Numerical modelling for the volatiles ignition of a particle

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By - Tejas Ashar

Supervisors: Professor Lin Ma, Professor Mohamed Pourkashanian, Professor Derek Ingham, Dr Alastair Clements

Industrial Supervisor: Angus Duncan

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Outline of the Presentation

1. Ignition overview

2. Different devolatilisation Models

3. Sensitivity analysis on different devolatilisation model

4. Single particle Ignition modelling

1. Ignition overview

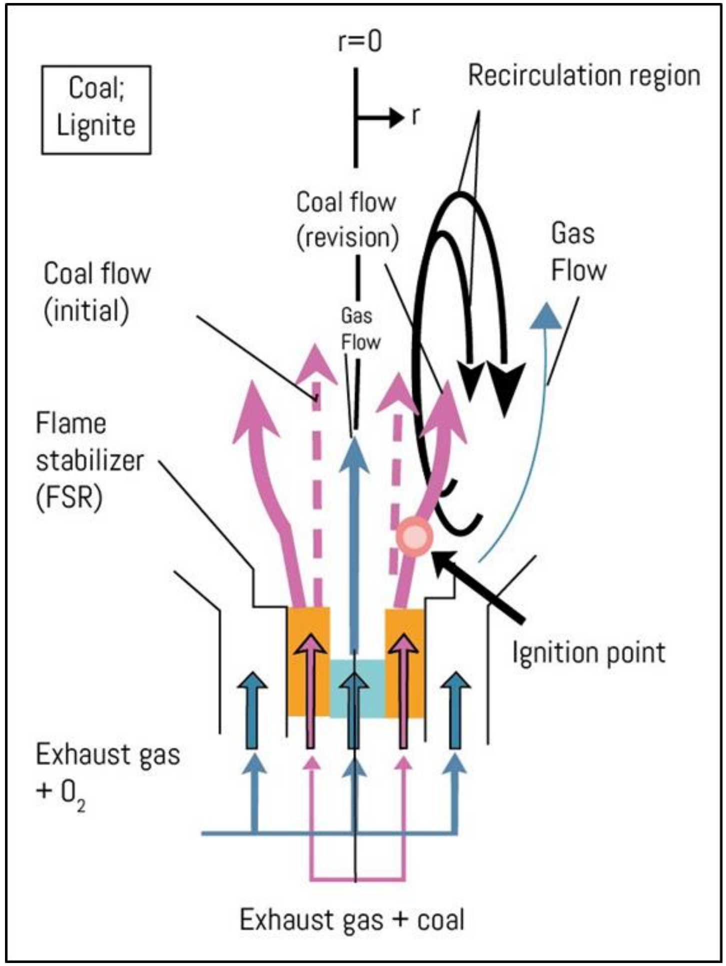
1.1 Importance of ignition

- Burners are designed to meet the specification of a design coal.
- Coal cost and availability fluctuates in the market

Possible Solution → Fuel Switching → Changes flame aerodynamics → Change in ignition and flame stability

- Computational fluid dynamics (CFD) is a tool which helps in visualising complex fluid flows by solving mathematical equations.

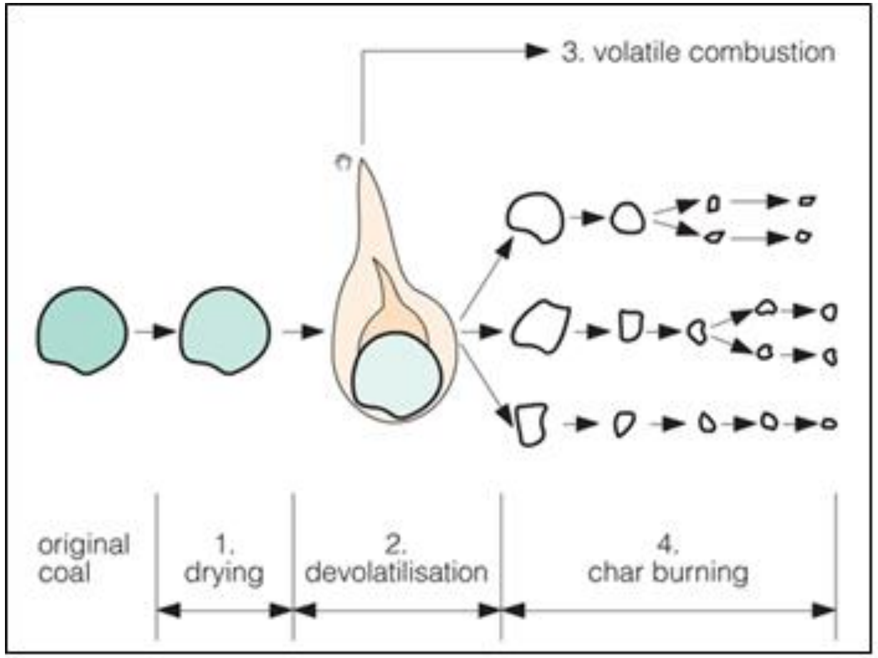
- Aim:
  - To do a sensitivity analysis on devolatilisation model.
  - To simulate single particle volatiles ignition.



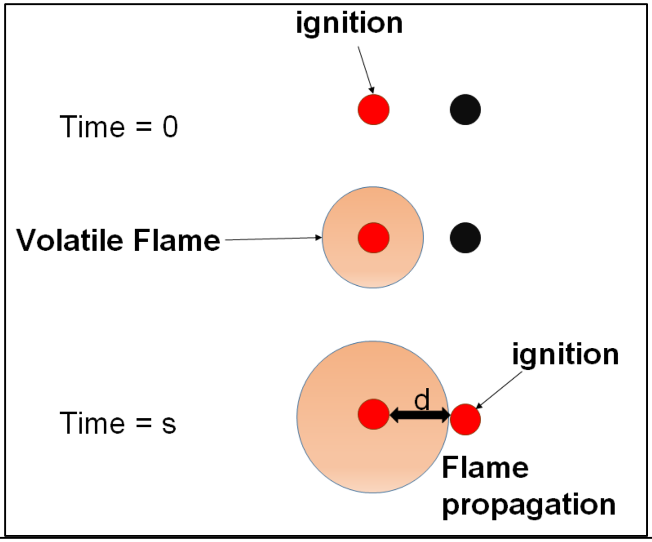
Aerodynamics of a burner [1]

[1] M Taniguchi, H Okazaki, H Kobayashi, S Azuhata, H Miyadera, H Muto, T Tsumura, et al. Pyrolysis and ignition characteristics of pulverized coal particles. Journal of Energy Resources Technology-Transactions of The ASME, 123(1):32–38, 2001.

