Case Study Template

1. Title of Case Study: Soot formation in turbulent flames

2. Grant Reference Number: EP/K026801/1

3. One sentence summary: This case study is about the development of comprehensive models for soot formation in turbulent flames, taking rigorously into account the soot – turbulence interaction.

4. One paragraph summary: Soot is particulate matter emitted from a variety of practical combustion devices such as diesel engines and gas turbines and can have particularly hazardous impact on public health, including respiratory problems and carcinogenic potential. On the other hand, in furnace combustion soot formation is desirable because it enhances the heat transfer rate through radiation, although it must still not be emitted. In the analysis of soot, the particle size distribution is of paramount importance because particles of different sizes have different properties and hazardous potential, and new regulations impose strict limits on the number of particles of different sizes emitted. The distribution can be modelled with the aid of the Population Balance Equation (PBE), but the numerical solution of this equation and its coupling with methods for modelling turbulent combustion poses major challenges. Our research group has been working over several years on developing methods that aim at resolving these issues and developing a complete method for the comprehensive modelling of sooting flames and combustion devices. The objectives are: a) to be able to predict soot formation and the full distribution (as opposed to a few properties such as number density and volume fraction) and b) to account correctly for the interaction of soot formation and turbulence in turbulent combustion.

5. Key outputs in bullet points:

- Development of a comprehensive approach for modelling the soot-turbulence interaction in turbulent flames that involves coupling the Population Balance Equation (PBE) with transported Probability Density Function (PDF) methods and Stochastic Fields, for prediction of the soot particle size distribution in turbulent flames.
- Development of a novel solution method for the Population Balance Equation (PBE).
- So far 9 journal and 11 conference papers, several more in preparation.

6. Main body text: Soot is particulate matter emitted from a variety of practical combustion devices such as diesel engines and gas turbines and can have particularly hazardous impact on public health, including respiratory problems and carcinogenic potential. New and more stringent regulations are constantly imposed on the manufacturers of combustion devices for reducing soot. On the other hand, in furnace combustion soot formation is desirable because it enhances the heat transfer rate through radiation, although again it must be fully consumed before the exhaust is emitted to the atmosphere. In the analysis of soot, the particle size distribution is of paramount importance. Particles of different sizes have different properties and hazardous potential. Traditionally, soot prediction and mitigation focussed solely on the prediction of soot mass fraction, and measurement methods such as soot filters collected only the larger particles. New regulations, however, impose strict limits on the number of particles of different sizes emitted. Furthermore, accurate knowledge of the distribution enables correct prediction of the soot formation and radiation rates, important in furnace combustion. The distribution can be modelled with the aid of the Population Balance Equation (PBE), a transport equation that relates the evolution of the particle number density to the kinetics of the fundamental processes that determine it, such as particle formation and growth. It is an integro-differential equation whose solution poses significant mathematical and numerical problems. Certain simplified methods can be applied in cases where the distribution shape can be assumed, but this is often not possible in soot and discretisation methods are appropriate. In its basic form, the PBE describes a homogeneous system, such as a perfectly stirred reactor. In an inhomogeneous system, however, the PBE must be coupled with fluid dynamics. Furthermore, the particle formation mechanisms are dependent on the local chemical environment, so the species transport equations must be solved as well. This gives rise to important theoretical and computational problems related to the coupling of turbulent flow and particle formation, where unclosed terms result. Our research group has been working over several years on a number of methods that aim at resolving these issues and developing a complete method for the comprehensive modelling of sooting flames and combustion devices. The objectives are: a) to be able to predict soot formation and the full dsistribution (as opposed to a few properties such as number density and volume fraction) and b) to account correctly for the interaction of soot formation and turbulence in turbulent combustion. Two important developments have resulted from our work. The first one is the developing of a method that deals with the numerical solution of a time-dependent PBE and which has been validated against a variety of analytical solutions. A recent development is the formulation of an adaptive grid approach that maps the number density to a reference space. This approach allows using a minimum number of discretised number densities, while attaining accuracy and covering a wide range of particle sizes. The second major development is a method that addresses the turbulence-soot closure problem: the population balance equation – probability density function (PBE-PDF) approach, based on a transport equation for the joint pdf of both reactive scalars and particle number density. The major advantage of this approach is that it overcomes the need for closure of the unresolved correlations. The method has been coupled with Large-Eddy Simulation (LES) of turbulent flames, an approach that allows for greater detail in the resolution of the flow structure in turbulent combustion and therefore greater accuracy in the overall combustion simulation. The coupling has been accomplished with the Stochastic Field method, a numerical method that takes into account the probability density function of the transported scalars. The LES-PBE-PDF approach simulations were carried out in the ARCHER UK National Supercomputing Service (http://www.archer.ac.uk), which we duly acknowledge. The availability of the ARCHER resource to our group was through the UK Consortium on Turbulent Reacting Flows (UKCTRF), through which we have had the opportunity for fruitful interactions with the combustion community and development of collaborations.

7. Names of key academics and any collaborators: Dr Stelios Rigopoulos (leading), Dr Ben Williams (collaborator), Dr Salvador Navarro-Martinez (collaborator), Dr George Papadakis (collaborator), Dr Fabian Sewerin (initially PhD student, now collaborator as an academic in Germany)

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9. Who should we contact for more information? Dr Stelios Rigopoulos, Imperial College, s.rigopoulos@imperial.ac.uk, 02075947108

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