Development and application of a novel radiation property model for oxy-coal combustion

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Overview

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- Background
- The Full Spectrum k-Distributions (FSCK) model
- Application
  - Doosan Babcock Clean Coal Test Facility (CCTF)
  - Results
- Conclusions and way forward

Radiation modelling

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- High temperatures in coal combustion mean that radiation dominates the heat transfer

- Numerical solution of the **radiative transfer equation** (RTE)

Change in intensity over a pathlength ds in elementary solid angle = Emission - Absorption and out scattering + In scattering of intensity from all other directions

- Radiative property model needed

Air-fuel combustion environment ≠ Oxy-fuel combustion environment

Radiative Property Models

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Line-by-line [dη< 2cm^{-1}, N > 10^6]

Narrow-band models

- Statistical narrow band [dη ≈ 25cm^{-1}, N > 300]
- Correlated-k [dη > 50cm^{-1}, N > 300]

Wide-band models

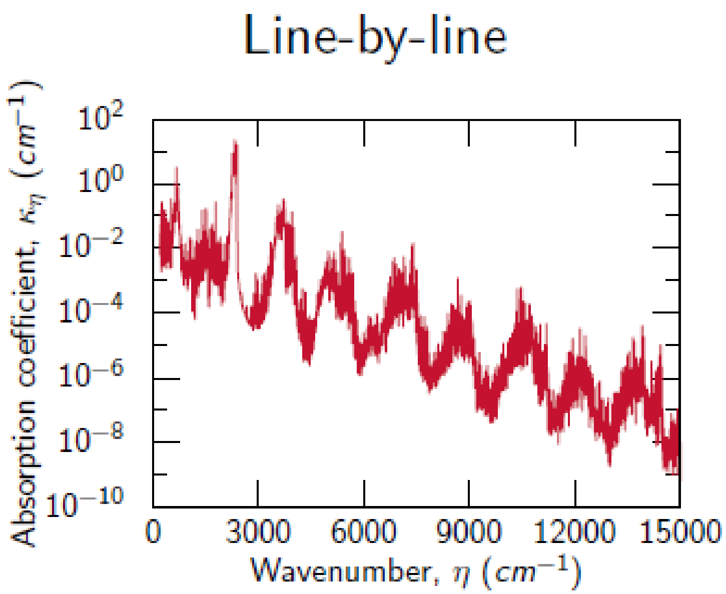
- Exponential wide-band model [dη ≈ 1000cm^{-1}, N > 7]

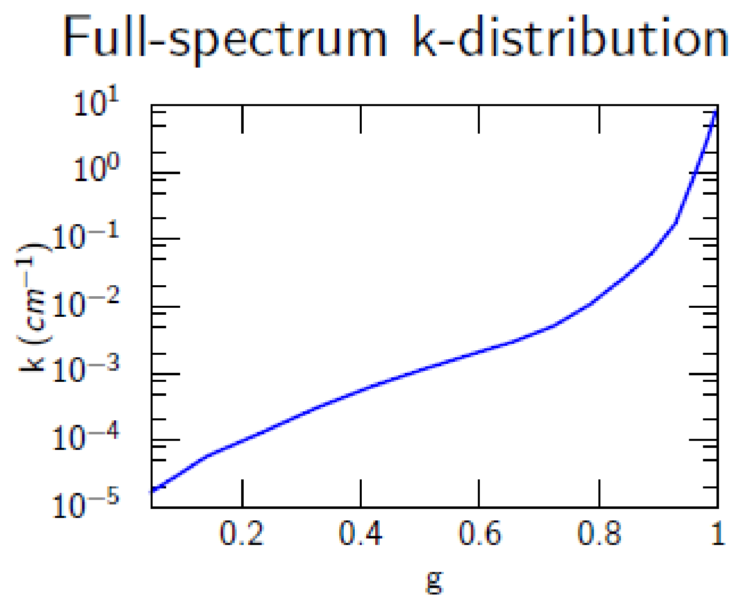
Global models

- Weighted sum of grey gases [N > 3]
- Grey weighted sum of grey gases [N = 1]
- Full-spectrum k-distribution [N > 4]