1.2. Ignition phenomena



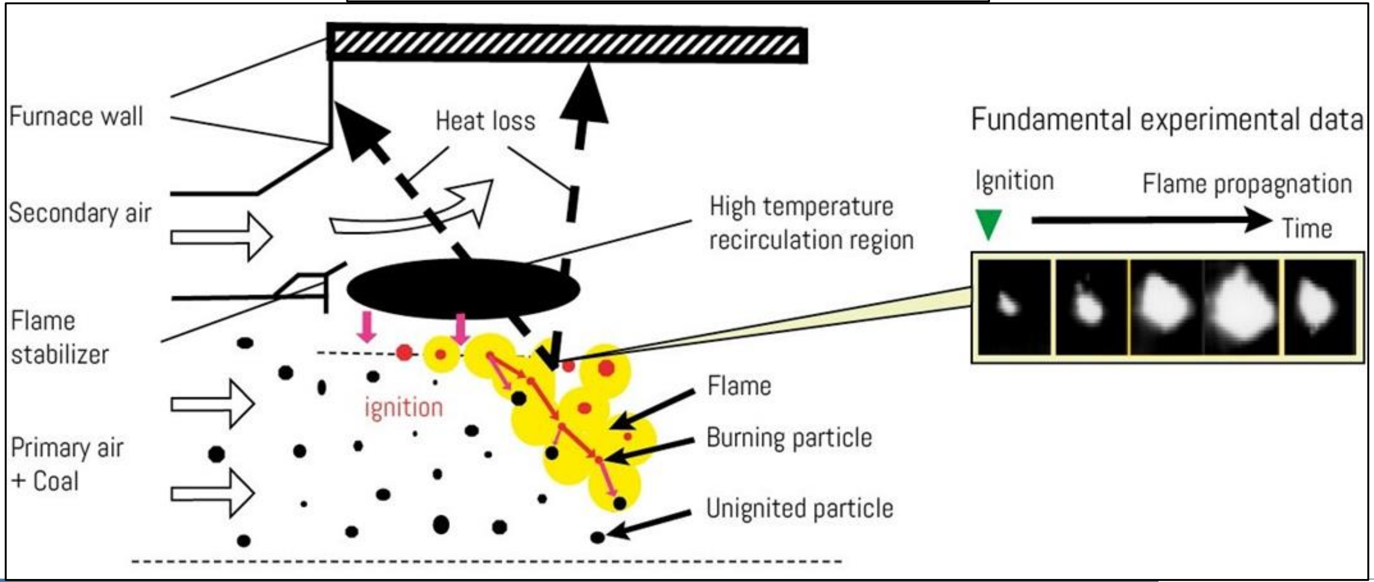
Single particle ignition [2]



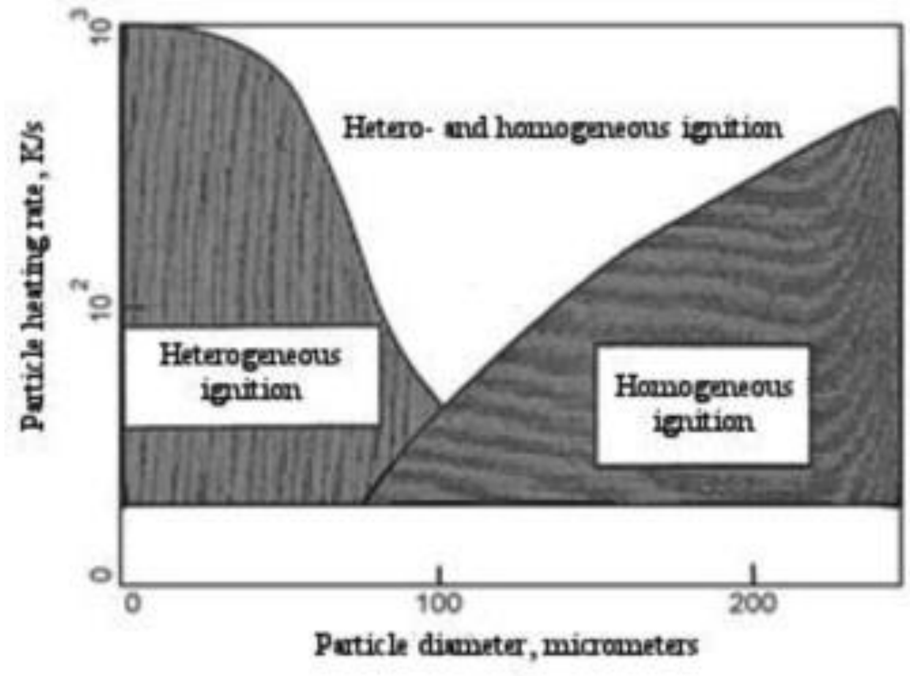
Flame propagation

[2.] E. J. Anthony and F. Preto, *Pressurized combustion in FBC systems, in Pressurised Fluid Bed Combustion*. Glasgow: Blackie, 1995

