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Clean Coal Technologies 2019

Modelling of Trace Element Fate in an Entrained-flow Solid Fuel Combustion Unit

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Background

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- Increasing Global Carbon Emission
- Co-firing Coal Combustion with Biomass
  - Carbon Emission Reduction
  - Burnout Efficiency
- EU Renewable Energy Directive
  10% Energy Share → 50% Deforestation (Hennenberg et al, 2017)

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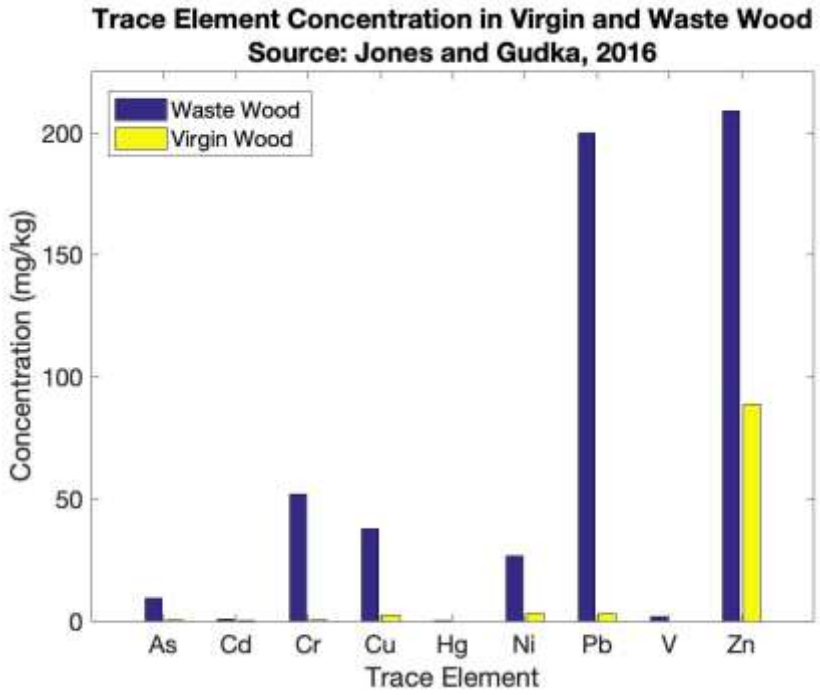
- Treated Wood as Alternatives
  - Abundance (3.7M tonnes in the UK and 53M tonnes in the EU)
- Potential in the Future

- Trace Element in Treated Wood



- Trace Element Origin

  As, Cu, Cr (Preservative); Pb (Paint); Ni, Co, V (Coating); Hg, Cd (Natural Deposition)

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Background

Trace Element Health Impact

As

- Lung Cancer
- Nausea
- Skin Irritation

Cd

- Respiratory Irritation
- Kidney Failure
- Bone Deformities
- Osteoporosis
- Renal Dysfunction
- Liver Fibrosis
- Oxidative Stress

Cr

- Cell Growth Failure
- Cell Apoptosis

Pb

- Ca Deficiency
- Neurotoxicity
- Cognitive Failure
- Reproductive Failure
- Parkinson's Disease

Hg

- Neurotoxicity
- Neural Inflammation
- Oxidative Stress

Directive 2010/75/EU

Element and Its Compound	Emission Limit (mg/Nm3)
Cd	Total: 0.05
Tl	
Hg	0.05
Sb	Total: 0.5
As	
Pb	
Cr	
Co	
Cu	
Mn	
Ni	
V	

- Trace and Ash-forming Element Fate and Occurrence Prediction
  - Gas Emission
  - Particle Eutectic
- Predictive Tool Establishment
- Assessment and Optimisation
  - Gas Cleanup
  - Slagging and Fouling

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Experiment

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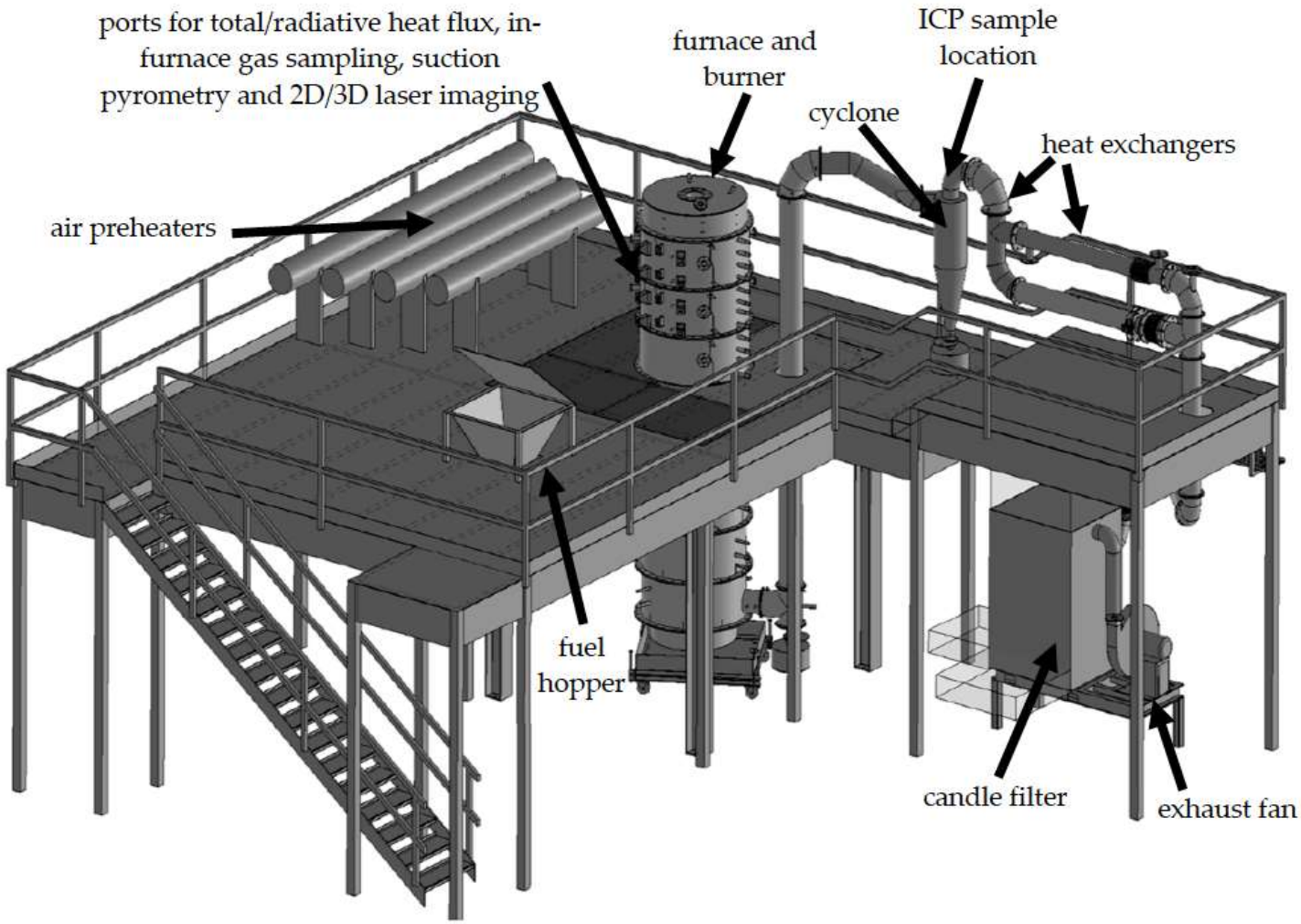
Combustion Experiment

