International Collaboration on Computational Modelling of Fluidised Bed Systems for Clean Energy Technologies (iComFluid)

*Final Publishable Summary Report*

iComFluid was a EU-Asia-Africa-North America network for fluidised bed technology research by uniting activities among top ranking European, Indian, Chinese, South African and American universities. A combination of Early Stage Career and Established Researchers were exchanged and trained on latest techniques covering the full range of thermal conversion for clean energy generation. iComFluid has successfully set foundations for long-term strategic collaboration between involved universities to work on the challenge of climate change and clean energy generation in a global framework. iComFluid aimed at researching in particular modelling of fast and catalytic pyrolysis, gasification and co-firing, targeting to fulfil a series of objectives that would significantly benefit the existing body of knowledge and inspire future research. A short description of the scope and outcome is included in this summary report.

Fluidised bed technologies concern the phenomenon of mixing a solid particulate substance (feedstock and inert bed materials) within a pressurised fluid (carrier gas) to lead to a behaviour of the mixture as a fluid, harvesting the benefits of properties and characteristics of normal fluids. Fluidised bed reactors are configurations employed to perform multiphase chemical reactions such as combustion, gasification or pyrolysis. In such systems, high velocities are applied to the low density carrier gas in order to enable suspension of the high density solid particles, and hence perform the process as involving fluid elements. Advantages of fluidised bed reactors include the uniformity of particle mixing and effective heat transfer, enabling rapid heating of the solid particles, uniform temperature gradient, and operation at continuous mode. Such technologies have been applied in a series of applications including coal-fired power plants, oil and bio-oil refinery plants, and food, pharmaceutical and biochemical industrial processes. Current research focuses on the interaction of the feedstock particles and the bed material, and the reduction of reactor size as well as increasing the efficiency of operation.

In fast pyrolysis, biomass is converted in a single step into liquid bio-oil that can be used as a substitute for conventional fossil fuels and precursor for chemical production. Fluidised bed reactors are regarded as the most suitable equipment for biomass fast pyrolysis and with the highest market attractiveness. Computational modelling of biomass fast pyrolysis in fluidised bed reactors can greatly aid the process equipment design and scale-up by identifying the key parameters that affect the process. During the project, integrated computational models were developed by incorporating chemical kinetics for different biomass feedstocks, followed by a parametric study to investigate the effect of biomass particle type and size and temperature on the product yields. A comparative study of yield prediction including global and advanced kinetic schemes helps to improve the understanding of the performance of fluidised beds at industrial scale. Further, the physical phenomena occurring within fast pyrolysis fluidised bed reactors were investigated through employing a 3-parameter shrinkage model. The model was used to calculate the particle shrinking rate and the variations of the apparent density of the biomass particles during the pyrolysis process. This model addresses the physical changes of the biomass particles during fast pyrolysis and gives detailed information of the effect of those changes on the fluid dynamics within the fluidized bed. Results from the model can therefore help to optimise the real fluidized bed operating parameters in the industry. The effects of different tube shapes on the flow characteristics and local heat transfer coefficients were also investigated and the time-averaged heat-transfer coefficient was compared with the experimental data in the literature. These were found to be in the same order as the experimental data which indicates that the project results can be quantitatively employed to aid the configuration of heating tubes during industrial design of the fluidized bed reactors. Finally, advanced modelling techniques for liquid collection systems (LCS) were studied through developing models which can significantly aid in the design and optimization of different types of LCSs and enhance understanding towards eliminating the flooding phenomena for future pilot or industrial scale applications.

The bio-oils produced from fast pyrolysis have high oxygen content and make them unsuitable as transportation fuels without applying further upgrading. Catalytic pyrolysis is one of the methods developed to produce better quality liquid fuels directly from the thermochemical conversion process. The major difference with conventional fast pyrolysis is that the bed material contains an amount of catalyst for the reforming and cracking of the oxygenated heavy molecular weight components of bio-oil, resulting in a less oxygenated final liquid product. The quantity and quality of the final bio-oil and gas products depend on the presence and type of catalyst. Computational modelling of the catalytic pyrolysis process greatly enhances our understanding of the major parameters that affect the process. By applying kinetic mechanisms developed for different catalysts we are able to identify the optimum reactor operating conditions as well as predict the final bio-oil and gas yields and composition. Through numerical simulations on the effect of catalysts a new technology has been explored in this project to use fluidised bed system with reduced pressure which aims at reducing H2 consumption and more importantly the deactivation of catalysts. The CFD model developed has demonstrated good performance of fluidised bed reactors with in-situ catalytic upgrading. Physical phenomena occurring in catalytic fast pyrolysis fluidised bed reactors have also been investigated together with a study on the effect of catalyst type and amount on the final bio-oil composition and yields. This study has allowed identifying the best catalyst for producing aromatic monomers from lignin. A parametric study for optimum bio-oil and gas yields production has shown that the heterogeneous upgrading reactions can perform significant effects on the hydrodynamics of fluidised beds, while different space time, and the ratio of catalyst mass to bio-oil precursors flow rate vary the yield distribution of products. New reactor concepts have also been investigated.