FSK Models

Simplify spectral integration of intensity by rearranging κ_η





85% CO_2, 10% H_2O, 5% N_2 mixture at 1000K

Models first proposed by Modest and Zhang (2002)

The FSCK Model

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The RTE for the FSCK method:

$$\frac{\mathrm{d}I_\eta}{\mathrm{d}\hat{\mathbf{s}}} = \kappa_\eta I_{b\eta}(T) - \kappa_\eta I_\eta - \sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi}\int_{4\pi} I_\eta(\hat{\mathbf{s}}')\Phi(\eta, \hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\,\mathrm{d}\Omega$$

$$\frac{\mathrm{d}I_g}{\mathrm{d}\hat{\mathbf{s}}} = k^*(T_0, \underline{\phi}, g_0)\left(a(T_0, T, g_0) I_b(T) - I_g\right) - \sigma_s I_g + \frac{\sigma_s}{4\pi}\int_{4\pi} I_g(\hat{\mathbf{s}}')\Phi(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\,\mathrm{d}\Omega$$

Integration can be done through a Gauss-quadrature scheme

$$\int_0^\infty I_\eta\,\mathrm{d}\eta = \int_0^1 I_g\,\mathrm{d}g_0 \approx \sum_{i=1}^{N_q} w(i) I_{gi}$$

Previously demonstrated in CFD by Porter et al. (2010)

Particle Radiation Interaction

Effective particle radiation:

$$\kappa_{\mathrm{P}} = \frac{1}{V}\sum_{\mathrm{P}} Q_{abs}\pi r^2$$

$$E_{\mathrm{P},g} = \frac{1}{V}\sum_{\mathrm{P}} Q_{abs,\mathrm{P}}\pi r_{\mathrm{P}}^2 a(T_0,\, T_{\mathrm{P}}, g_0) I_b(T_{\mathrm{P}})$$

$$\sigma_{s,\mathrm{P}} = \frac{1}{V}\sum_{\mathrm{P}} Q_{sca}\pi r^2$$

The RTE for the FSCK method with particles:

$$\frac{\mathrm{d}I_g}{\mathrm{d}\hat{\mathbf{s}}} = k^*(T_0, \underline{\phi}, g_0)\left(a(T_0, T, g_0)I_b(T) - I_g\right) + E_{\mathrm{P},g} - \kappa_{\mathrm{P}} I_g - (\sigma_s + \sigma_{s,\mathrm{P}})\, I_g + \frac{(\sigma_s + \sigma_{s,\mathrm{P}})}{4\pi}\int_{4\pi} I_g(\hat{\mathbf{s}}')\Phi(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\,\mathrm{d}\Omega$$

Application Details

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Gas Radiation

- Directional radiation transfer by the DO method
- Solid angle discretisation $N_\theta = N_\Phi = 3$
- Radiation included from CO_2, H_2O and CO
- Mixing scheme from Modest and Riazzi (2005)
- k-distributions calculated from NB k-g database

Particle Radiation

- Particle absorption efficiency $Q_{abs} = 0.9$
- Particle scattering efficiency $Q_{sca} = 0.01$
- Isometric scattering phase function

