Sandia piloted jet diffusion flame D:

NO$_x$ (Vujanović et al., 2004)
Soot model parameter analysis (Ban et al., 2004)

FM530 HD Engine
- bore – 130 mm
- stroke – 150 mm
- swept volume 1.99 l
- connecting rod length – 263.8 mm
- head temperature – 500 K
- liner temperature – 410 K
- piston temperature – 510 K

5 different load cases combining:
- load: 25%, 50% and 75%
- speed [rpm]: 1130, 1420 and 1710
- moment of fuel injection: 0°CA (TDC) and −4°CA

Presumed mechanism

RESULTS

Advanced soot model – optimized parameter set

SOOT SOURCE
= Particle Inception + Surface Growth + Fragmentation + Oxidation

Nox Zeldovich model – optimized parameter
DTRM (Baburić et al., 2002)

Radiation modeling – discrete transfer radiation method (DTRM)

- Recurrence formula

\[ i_{n+1} = i_n (1 - \varepsilon) + \frac{\sigma T_g^4}{\pi} \cdot \varepsilon \]

- Boundary condition

\[ i = \frac{q_{\text{out}}}{\pi} = (1 - \varepsilon_w) \frac{q_{\text{in}}}{\pi} + \varepsilon_w \frac{\sigma T_w^4}{\pi} \]

- Source terms

\[ S_{j,i} = (i_{n+1} - i_n) A_j \cos \Theta_{j,i} \Delta \Omega_{j,i} \quad S_{j,tot} = \sum_i S_{j,i} \]

- Radiative properties → Weighted sum of gray gases model (WSGGM)
DTRM (Baburić et al., 2002)

DTRM – verification

Nondimensional heat flux against optical thickness for different emissivities of lower wall (upper wall is held at constant emissivity 0.8) – two infinitely long parallel plates.

Nondimensional heat flux against nondimensional wall distance for different optical thicknesses (18 rays) – finite cylinder.
DTRM (Baburić et al., 2002)

- **DTRM – IJmuiden experimental furnace**

**Fuel:**
- **Composition**
  - Carbon: 0.869
  - Hydrogen: 0.118
  - Sulphur: 0.013
- **Lower calorific value**: 41072.5 kJ/kg

**Boundary conditions:**
- Secondary air flow: 1849 kg/h
- Primary air flow (swirl): 434 kg/h
- Secondary air temperature: 47 °C
- Primary air temperature: 26 °C
- Fuel flow: 155 kg/h
- Fuel temperature: 116 °C

**IJmuiden furnace layout**

- Cooling tubes arrangement
- Burner arrangement

**Cooling tubes positioning**

**Water cooled doors for instrument access**

**Boundary conditions:**
- Secondary air flow: 1849 kg/h
- Primary air flow (swirl): 434 kg/h
- Secondary air temperature: 47 °C
- Primary air temperature: 26 °C
- Fuel flow: 155 kg/h
- Fuel temperature: 116 °C
DTRM (Baburić et al., 2002)

- DTRM – IJmuiden experimental furnace (computational mesh)

Unstructured computational mesh:
A) Vertical cut along the axis (part; flame expecting region)
B) Cooling tubes (side view; cut)
DTRM (Baburić et al., 2002)

- DTRM – IJmuiden experimental furnace (results)

**Measured and predicted axial temperature profiles at centreline position**

**Predicted net radiative heat flux axial profiles at the walls**

<table>
<thead>
<tr>
<th>Boundary region</th>
<th>Measured heat flow [kW]</th>
<th>Predicted heat flow [kW]</th>
<th>Predicted heat flow [kW]</th>
<th>Predicted heat flow [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>DTRM (4 rays)</td>
<td>DTRM (8 rays)</td>
<td>DTRM (8 rays; non-conservative)</td>
</tr>
<tr>
<td>Mass-flow inlets</td>
<td>1805.6</td>
<td>1802.2</td>
<td>1801.5</td>
<td>1798.6</td>
</tr>
<tr>
<td>Outlet</td>
<td>-924.3</td>
<td>-972.1</td>
<td>-968.6</td>
<td>-952.5</td>
</tr>
<tr>
<td>Cooling tubes</td>
<td>-603.7</td>
<td>-631.7</td>
<td>-638.3</td>
<td>-601.9</td>
</tr>
<tr>
<td>Other walls</td>
<td>-239.0</td>
<td>-230.5</td>
<td>-228.6</td>
<td>56.7</td>
</tr>
<tr>
<td>Unaccounted</td>
<td>-38.6</td>
<td>-32.1</td>
<td>-34</td>
<td>300.9</td>
</tr>
<tr>
<td>Unaccounted [%]</td>
<td>2.14</td>
<td>1.78</td>
<td>1.89</td>
<td>16.73</td>
</tr>
</tbody>
</table>
The end

Thank You for Your Attention!

http://powerlab.fsb.hr/avl