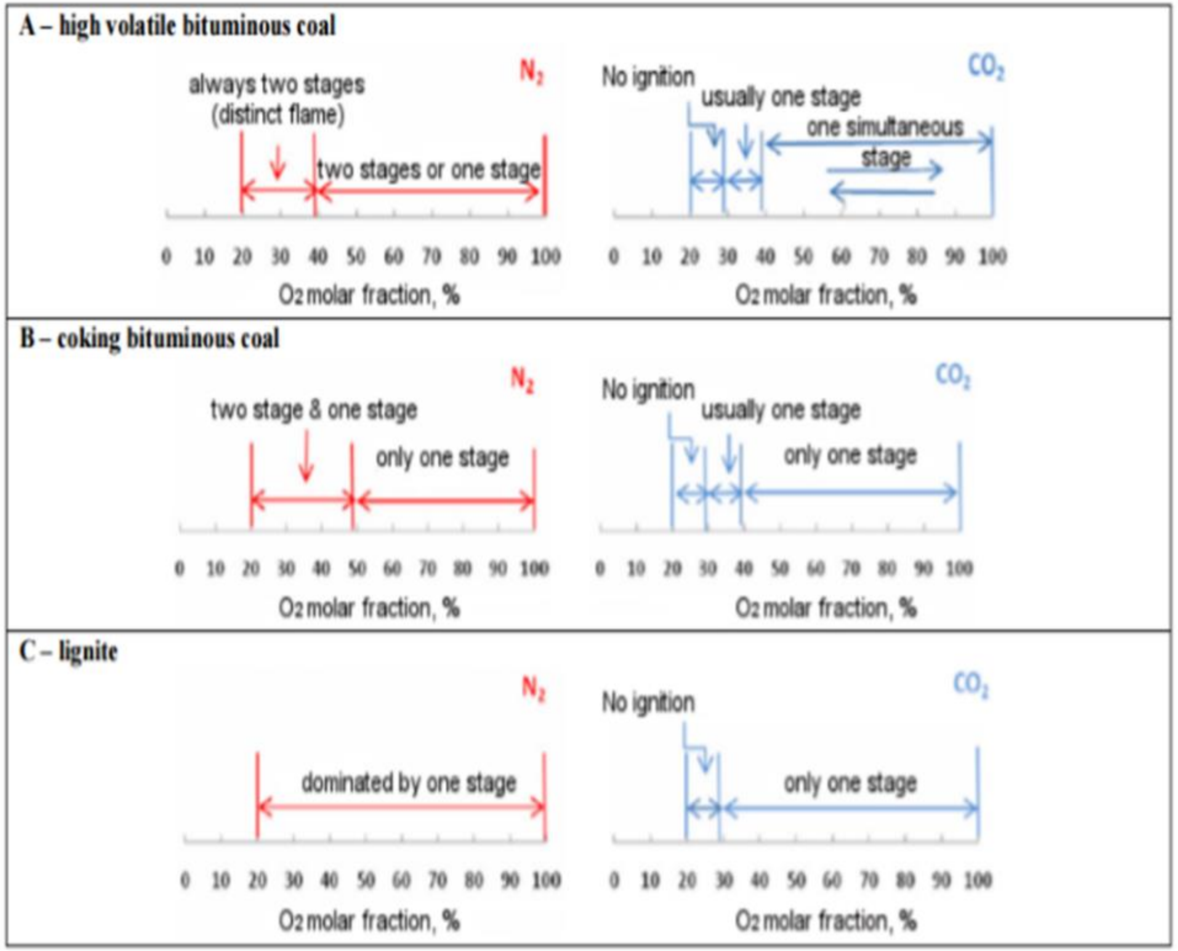
Ignition in a furnace



1.3 Experimental studies



Region defining ignition mechanism [3]



Work done by Khatami et al in drop tube furnace [4]

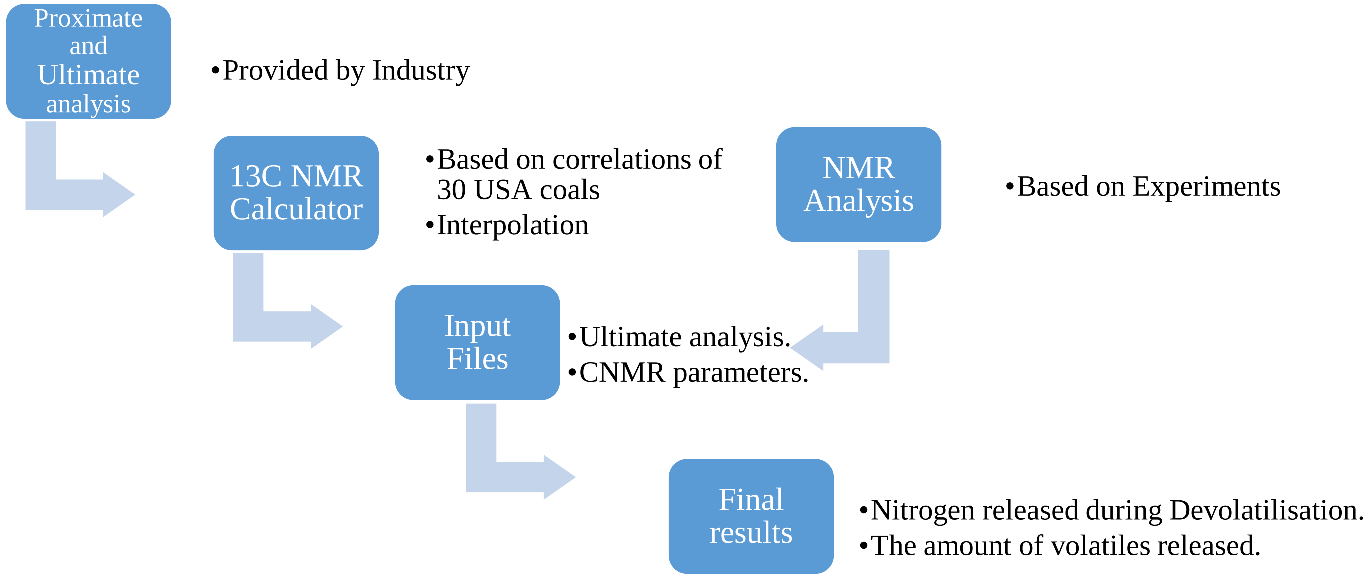
[3] H Ju¨ntgen and KH Van Heek. An update of german non-isothermal coal pyrolysis work. Fuel Processing Technology, 2(4):261–293, 1979.
[4] Reza Khatami, Chris Stivers, Kulbhushan Joshi, Yiannis A Levendis, and Adel F Sarofim. Combustion behavior of single particles from three different coal ranks and from sugar cane bagasse in o 2/n 2 and o 2/co 2 atmospheres. Combustion and flame, 159(3):1253–1271, 2012.

EPSRC Engineering and Physical Sciences Research Council

2. Different devolatilisation models

2.1 CPD (Chemical Percolation Devolatilisation model)

- It is an open source model developed by Sandia National Lab and University of Utah [7]
- It describes the devolatilization behaviour of rapidly heated coal based on the chemical structure of the parent coal.

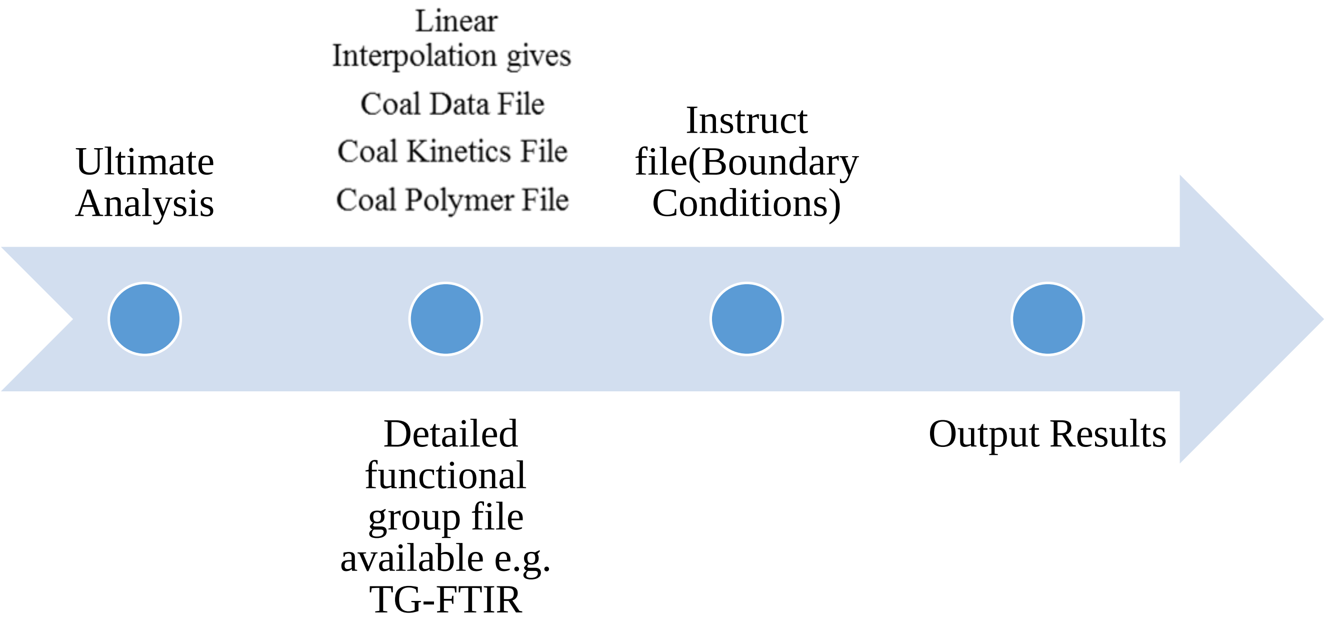


[7]. T. H. Fletcher, A. R. Kerstein, R. J. Pugmire, M. S. Solum, and D. M. Grant, “Chemical Percolation Model for Devolatilisation . Direct Use of 13C NMR Data To Predict Effects of Coal Type,” *Energy & Fuels*, vol. 6, no. 10, pp. 414–431, 1992.