Case description

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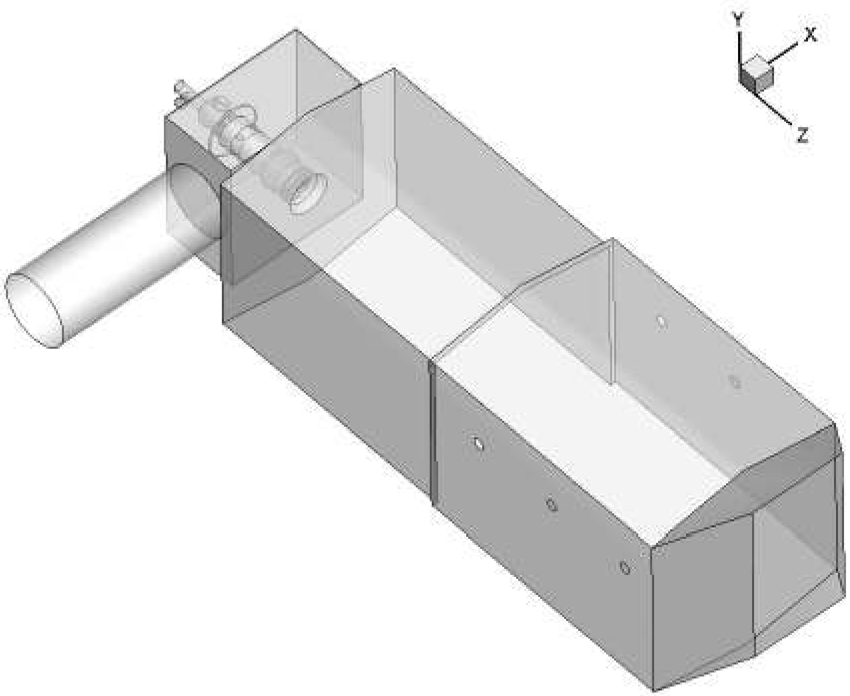
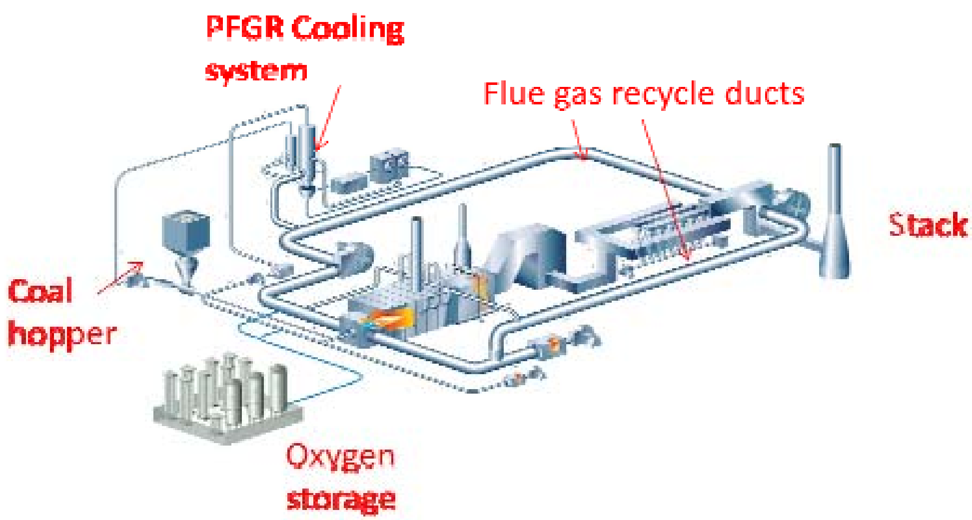
Doosan Babcock Clean Coal Test Facility (CCTF)



$40MW_{th}$

Air- and oxy-coal combustion

Single, low NO_x burner



Test conditions

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Operating Conditions		
Burner zone stoichiometry		1.0
FGR rate %		60.0
Mass flow (kg/s)	Windbox	8.61
	Primary	3.32
	Core	0.4
	Total	12.33
Coal flow rate (kg/s)		1.18
O_2 in primary		19.7
O_2 in windbox		30.0
CO_2 in primary		63.04
CO_2 in windbox		50.88
H_2O in windbox		7.41

Coal analisys (%) El Cerrejon	
HCV as r.	3.159e+7 MJ/kg
Ash	2.3
Moisture	2.9
FC	58.5
VM	36.3
C	77.90
H	5.06
N	1.68
S	0.68
Cl	0.02
O	9.49

Modelling approach

- CFD simulation using ANSYS Fluent v12.1
- RANS, full 3D model, 4M cells
- Turbulence-chemistry interaction: eddy dissipation
- Two-step global reaction for volatile combustion
- Devolatilisation: single rate

  (A_0 = 14841 s^{-1}; E_a = 35.3 MJ/kmol)
- Char combustion: intrinsic model

  (A_0 = 4.0e-04 kg/m^2-s-Pa; E_a = 66 MJ/kmol)