250kW PACT Facility Burner



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Combustion Experiment

Biomass and Gas Properties

Boiler – **250-kW PACT Facility**
Type – **Entrained Flow without Bottom Bed**
Location – **Sheffield, England**
Biomass – **US White Wood Pellet / Recycled Wood**
Biomass Flow Rate (US White Wood Pellet / Recycled Wood) – **39.8 kg/h / 42.11 kg/h**
Gas – **Air / Oxy27**
Gas Flow Rate (Air / Oxy27) – **2.789 mol/s / 1.913 mol/s**

Proximate Analysis (Mass Fraction)
Moisture (US White Wood Pellet / Recycled Wood) – **6.69% / 5.8%**
Volatiles (US White Wood Pellet / Recycled Wood) – **78.1% / 73.9%**
Fixed Carbon (US White Wood Pellet / Recycled Wood) – **14.51% / 17.1%**
Ash (US White Wood Pellet / Recycled Wood) – **0.7% / 3.2%**

Ultimate Analysis (Mass Fraction)
N (US White Wood Pellet / Recycled Wood) – **0.15% / 0.4%**
C (US White Wood Pellet / Recycled Wood) – **48.44% / 51.9%**
H (US White Wood Pellet / Recycled Wood) – **6.34% / 6%**
S (US White Wood Pellet / Recycled Wood) – **less than 0.02% / less than 0.02%**
Cl (US White Wood Pellet / Recycled Wood) – **less than 0.01% / less than 0.01%**
O (US White Wood Pellet / Recycled Wood) – **37.69% / 41.7%**
GHV (US White Wood Pellet / Recycled Wood) – **19.41 kJ/kg / 18.4 kJ/kg**

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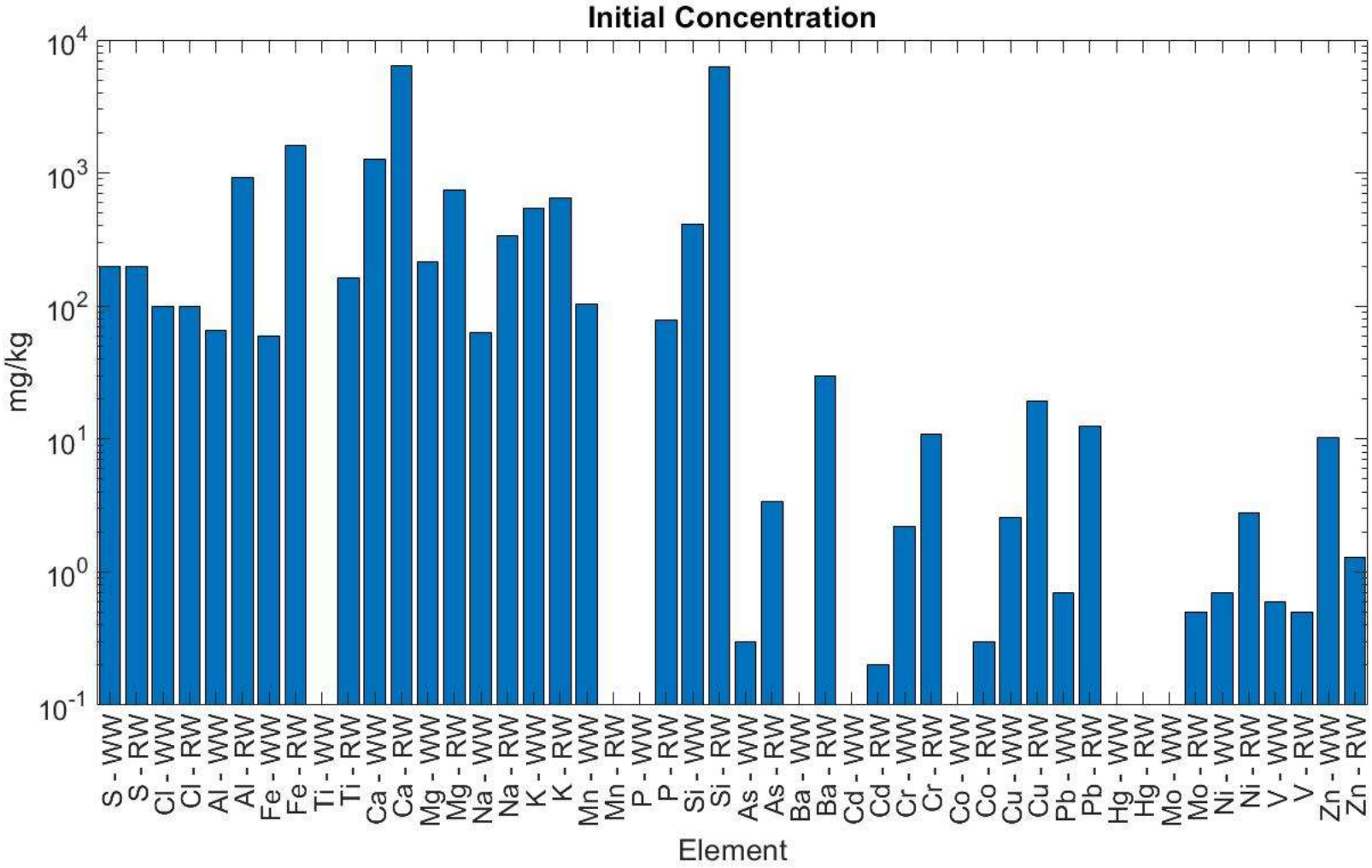
Combustion Experiment

