Modelling Intumescent Coating Behaviour in Fire

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Outline

- General background and Aims
- Model building and validation
- Sensitivity study
- Implementation
- Conclusion and future works
Background

- The intumescent coating is widely used worldwide
- Intumescence is highly dynamic and depends on fire conditions
- Test data are based on standard fires

Aims

- To understand the mechanisms determining the fire-resistant properties of intumescent coating
- To provide a robust scientific footing to model intumescent coating performance under various fire exposure conditions
- To identify and evaluate the main parameters which can describe the intumescence performance with sufficient accuracy
General illustration of intumescence

Pre heating
- Virgin Zone
- Melting
- Blowing
- Fully Expanded Char
- Protected Substrate

During Heating
- Heat

Post heating
- Heat
Energy conservation in the coating:

Influential issues:

• Expansion
• Thermal conductivity
• Decomposition heat
• Mass loss rate
• Convection heat loss (gas transportation)

\[
\frac{\partial}{\partial x} (\lambda \frac{\partial T}{\partial x}) \times A + \Delta h_{\text{decomposition}} \left( - \frac{\partial m_{\text{reactive}}}{\partial t} \right) = \\
(m_{\text{solid}} C_{\text{solid}} + m_{\text{gas}} C_{\text{gas}}) \frac{\partial T_i}{\partial t} \\
+ (C_{\text{gas}} T_i \frac{\partial (\varepsilon_{\text{porosity}} A_{\text{area}} \Delta x_{\text{thickness}} \rho_{\text{gas}})}{\partial t} + C_{\text{solid}} T_i \frac{\partial m_{\text{solid}}}{\partial t}) \\
+ \frac{\partial \Delta m_{\text{gas}}}{\partial x} C_{\text{gas}} T_i
\]
Chemicals in the coating

- 1, inorganic acid sources

\[ \text{NH}_4\text{H}_2\text{PO}_4 \xrightarrow{\Delta} \text{NH}_3 + \text{H}_3\text{PO}_4 \]

- 2, Blowing agent (organic amine or amide)

- 3, Charring material (carbon-rich polyhydric compound)
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Decomposition process

Reaction rate constant
(Arrhenius equation)

\[
K_j = A_j \exp\left(-\frac{E_j}{\mathcal{R}T}\right), \quad j = 1, 3
\]

Mass loss rate

\[
\frac{\partial m_{\text{solid}}}{\partial t} = m_0 \left(-K_1 Y_1 - K_2 Y_2^2 - K_3 Y_3 + \nu_c K_3 Y_3 \right)
\]

Decomposition heat

\[
\Delta H = m_0 \left(K_1 Y_1 H_1 + K_2 Y_2^2 H_2 + K_3 Y_3 H_3 \right)
\]

Expansion

Total thickness

\[
x = x_0 + \Delta b
\]

Expansion rate

\[
\frac{\partial \Delta b}{\partial t} = \beta \frac{m_0 K_2 Y_2^2}{\rho_{\text{gas}}}
\]
Gas transportation

\[ \Delta m_{\text{gas}}^{\text{diff}} C_i T_i = \left( \rho_{\text{in}} u_{\text{in}} C_{i-1} T_{i-1} - \rho_{\text{out}} u_{\text{out}} C_i T_i \right) \times \Delta t \]

- Gas leaves this discretized layer (gas-out) is:
  - Gas transferred from lower layer (gas-in) PLUS gas produced from solid decomposition
  - Subtract contribution responsible for bubbling

- Decompositions happen to produce gas product

- Retained gas change in mass:
  - Total volume, Porosity and Density

\[ \rho_{\text{out}} u_{\text{out}} = \rho_{\text{in}} u_{\text{in}} + m_0 \left( K_1 Y_1 + K_2 Y_2^2 + (1 - \nu_c) K_3 Y_3 \right) - \frac{\partial (\varepsilon \Delta x \rho)}{\partial t} \]
Thermal conductivity & Bubble size

Thermal conductivity:

\[ \lambda^* = \lambda_s \frac{\frac{\lambda_g}{\varepsilon^3} + 1 - \frac{2}{\varepsilon^3}}{\frac{\lambda_s}{\varepsilon^3} - \varepsilon + 1 - \frac{2}{\varepsilon^3} + \varepsilon} \]

Gas phase conductivity:

\[ \lambda_g = \lambda_{\text{cond}} + \lambda_{\text{rad}} \]

Conduction part:

\[ \lambda_{\text{cond}} = 4.815 \times 10^{-4} T^{0.717} \text{W/m·K} \]

Radiation part:

\[ \lambda_{\text{rad}} = \frac{8}{3} d e \sigma T^3 \]
## Modelling Intumescent Coating Behaviour in Fire