Results

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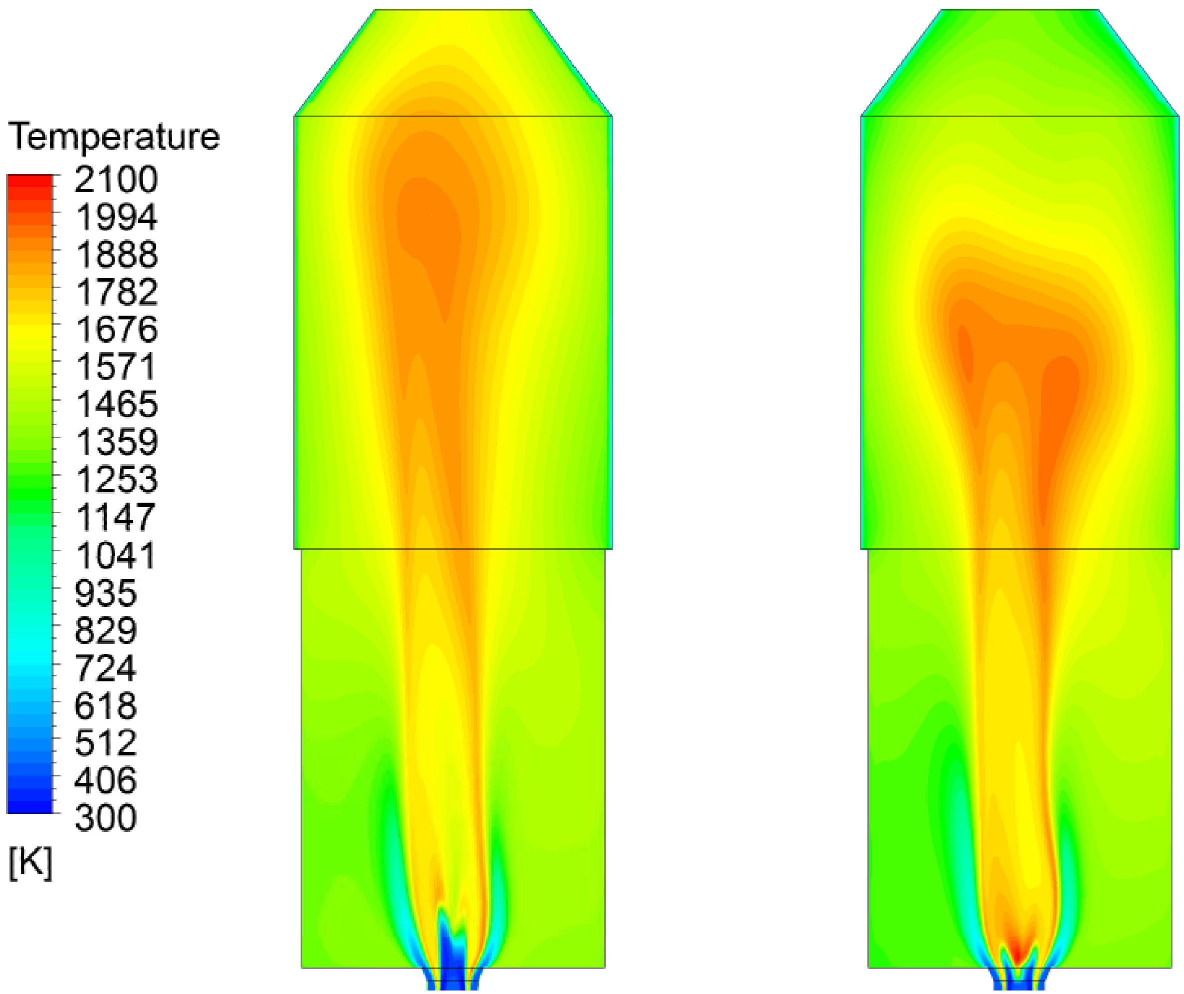