Biomass and Gas Properties



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Model

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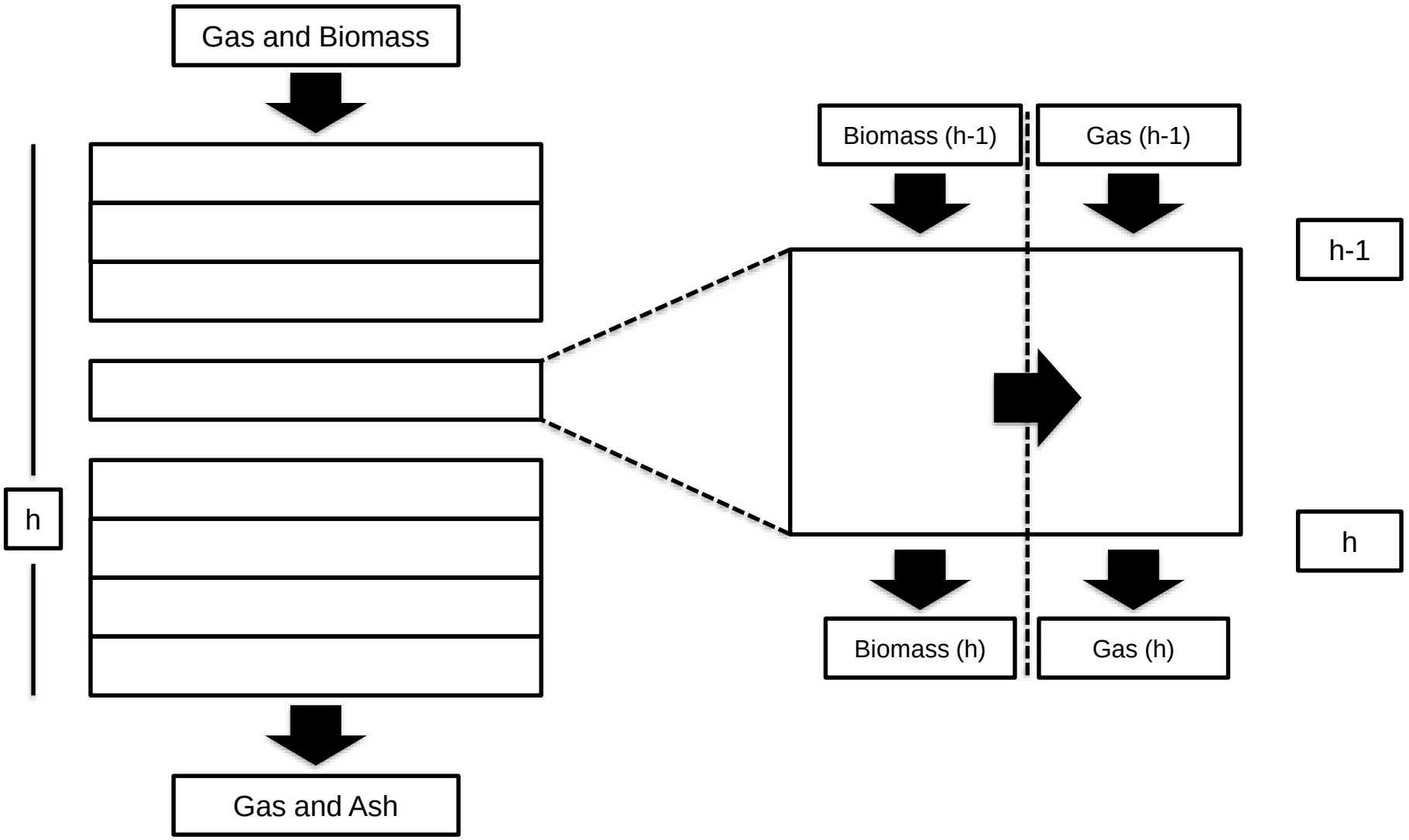
Combustion Model

Model Hierarchy



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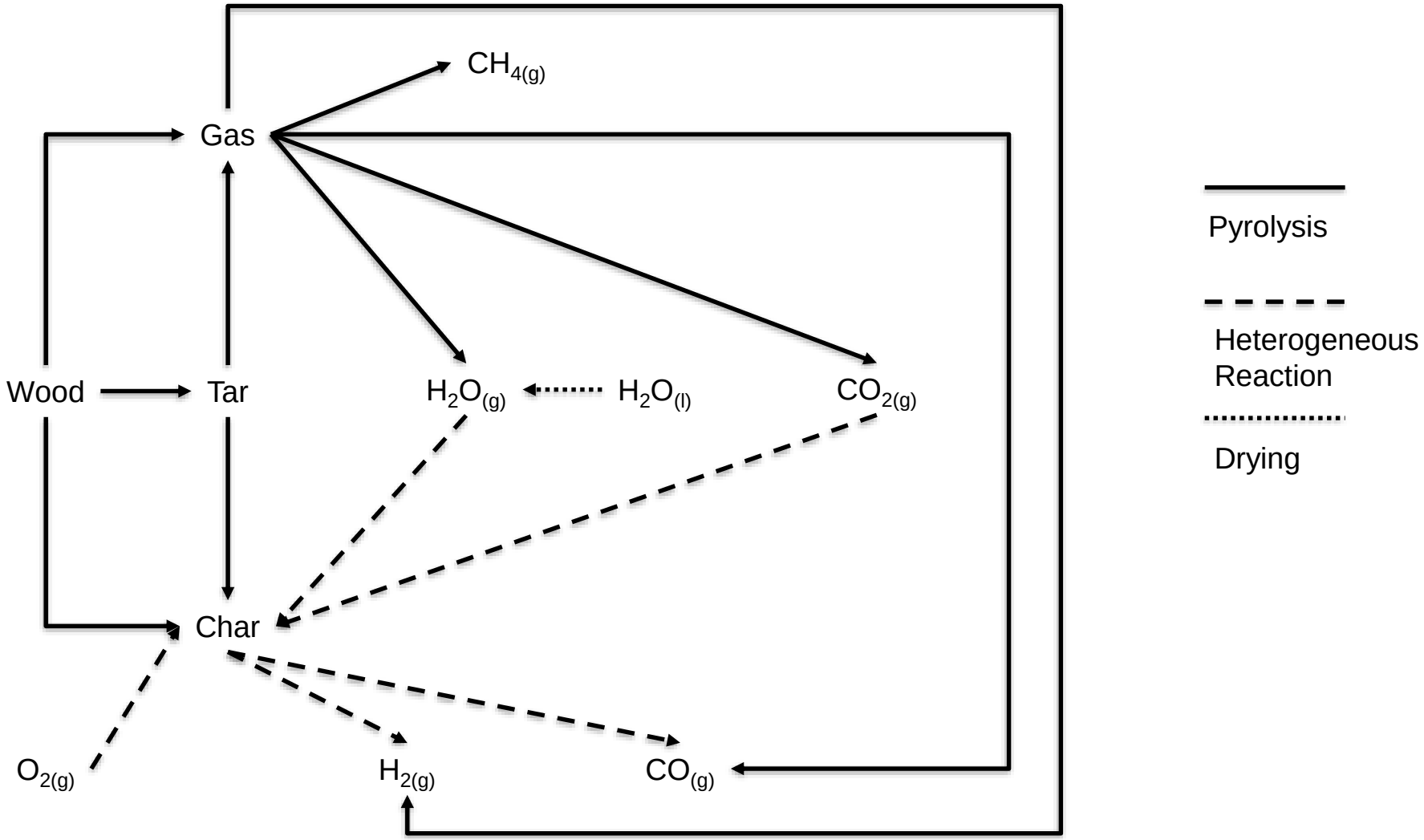
Combustion Model