EPSRC Engineering and Physical Sciences Research Council

2.2 FG-DVC (The Functional Group, Depolymerisation, Vaporisation, Cross Linking

- The code for this model was developed by Solomon and workers [8] and requires licencing.
- The FG-DVC requires the ultimate analysis for the coal as input but better results are obtained if the functional group data for the coal is used.



Advantage:

It gives detailed final gas species.

Disadvantage:

It gives higher error if operated without sufficient data (functional group).

[8]. P. R. Solomon and M. A. Serio, “A characterization method and model for predicting coal conversion behaviour. Reply to Herod, A. and Kandiyoti, R. Fuel 1993, 72, 469,” *Fuel*, vol. 73, no. 8, p. 1371, 1994.

3. Sensitivity analysis on different devolatilisation model

3.1 Experimental Data

The data provided in [9] are as follows:

- TGA proximate analysis (Ash df and VM daf basis)
- Elemental analysis daf basis (C,H and N)
- Measured values of:
  - High Temperature Volatile Yield
  - Nitrogen release.

Experiment Type	High Temperature Wire Mesh (HTWM)
Heating Rate	10000 K/s
Final Temperature	1873.15 K
Hold Time	2 s
Amount of Coal	10 -12 mg
Size of the Coal	125 – 150 µm

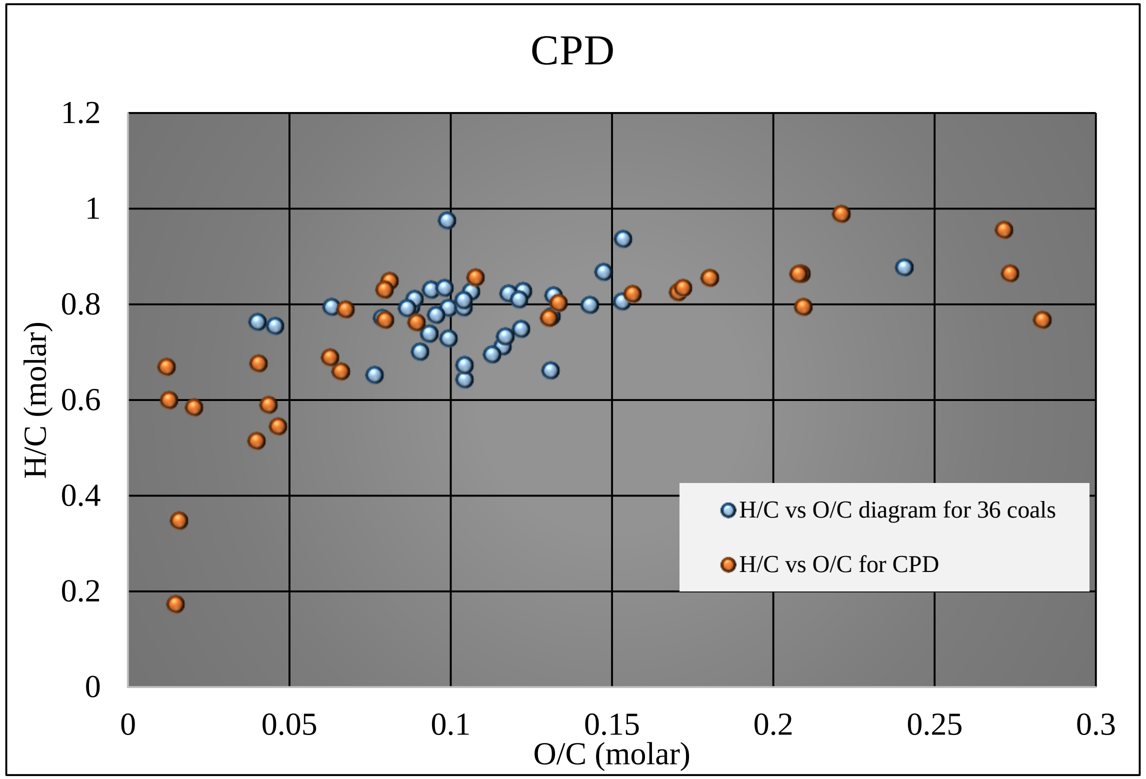
HTWM devolatilisation experimental conditions for the 36 coals [9].

Coal	Country of origin	TGA micro-proximate analysis		Elemental analysis (% daf)			HTWM volatile yield (% daf)	Volatile N (%coal N)
		Ash (wt% db)	VM (wt% daf)	C	H	N		
1	VEN	4.3	38.3	83.0	5.5	1.8	54.3	58.2
2	COL	9.4	38.6	82.8	5.6	1.8	59.1	62.2
3	COL	3.0	38.5	77.4	5.2	1.6	60.7	74.2

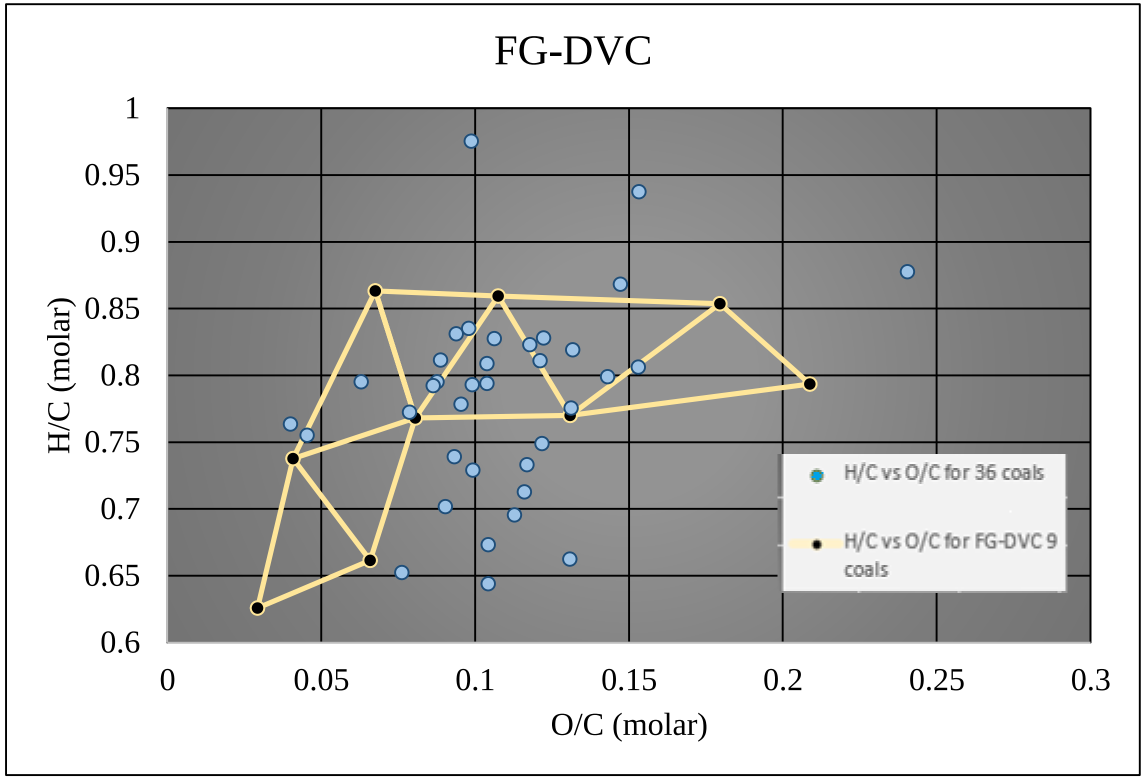
Coal origins, properties and high temperature wire mesh test results[9].