WSGG – Smith et al. (1992)
Y = 0m

FSCK model
Y = 0m

	Exit T.
Measured	**1372K**
WSGGM	**1496K**
FSCK	**1370K**

Results

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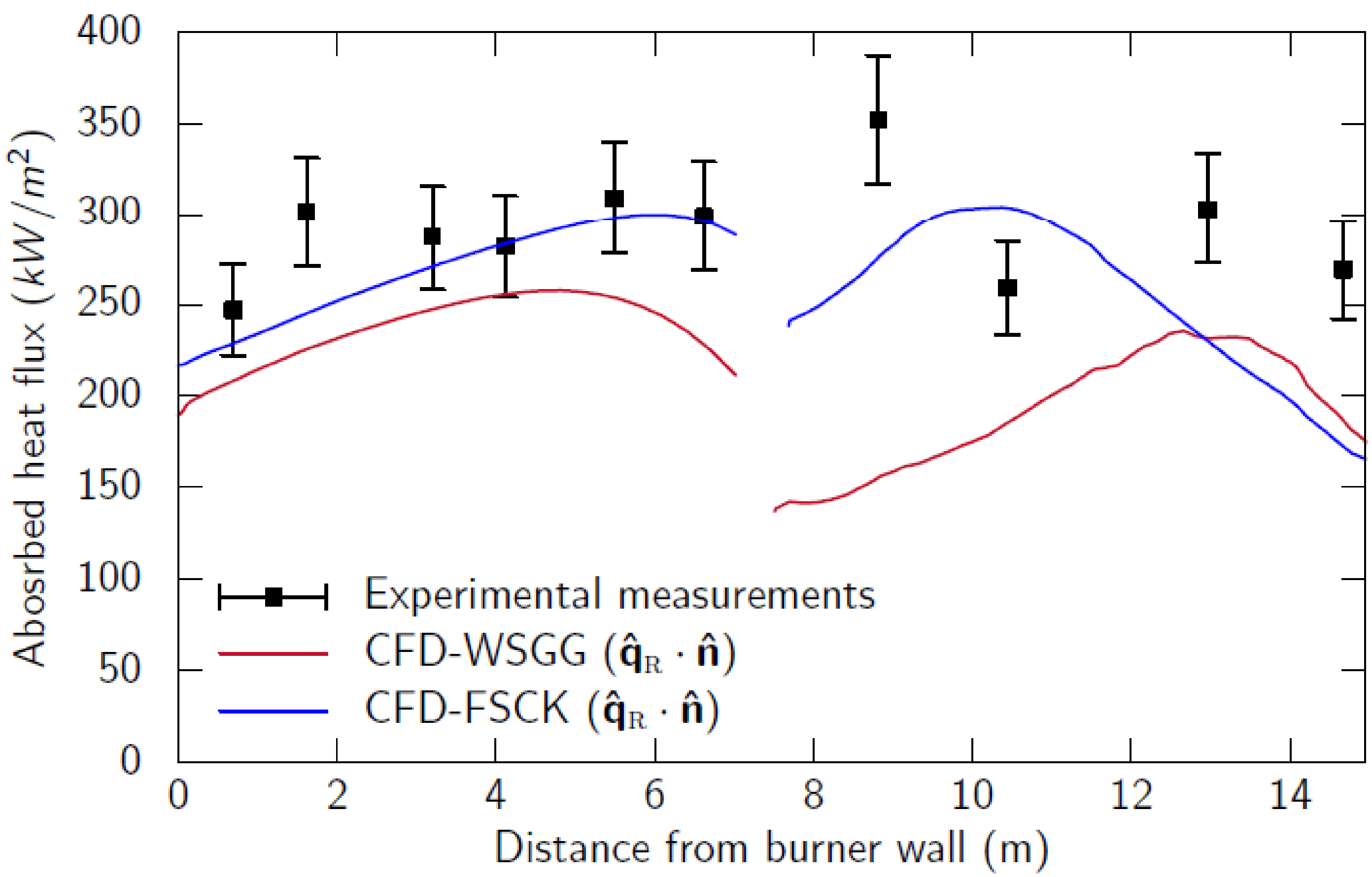

Conclusions and way forward

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- Radiation models significantly affect temperature in CFD
- Accurate gas-radiation properties are important for oxyfuel
  - Far higher concentrations of participating gasses
  - Including the FSCK model improves temperature predictions
- Both gas- and particle-phase radiative sources are important
- Further insight required for particle radiation interaction

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