Particle Thermal Conversion Route



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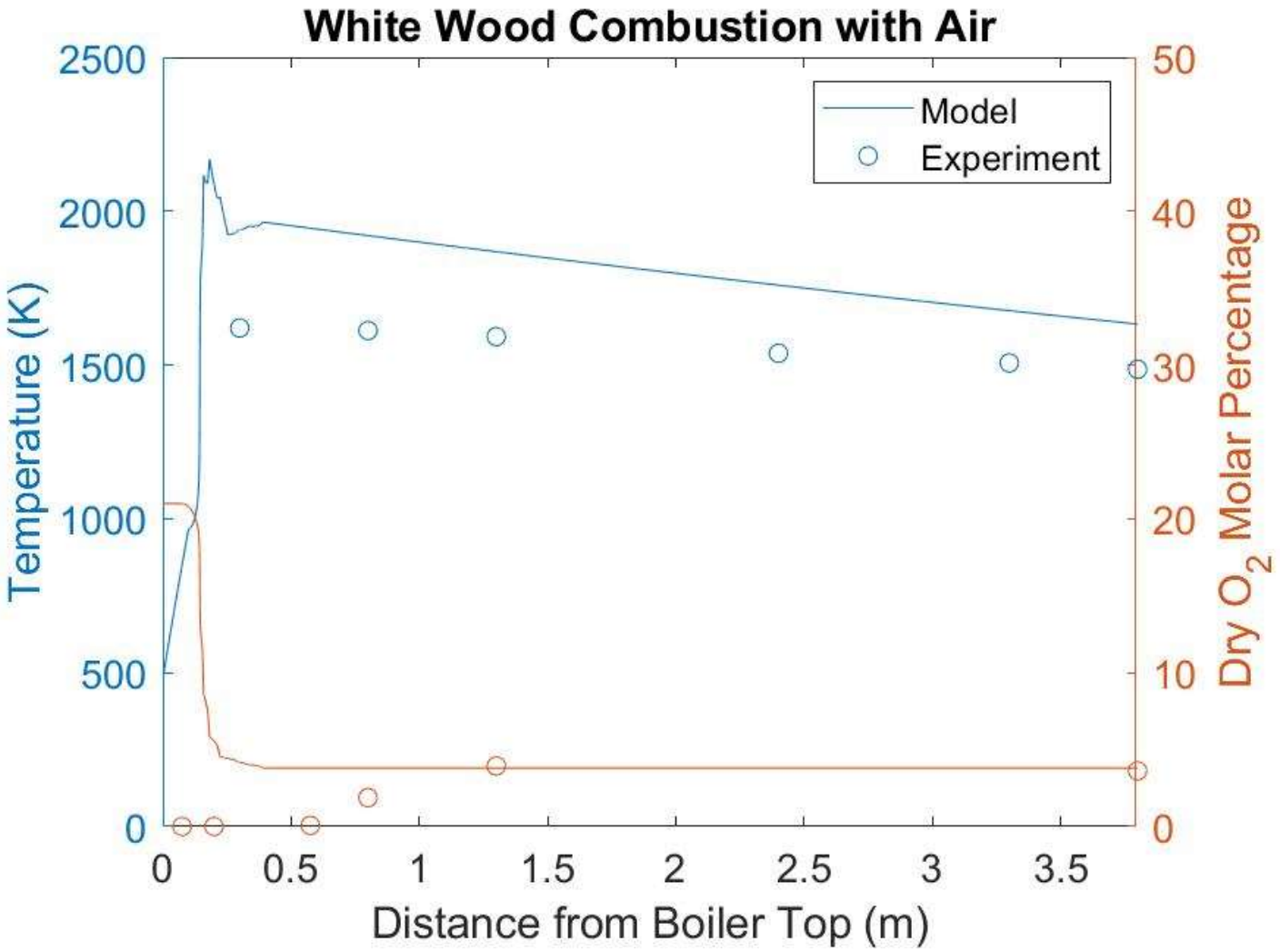
Combustion Model

Temperature and Gas Concentration



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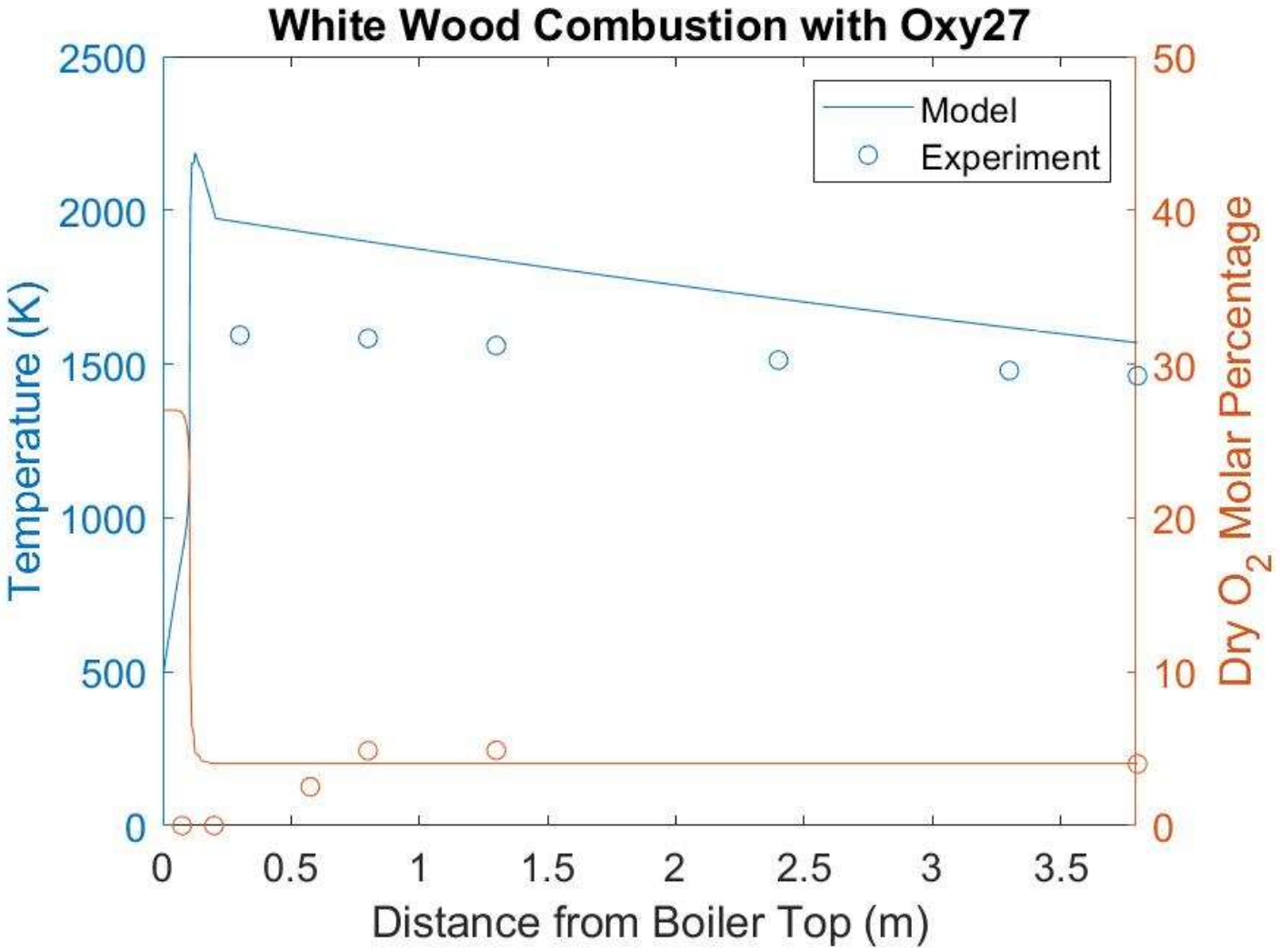
Combustion Model

Temperature and Gas Concentration



Trace element and ash-forming element phases and amounts are calculated based on minimisation of Gibb's energy.