[9]. C. K. Man, J. R. Gibbins, J. G. Witkamp, and J. Zhang, "Coal characterisation for NOx prediction in air-staged combustion of pulverised coals," in *Fuel*, 2005, vol. 84, no. 17, pp. 2190–2195.

3.2 Comparison of the interpolating coals

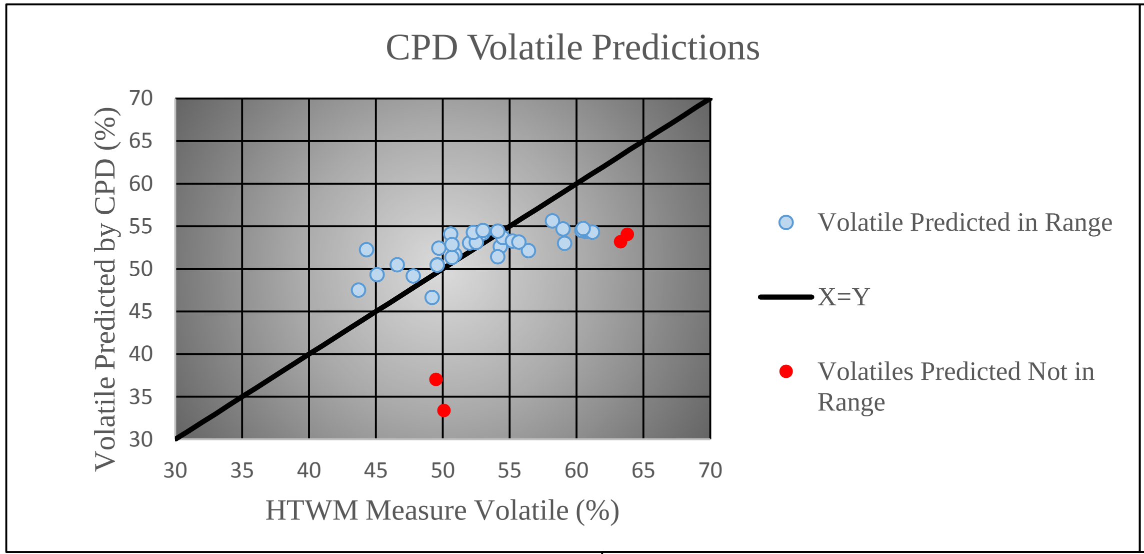


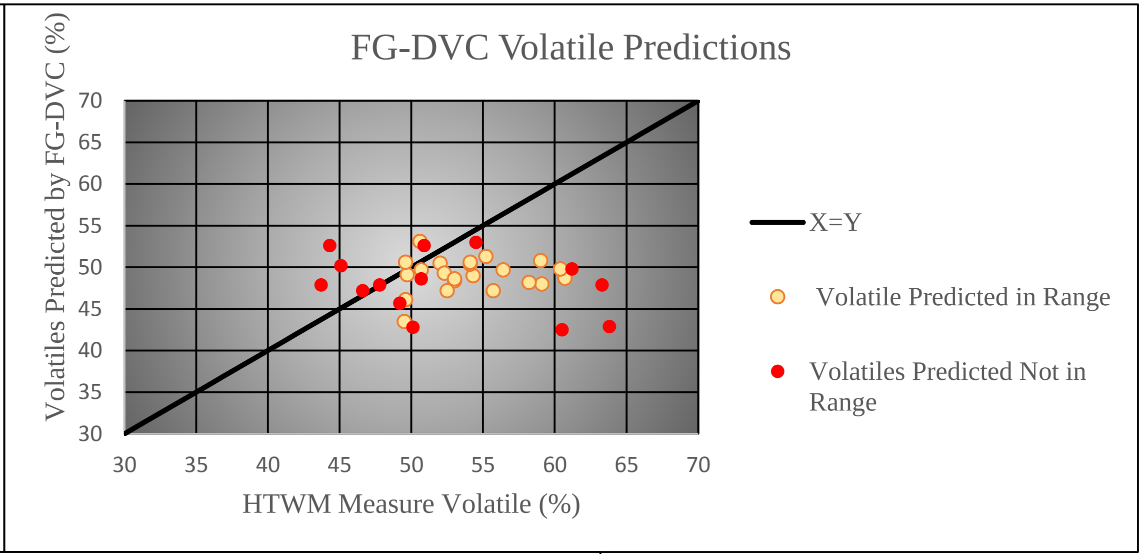
Coalification chart of the 30 coals used for the CPD and the coals under investigation

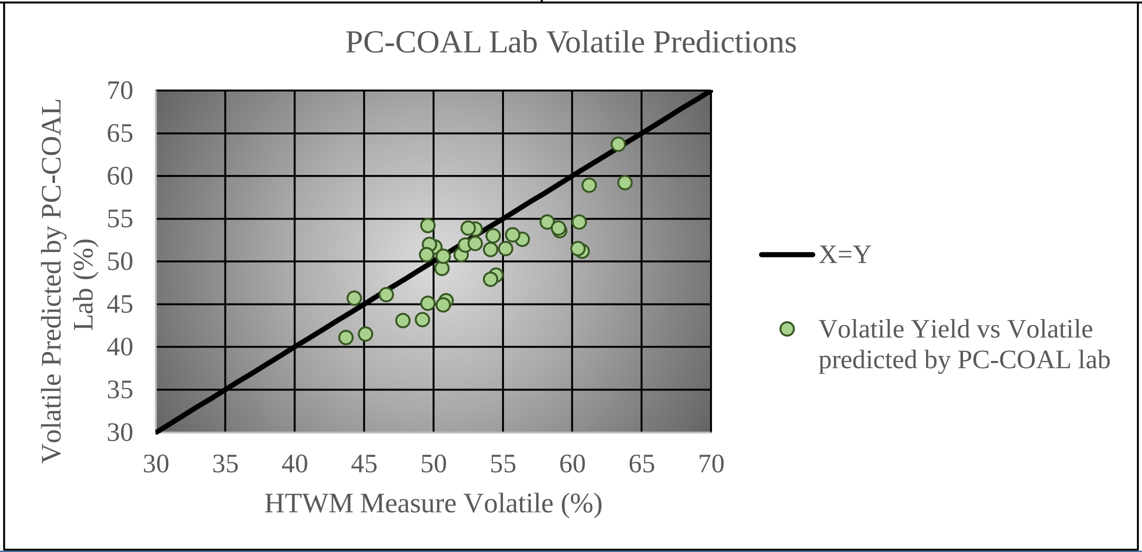


Position of the 36 coals on the triangular mesh of the FG-DVC.

