Case Study 3

1. Title of Case Study: High-fidelity simulation study of turbulent solid-fuel combustion and emissions

2. Grant Reference Number: IE150727 (Royal Society); EP/K025171/1 (EPSRC).

3. One sentence summary: Alkali-metal minor-species formation and dynamics in turbulent solid-fuel combustion has been investigated by incorporating tabulated detailed alkali metal chemistry in high-fidelity simulation of the gas-solid two-phase flame, for the first time.

4. One paragraph summary: Turbulent solid-fuel combustion occurs in a variety of power-generating combustion devices burning coal, biomass or their blends. Alkali metal minor-species emissions, including sodium species rich in some coal and potassium species usually rich in biomass, accelerate ash deposition on heat exchanging surfaces and degrade heat transfer efficiency, thus leading to severe operating issues of the industrial combustion devices. Although global combustion characteristics of a turbulent gaseous flame can be reasonably predicted nowadays, reacting dynamics of minor species in a turbulent multiphase flame is still an open challenge. In this work. A detailed sodium chemistry has been tabulated and incorporated into high-fidelity simulation of a turbulent pulverised-coal flame. This first attempt has made numerical experiments of minor species formation and reacting dynamics prediction possible in laboratory- and industrial-scale turbulent solid-fuel combustion.

5. Key outputs in bullet points:

(1) K.D. Wan, J. Xia, L. Vervisch, Z.H. Wang, K.F. Cen, "Modeling alkali metal emissions in large-eddy simulation of a preheated pulverized-coal turbulent jet flame using tabulated chemistry", **Combust. Theory Modelling**, under review.

(2) K.D. Wan, J. Xia, Z.H. Wang, M. Pourkashanian, K.F. Cen, "Large-eddy simulation of pilot-assisted pulverized-coal combustion in a weakly turbulent jet", **Flow Turbulence Combust.**, revision submitted.

(3) K.D. Wan, J. Xia, Z.H. Wang, L.C. Wrobel, K.F. Cen, "Online-CPD-coupled large-eddy simulation of pulverized-coal pyrolysis in a hot turbulent nitrogen jet", **Combust. Sci. Tech.** 189 (2017) 103–131.

(4) K.D. Wan, Z.H. Wang, Y. He, J. Xia, Z.J. Zhou, J.H. Zhou, K.F. Cen, "Experimental and modeling study of pyrolysis of coal, biomass and blended coal-biomass particles", **Fuel** 139 (2015) 356–364.

6. Main body text

In both the UK and China, burning solid fuel such as coal, biomass and their blends produces a considerable proportion of power and energy. Solid fuel properties are complex and therefore the prediction of solid fuel combustion is difficult. For coal and biomass, the burning starts with pyrolysis, which is thermal decomposition due to heating, and then gaseous volatile and solid char combustion. Since volatile species production during pyrolysis is an important initial condition for solid-fuel combustion, an advanced pyrolysis model, the chemical percolation devolatilization model [4], has been directly incorporated into a large-eddy simulation solver, in order to better predict gaseous volatile species production in real time [2,3]. Prediction of alkali metal emissions during high-sodium coal burning is then attempted for the first time thanks to collaborations with leading scientists in China and France, and computing support via EPSRC-funded UKCTRF. This is achieved through tabulating a detailed chemistry of sodium species upon local initial conditions for sodium reactions determined by turbulent gas-phase combustion [1]. Although important assumptions and simplifications have been made, this work has enabled future high-fidelity simulation studies on properly predicting combustion characteristics and emissions of laboratory- and industrial-scale turbulent solid-fuel combustion using high-fidelity simulation techniques.

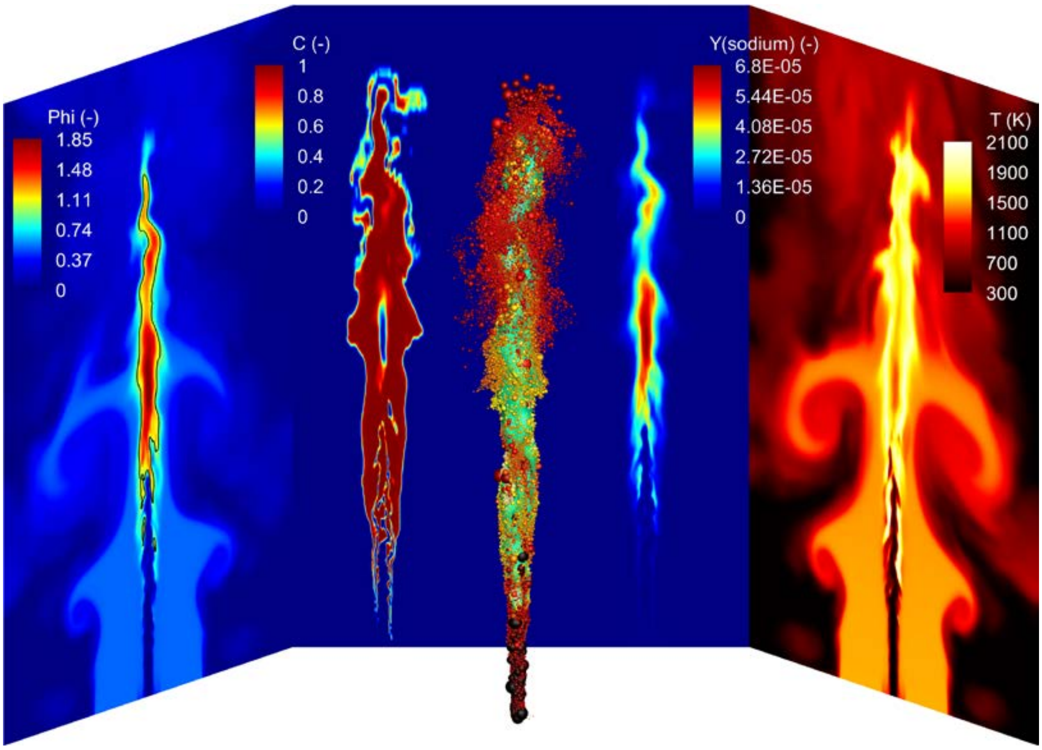

Figure 1: Sodium chemistry tabulation in LES of a weakly turbulent preheated pulverised-coal jet flame [1]. The four planes show a snapshot of the equivalence ratio Φ, the progress variable C, the mass fraction of the sodium element Y_{Na}, and the gas-phase temperature T_g: the four coordinates of the chemical lookup table for a subset of a detailed sodium chemistry. The 3D plot shows the coal-particle distribution with particle size and temperature information and the $Y_{NaOH}=2\times10^{-5}$ iso-surface.

7. Names of key academics and any collaborators:

(1) Academic: Dr J. Xia, Brunel University London;

(2) PhD researcher: Dr K.D. Wan, Brunel University London & Zhejiang University;

(3) Collaborators: (a) Profs Z.H. Wang & K.F. Cen, State Key Laboratory of Clean Energy Utilization, Zhejiang University, China; (b) Prof L. Vervisch, INSA de Rouen & CORIA – CNRS, France.

8. Sources of significant sponsorship (if applicable): N/A

9. Who should we contact for more information? Dr Jun Xia; jun.xia@brunel.ac.uk; 01895 265 433.

10. Please indicate if you would like this case study to be included on the Consortium's ARCHER web-page. Yes