1. Lack of available reaction kinetic data
2. Reduce calculation complexity of multi-elements

Equilibrium phase and mass are calculated using Equilib module in FactSage™.

$$G = \sum_{\substack{ideal \\ gas}} n_i(g_i{}^o + RT \ln P_i) + \sum_{\substack{pure \\ condensed \\ phase}} n_i\, g_i{}^o + \sum_{solution\ 1} n_i(g_i{}^o + RT \ln X_i + RT \ln \gamma_i)$$

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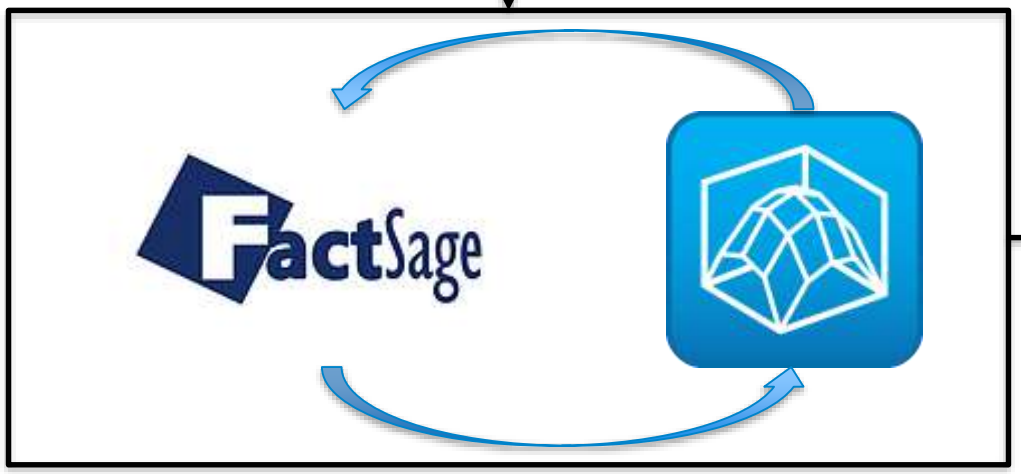
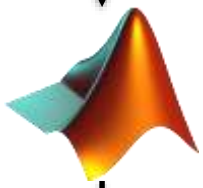
Chemical Equilibrium Model

Chemical Equilibrium Surrogate

Trace Element
- Concentration Index Range
- Temperature Range



Trace Element
- Element Concentration
- Temperature



Chemical Equilibrium Surrogate

Trace Element
- Product Concentration

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Chemical Equilibrium Model

Chemical Equilibrium Library

Transparent Data File (.cst)

Trace Element
- Element Concentration
- Temperature

Visual Studio

- Dynamic Link Library (.dll)
- ChemApp Interface (.c)
- Transparent Data File (.cst)
- Binary Data File (.bin) for Fortran

Mex File

Trace Element
- Product Concentration

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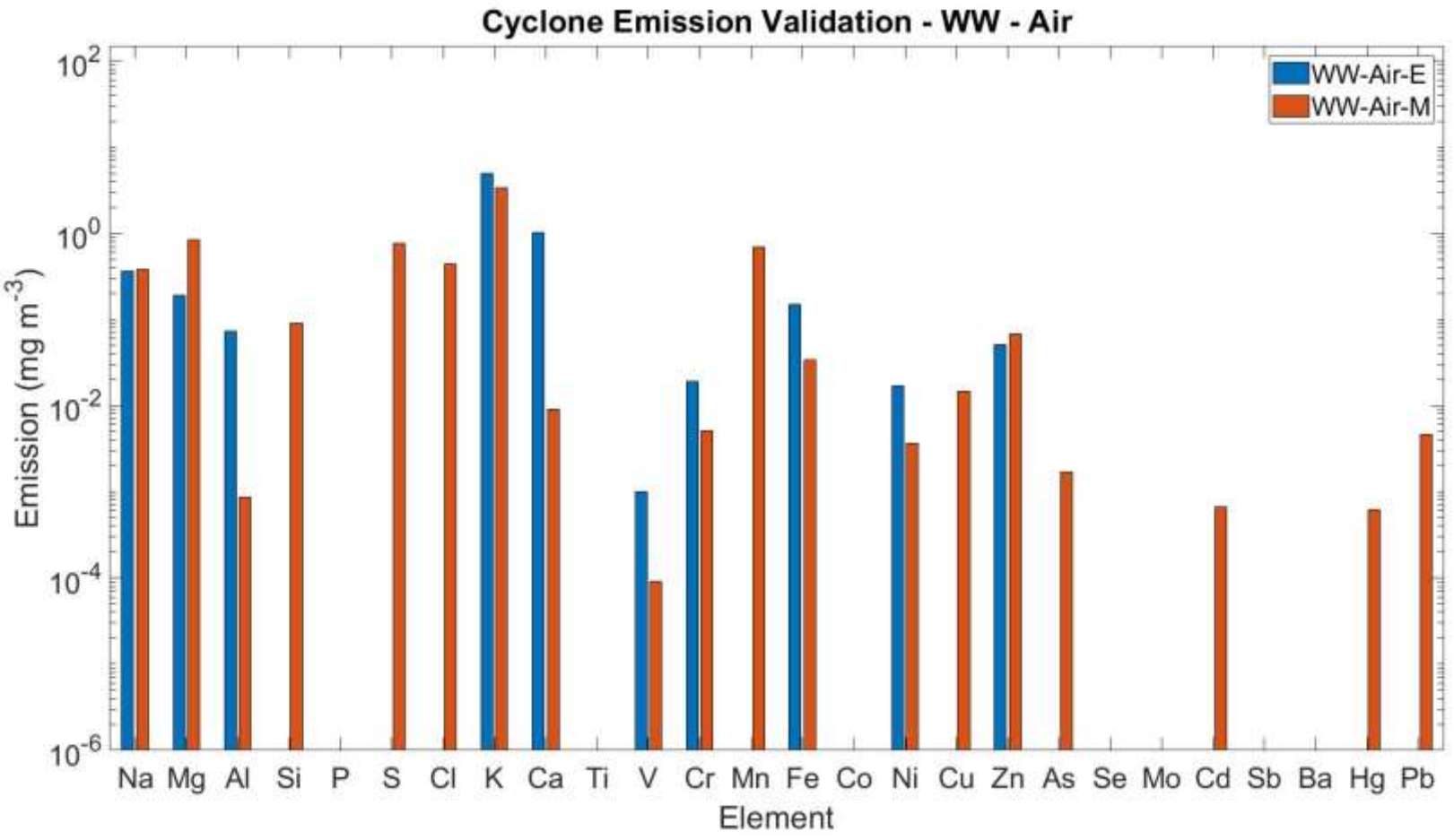
Chemical Equilibrium Model