3.3 High Temperature Volatiles Predictions

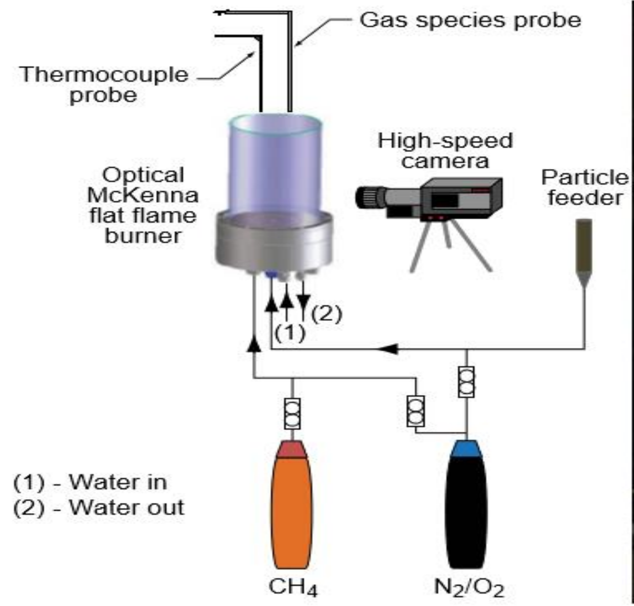


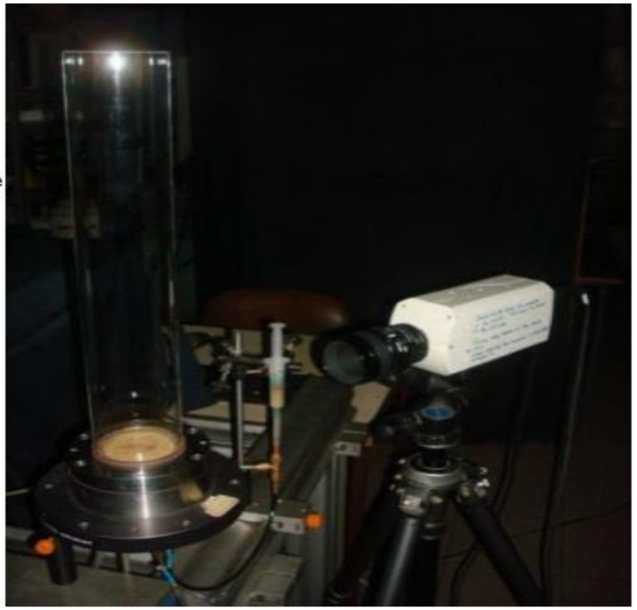




4. Single particle Ignition modelling

4.1 Experimental data for the coal [8]





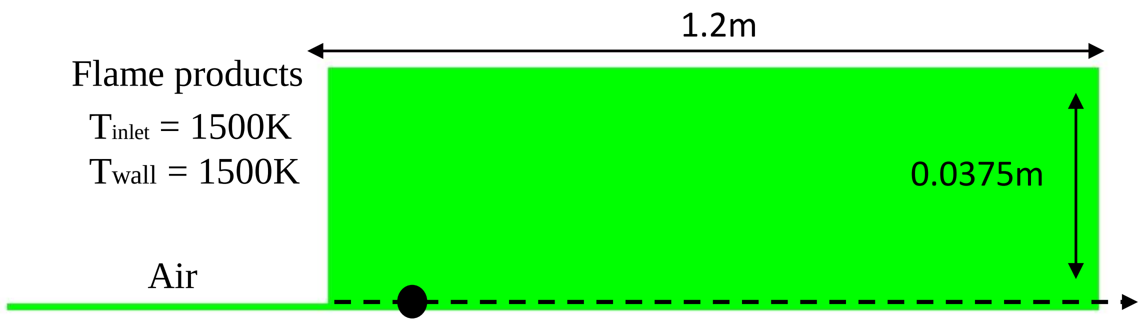
Fuel type	Density(kg/m^3)	Specific heat(J/kgK)	Diameter(μm)
Bituminous coal	1300	1680	80-90

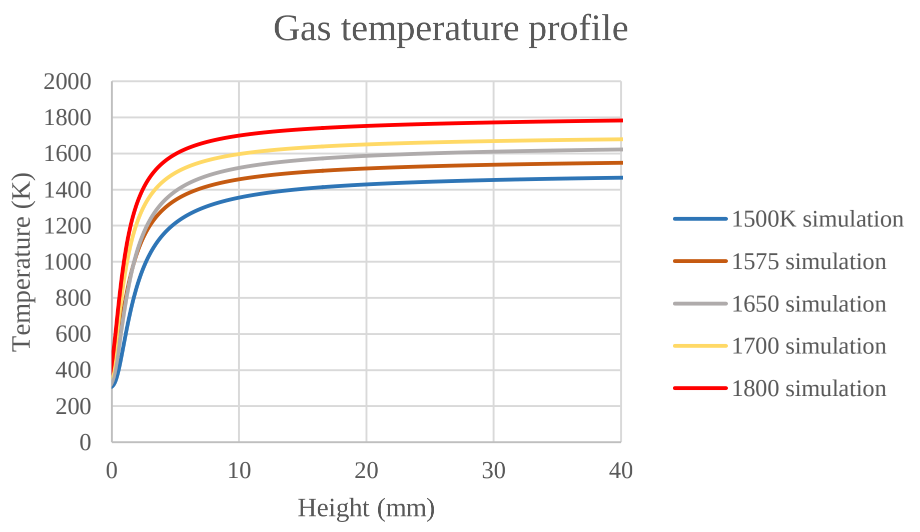
Parameter	Pine bark	Wheat straw	Bituminous coal
Proximate (wt % as received)			
Moisture	13.9	8.9	**1.6**
Volatile matter	58.9	64.9	**37.6**
Fixed carbon	25.9	11.5	**58.8**
Ash	1.3	14.7	**2.0**
Ultimate (wt% as received)			
Carbon	47.8	39.4	**76.9**
Hydrogen	4.3	5.2	**5.1**
Nitrogen	0.3	0.5	**1.6**
Sulphur	<0.02	<0.02	**0.7**
Oxygen	32.4	31.3	**12.1**
Low heating value(MJ/kg)	17.1	18.8	**32.7**

[8] de Barros Magalhãe, Duarte Nuno Matos. "Ignition behaviour of single biomass and coal particles." *European Combustion Meeting*. 2003.