Gasification is the most effective thermochemical process for the conversion of solid fuels into combustible gases (syngas), and into liquids through further catalytic conversion of syngas. In gasification, an oxydising medium of reaction is required which can oxygen (below stoichiometric ration), steam, carbon dioxide, hydrogen or a combination of them; supercritical water can also be used. Depending on the type of feedstock, gasifying medium, plant operating parameters and configuration, final product composition and purity vary. Computational modelling of gasification process can strengthen our understanding of the major heat, momentum and mass transport phenomena occurring in fluidised beds applied to gasification, enabling us to optimise the process by conducting various parametric studies. Also, computational modelling aids the development of advanced syngas purification technologies, which are current bottlenecks for the deployment of biomass gasification technologies. Fluidised bed gasification for biomass is still relatively new development and the majority of technology development has yet moved into demonstration scale. Circulating fluidised bed (CFB) gasifiers have solid’s residence times up to 30 minutes, allowing them to achieve high gasification yields at lower temperatures than those used in well-established coal-fed entrained flow gasifiers. This is critical for the operation of biomass gasifiers in order to avoid ash melting and, consequently, improving system reliability and energy efficiency. Additionally, CFB gasifiers can achieve very high gasification yields (over 95%) for reactive fossil fuels such as subbituminous coal and lignite. As part of the project, an extensive review for mathematical modelling applied to the fluidised bed gasification systems was completed and these models were broadly classified as equilibrium and kinetic models. A multiphase CFD model for fluidised bed gasification was developed and applied for chemical looping combustion (CLC) processes to describe physical and chemical phenomena. However, the model predictions for continuous CLC process operations were not satisfactory, and the modelling methods could be improved. CFD models for in-situ gasification chemical-looping combustion (iG-CLC) including reactor fluid dynamics, and the reaction kinetics for the gasification of coal with oxygen as carrier gas were developed. The model was validated by comparing the species concentration at the reactor outlet with literature experimental data. Then results were discussed in terms of fluid dynamics of fuel reactor, concentration of various species, conversion of char and oxygen carrier in the reactor. A multi-fluid CFD model of the desulphurization process within a bubbling fluidized bed coal gasifier was also established using one gaseous phase and five particulate phases; devolatilization, heterogeneous, and homogeneous chemical reactions as well as calcination and desulphurization reactions were incorporated.

In an attempt to minimise greenhouse gases, NOx and SOx emissions, the development of coal and biomass co-firing facilities have been greatly encouraged as it is one of the most economically attractive method for reducing pollutant emissions. Co-firing consists on the combustion of biomass alongside coal for heat and power generation. Due to the lower nitrogen and sulphur content of biomass, co-firing emissions are significantly reduced. It also leads to the substitution of fossil fuels and a net reduction of CO2 emissions. Fluidised bed co-firing appears to be an attractive system, since it is a more flexible technology in dealing with the fouling and slagging issues that ash from biomass usually causes. Computational modelling of coal and biomass co-firing in fluidised beds can greatly enhance our knowledge and understanding of the complex thermochemical phenomena occurring in this type of systems. Parametric studies can identify the limits of operation conditions of such systems and the maximum blending percentages of coal and biomass for high efficiency unit operation with minimal changes to the exiting fossil-based infrastructure. Experiments on CFB were carried out as part of this project, observing that the operating pressure has significant effect on the hydrodynamics parameters of bed pressure drop and axial bed voidage profiles. The effect of aeration rate on bed hydrodynamics in the riser of a pressurized circulating fluidized bed (PCFB) has been studied and it was found that the suspension density increases along the riser height with the decrease in aeration rate; the solid circulation rate increases with the increase in aeration rate as well as primary air flow rate. As an additional objective, fluidised bed carbon capture reactors using new materials were also investigated.