Gas Emission Validation – WW Air



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Background

Trace Element Emission Regulation

Elements	EU ($mg\ m^{-3}$)	WW-Air ($mg\ m^{-3}$)		WW-Oxy27 ($mg\ m^{-3}$)		RW-Air ($mg\ m^{-3}$)	
Cd	Total: 0.05	0.00067	0.00067	0.00123	0.00123	0.00111	0.00111
Tl		N/A		N/A		N/A	
Hg	Total: 0.05	0.00062	0.00062	0.00123	0.00123	0.00052	0.00052
Sb	Total: 0.5	N/A	**0.71859**	N/A	**1.34767**	N/A	0.19149*
As		0.00171		0.00369		0.01821	
Pb		0.00468		0.00860		0.07004	
Cr		0.00508		0.02301		0.00245	
Co		N/A		N/A		0.00118	
Cu		0.01475		0.03195		0.09870	
Mn		0.68860		1.27183		N/A	
Ni		0.00368		0.00858		0.00088	
V		0.00009		0.00001		0.00003	

*Mn data availability would probably affect the total emission.

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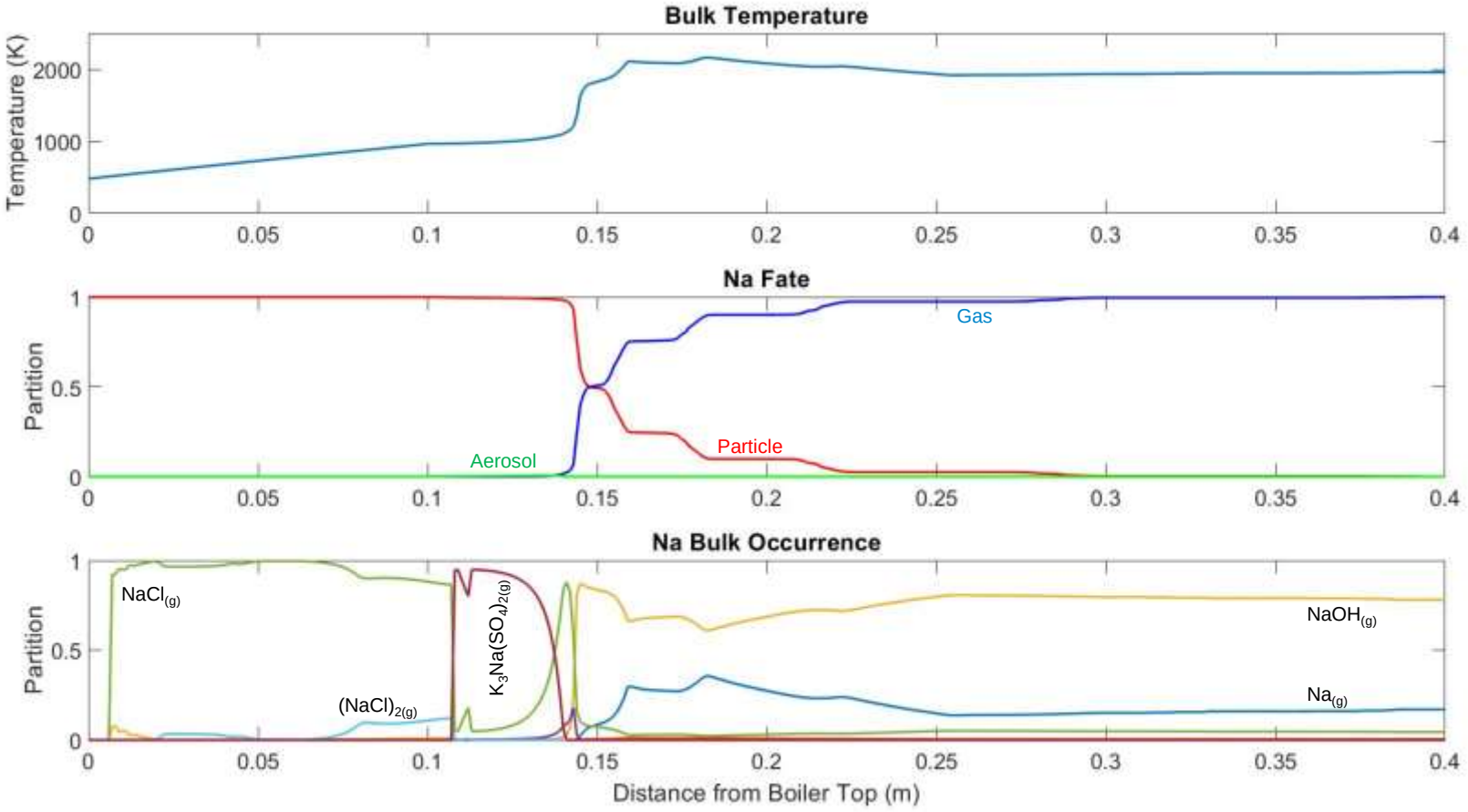
Chemical Equilibrium Model

Model Evaluation: Sodium – WW – Air



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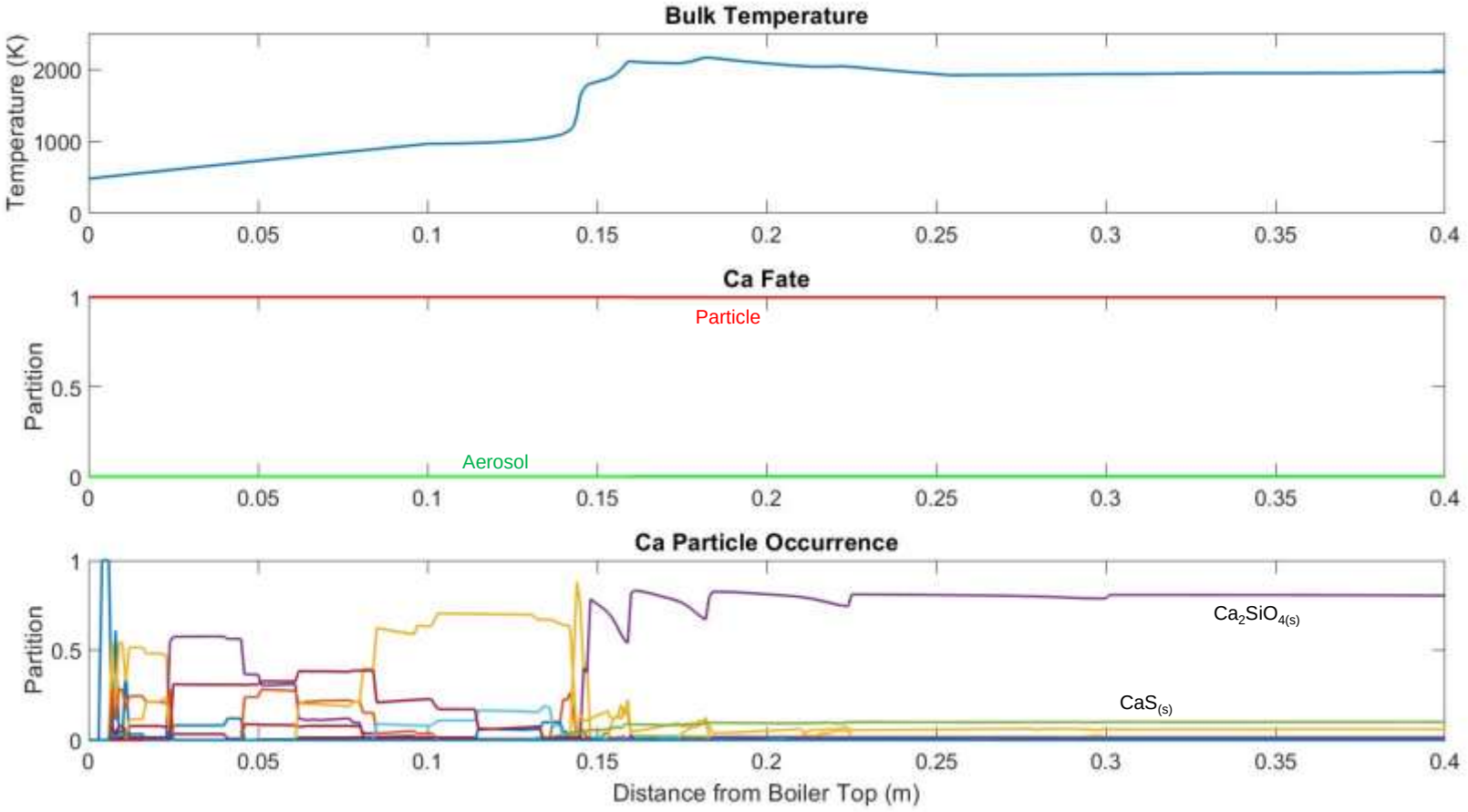
Chemical Equilibrium Model