4.2 Fluent case

- 2D Axisymmetric geometry
- 338783 cells, structured mesh
- Maximum aspect ratio 7.7
- URANS
- Viscous model: Laminar
- Reactions: Volumetric, 2-step
- Turbulence –Chemistry Interaction: Finite rate
- Devolatilisation Model: CPD
- Volatiles composition: $C_xH_yO_zN_aS_b$





Operating conditions

Parameter	Test 1	Test 2	Test 3	Test 4	Test 5
Thermal input (kW)	0.6	0.8	1	1.7	2
Methane flow rate (dm^3/min)	1.1	1.4	1.9	3	3.5
Transport air flow rate (dm^3/min)			0.14		
Primary air flow rate (dm^3/min)	15.5	19	25.1	40.5	47.5
Excess air coefficient (λ)			1.4		
Mean gas temperature in the ignition zone (K)	1500	1575	1650	1700	1800
Mean O_2 concentration in the ignition zone (dry vol. %)			7.6		

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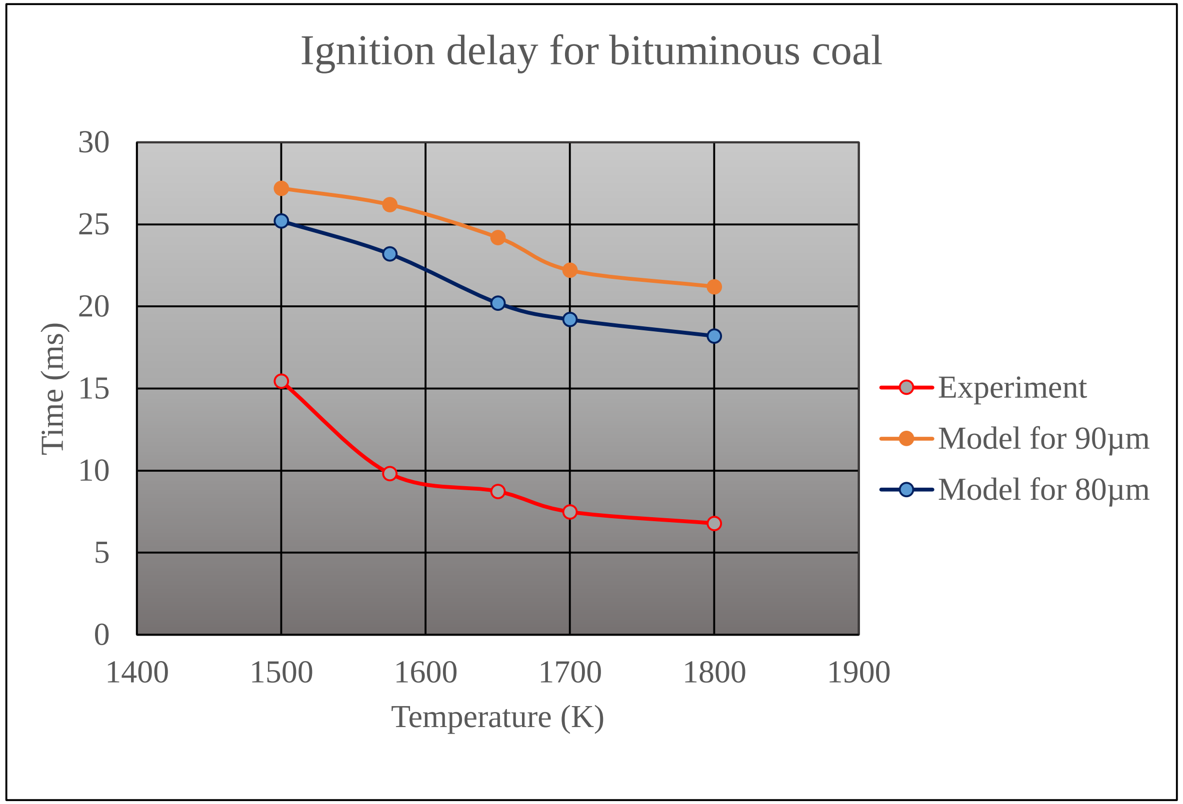
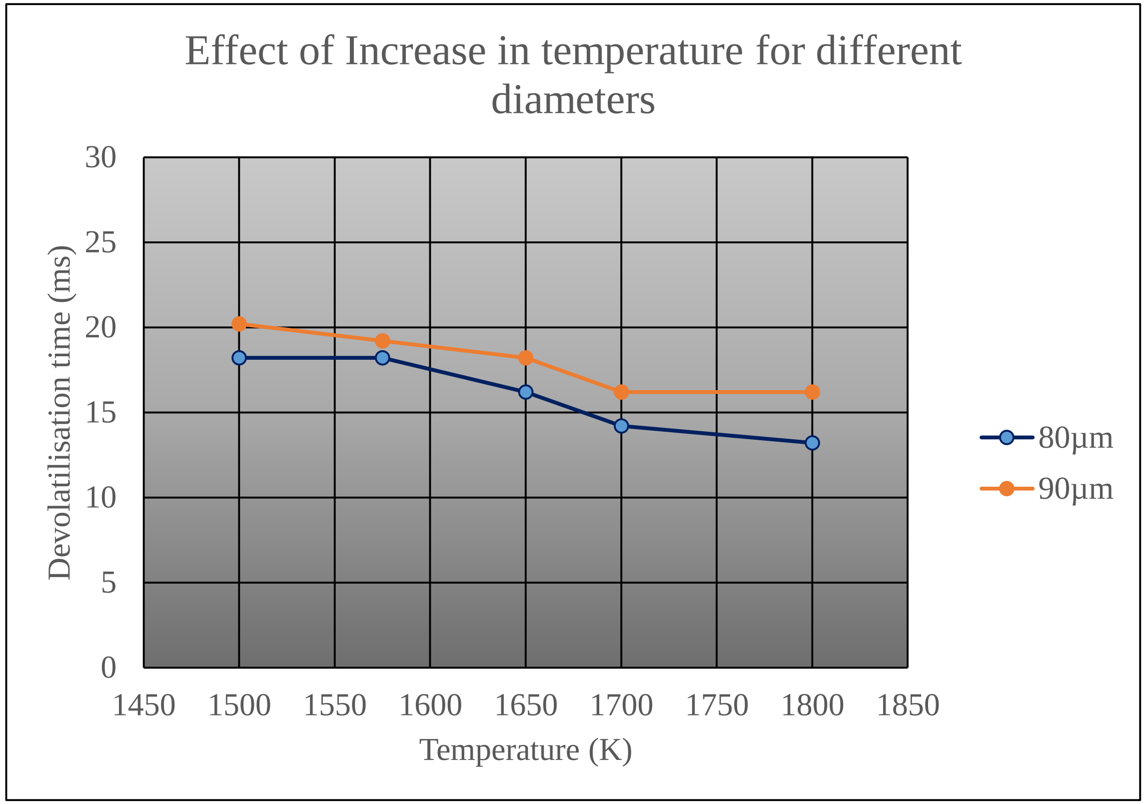
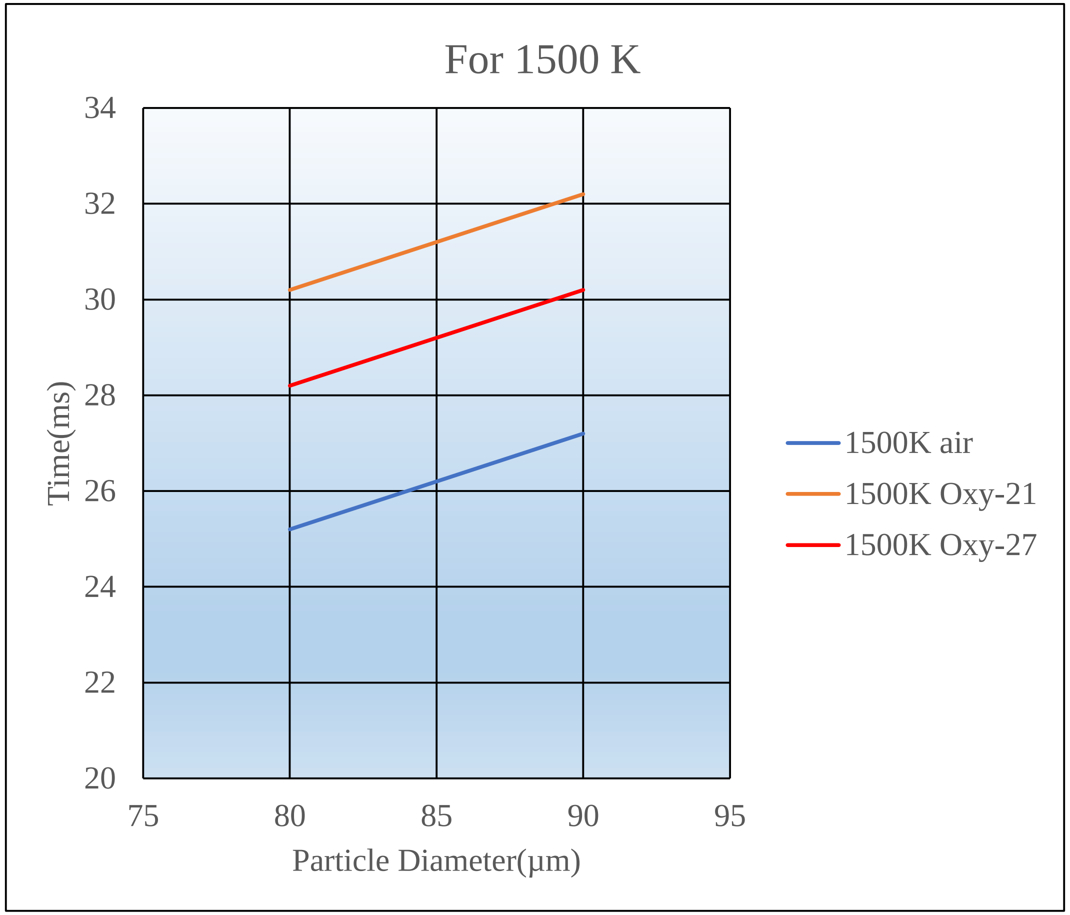
4.3 Results for ignition delay

