

An Indian-Australian research partnership

Project Title: **Mathematical modelling of fine ash particulate formation during oxy-fuel combustion of low-rank coal**

Project Number **IMURA0212**

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Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address?

(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1. **Advanced computational engineering, simulation and manufacture**
2. Infrastructure Engineering
3. **Clean Energy**
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research

The Research Problem

Define the problem

Coal combustion is the major way for power generation in both Australia and India. The ash formation is a major concern during coal combustion, potentially causing corrosion, slagging and fouling in the coal-fired furnace. Moreover, the ultra-fine/fine ash particulates formed pose significant environmental impact, due to the enrichment of toxic and carcinogenic heavy metals which are readily inhaled by the human beings. Shifting coal combustion in air to O₂/CO₂ mixture (*i.e.* oxy-fuel combustion) is one promising technology for mitigation of greenhouse gas emissions from coal combustion. The ash formation in oxy-fuel process is however still less understood. As the specific heat capacity of CO₂ is far larger than that of N₂, a lower flame/particle temperature is expected at the same O₂ content in O₂/CO₂ than in O₂/N₂. Accordingly, the vaporisation extent of ash within char matrix would be reduced. Moreover, as the mean free path of CO₂ is smaller than that of N₂, the collision frequency among primary nuclei of ash would be lessened, and hence, the ash formed in oxy-fuel mode would be eventually smaller than in air. Systematic investigation has not been conducted to elucidate these problems. Failing to do it would cause significant risk during retrofitting existing power generation plants with oxy-fuel combustion technology. The new problems relating to slagging/fouling and environmental pollutant release could occur.

Project aims

Define the aims of the project

This project aims to employ mathematical modelling to complement the ongoing experimental works in Monash to predict fine ash particulate formation during oxy-fuel combustion of a variety of low-rank coal samples. Particularly, the partitioning of two basic metals (Na, Ca) and their interaction with SO₂, HCl and refractory metals (Si, Al) will be modelled. The thermodynamic properties and kinetic/rate of two major routes including the vaporisation of metals and the coagulation of metallic vapours in N₂ versus CO₂ will be mainly modelled. Influence of gas impurities (HCl, SO₂ and steam) on the vaporisation of metals will also be modelled and compared with the experimental observations.

Expected outcomes

Highlight the expected outcomes of the project

Through the completion of this project, advanced mathematical model regarding oxy-fuel ash formation will be developed. Publication of two-three high quality papers in internationally renowned journals is desirable.

Capabilities and Degrees Required

List the ideal set (up to 8) of background and capabilities required in a student for this project noting that the more specific you make it, the less likely that you will get a candidate that matches the requirements exactly.

The potential candidate is expected to have the following background and/or research capabilities:

- 1) Bachelor degree of chemical engineering or chemistry.
- 2) Background knowledge regarding coal chemistry, inorganic minerals and phase diagram.
- 3) Familiar with a variety of programming softwares such as Fortran or C++.
- 4) Interested in clean energy research.