Model Evaluation: Calcium – WW – Air



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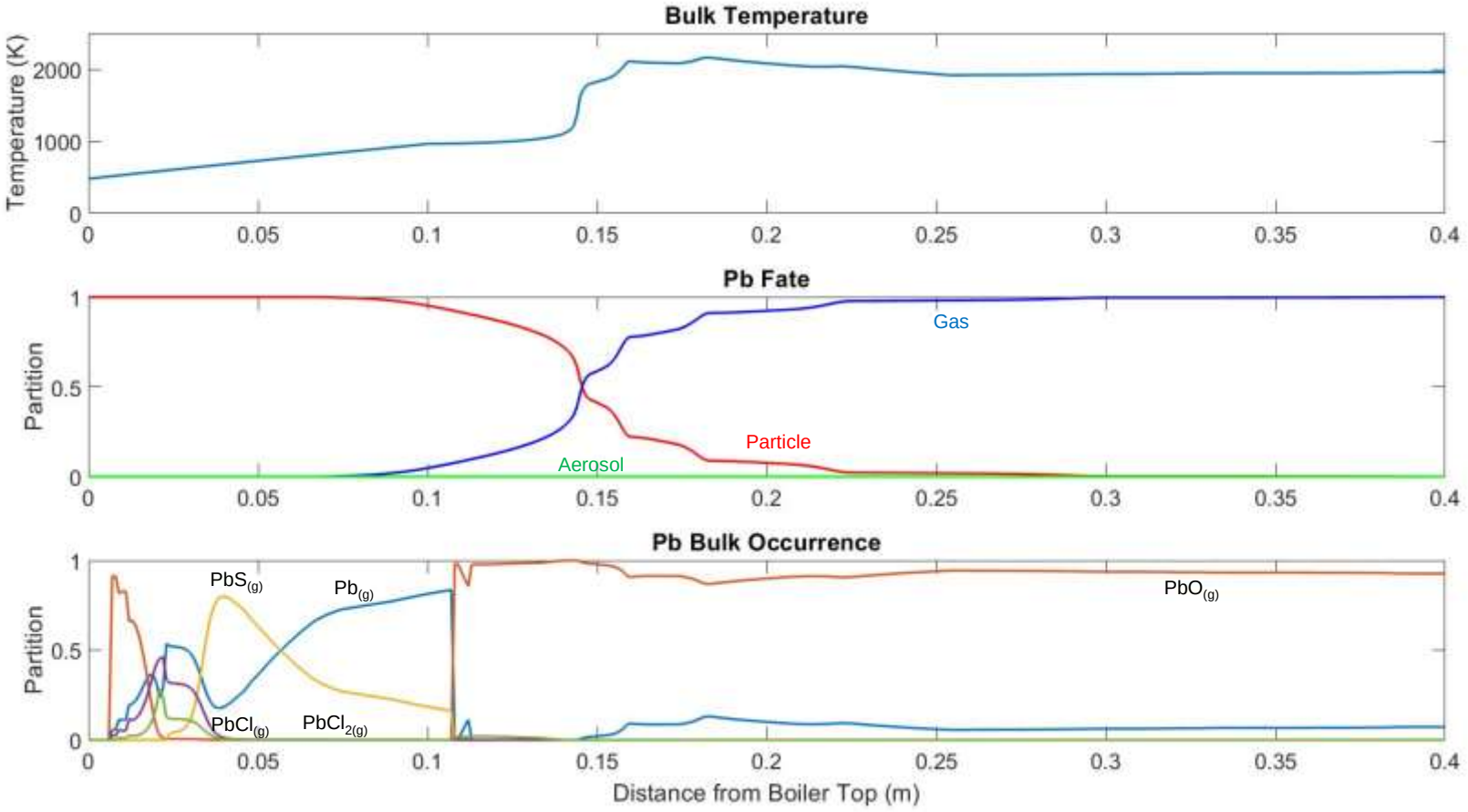
Chemical Equilibrium Model