<table>
<thead>
<tr>
<th>Variables</th>
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<tbody>
<tr>
<td>(A_1) (s)</td>
<td>800(+)</td>
<td>(\varepsilon_0)</td>
<td>0.3(*)</td>
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<tr>
<td>(E_1) (kJ/mol)</td>
<td>53.384(+)</td>
<td>(\lambda_c) (Kw/mK)</td>
<td>0.345×10^{-3}(+)</td>
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<td>(A_2) (s)</td>
<td>6.9×10^{6}(+)</td>
<td>(\lambda_f) (Kw/mK)</td>
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<td>(E_2) (kJ/mol)</td>
<td>93.035(+)</td>
<td>(\lambda_s) (Kw/mK)</td>
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<td>(A_3) (s)</td>
<td>5.0(+)</td>
<td>(\rho_c) (kg/m³)</td>
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<td>(E_3) (kJ/mol)</td>
<td>63.786(+)</td>
<td>(\rho_s) (kg/m³)</td>
<td>7850.0(+)</td>
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<tr>
<td>(v_c)</td>
<td>0.784(+)</td>
<td>(e_c)</td>
<td>1.0(+)</td>
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<tr>
<td>(v_g)</td>
<td>0.216(+)</td>
<td>(e_f)</td>
<td>0.8(+)</td>
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<tr>
<td>(\Delta h_1) (kJ/kg)</td>
<td>-1256(*)</td>
<td>(d_{c0}) (m)</td>
<td>5.0×10^{-6}(*)</td>
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<tr>
<td>(\Delta h_2) (kJ/kg)</td>
<td>-1256(*)</td>
<td>(d_{f0}) (m)</td>
<td>325.0×10^{-6}(*)</td>
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<tr>
<td>(\Delta h_3) (kJ/kg)</td>
<td>9789(+)</td>
<td>(E_{\text{max}})</td>
<td>3.0(+)</td>
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<tr>
<td>(Y_{10})</td>
<td>0.28(+)</td>
<td>(\beta)</td>
<td>1.0(*)</td>
</tr>
<tr>
<td>(Y_{20})</td>
<td>0.17(+)</td>
<td>(W_{v_2}), (W_p) (kg/mol)</td>
<td>30.0×10^{-3}(*)</td>
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<tr>
<td>(Y_{30})</td>
<td>0.55(+)</td>
<td>(h) (kW/m²)</td>
<td>20.0(*)</td>
</tr>
<tr>
<td>(C_1) (kJ/kg/K)</td>
<td>1.884(+)</td>
<td>(Q) (kW/m²)</td>
<td>157.0(+)</td>
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<td>(C_4) (kJ/kg/K)</td>
<td>1.63(+)</td>
<td>(\tau_{c0}) (m)</td>
<td>0.2×10^{-2}(+)</td>
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<td>(C_5) (kJ/kg/K)</td>
<td>0.42(+)</td>
<td>(\tau_s) (m)</td>
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<td>(C_6) (kJ/kg/K)</td>
<td>1.0(+)</td>
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Validation

To validate the mathematical model, a reference case (Cagliostro, 1975) has been studied.

Coating thickness: 2mm
Steel substrate thickness: 1.5mm
External heat flux: 157kW/m²
Sensitivity study

- E2 value has significant effect on intumescent performance
- 20% difference in E2 value can lead to 100K difference in coating performance
• E3 value demonstrate importance on post heating period
• Lower E3 value speeds up bubble growth, gives higher radiative thermal conductivity
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- Bubble size determines the radiative heat transfer
- Maximum expansion ratio has an effect on effective thermal conductivity

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• Decomposition heat $H$, blowing gas retaining ratio $\beta$, gas movement, and mass fraction of blowing agent have less effect on the performance
Key variables and determination

- **Kinetics:**
  E2 and E3
  Measuring by Thermogravimetric Analysis (TGA)

- **Maximum expansion factor:**
  Emax
  Use Viscosity-Temperature relationship

- **Bubble size:**
  d
  Back calculating from measured thermal conductivity
Implementation of the model

Intumescence under cone-calorimeter

Test B12:
Dried Coating Thickness (DFT): 0.4mm
Steel plate: 10mm
Temperature history in test B12

- Estimated \( E_2 = 115,000 \)
According to Expansion history and effective thermal conductivity data provided

Estimated final pore size: 3.5mm.
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Based on estimated E2 and Pore size, the prediction best fit experimental results when E3=55,000
Modelling against other tests

Predictions by use of parameters extracted from test B12

- Test A6: DFT=0.4mm, Steel plate =20mm
- Test A3: DFT=0.8mm, Steel plate =20mm
- Test B7: DFT=1.2mm, Steel plate =10mm
- Test A6: DFT=0.4mm, Steel plate =20mm
Conclusion

- The model, describing expanding coating and dynamic material properties, has been validated by experimental results.
- Chemical kinetics (E2, E3), Maximum expansion ratio, and Pore size demonstrate their importance on fire protection performance.

Future works

- TGA test will be conducted for accurate kinetic values.
- Further study with expanding process, including viscosity study, will assist to predict Emax.
- Validate model in real fire conditions and on larger scale tests.
Thank you for attention!