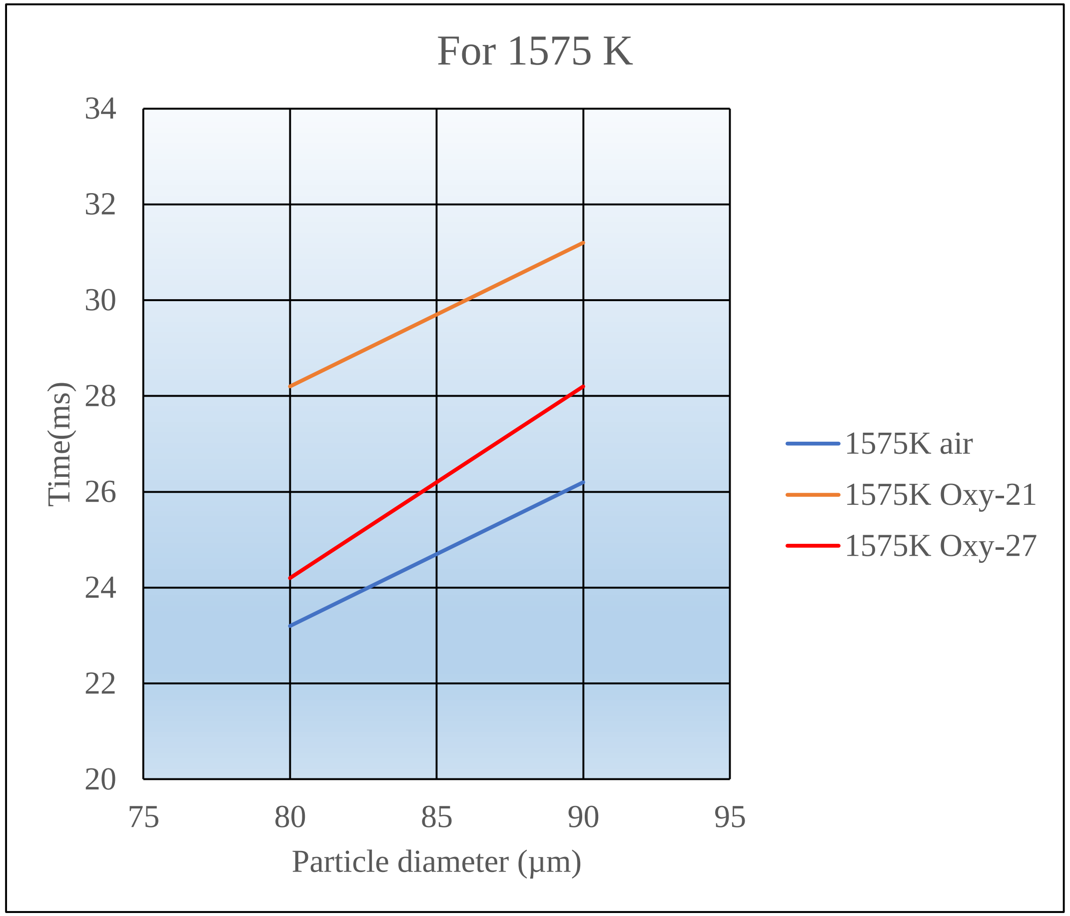




Ignition was detected based on initiation of CO

4.4 Impact of Oxy-fuel conditions





5. Conclusion and further work

- Three network models for predicting devolatilisation behaviour of coals has been evaluated and compared against experimental data of 36 different coals.
- The PC-Coal Lab covers a wider range of coals for correlation compared to the other two models whereas the FG-DVC accommodates very few coals, thus making it the least effective model for investigating the devolatilisation behaviour of coals.
- The numerical model is capable of predicting the ignition trends when compared to experiments for variation in gas temperature.
- The model is also capable to predict trends on switching from air to oxy-fuel.

Further work

- To simulate heterogenous ignition.
- Include more reactions to improve the accuracy of the ignition point.
- Validate the model for variation in size and solid fuels such as biomass.

Thank you for listening

Questions?