Model Evaluation: Lead – WW – Air



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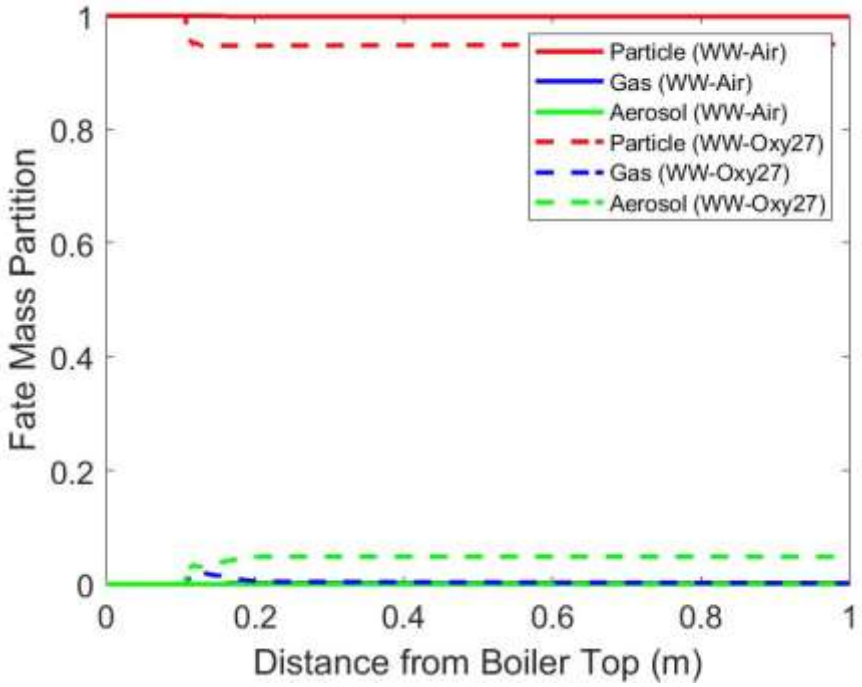
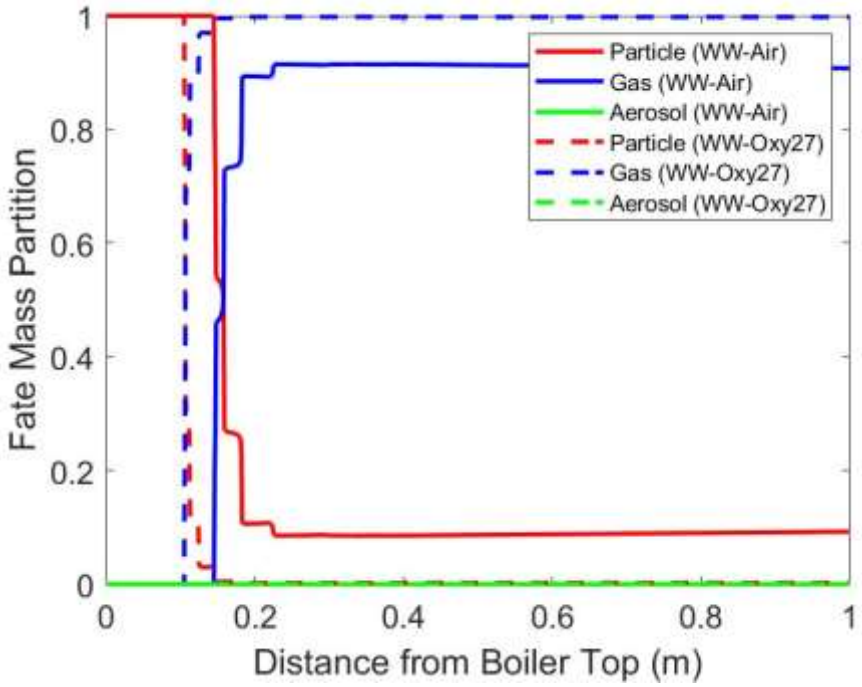
Chemical Equilibrium Model

Model Evaluation: Fate – WW – Air and Oxy27

Calcium



Nickel



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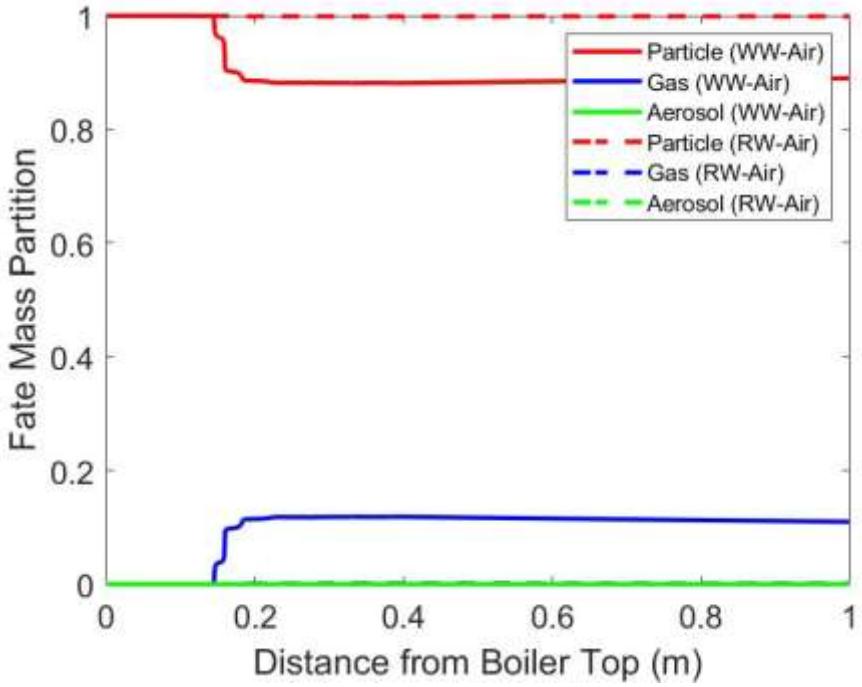
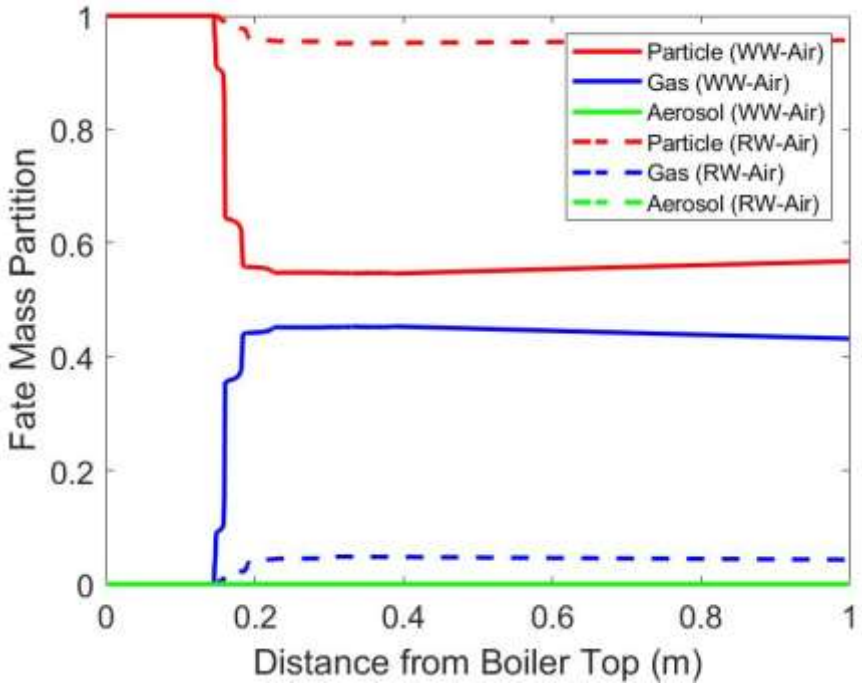
Chemical Equilibrium Model

Model Evaluation: Fate – WW and RW in Air

Iron



Chromium



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Conclusions

- Combustion Model Well Validation
- Successful Chemapp Integration with Modelling Environment
- Elemental Fate and Occurrence Validation
  - Kinetic Limitation
  - Particle Flow
- Initial Concentration Impact on Fate and Occurrence

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Future Work

- Co-firing with Coal: Impact on Fouling Tendency Reduction
- Evaluation on Downstream Aerosol Filtration