Institution: Oxford Brookes University

Unit of Assessment: 12, Engineering

Title of case study: Robust and reliable digitalisation of the automotive industry: improvements in 3D CFD modelling to help reduce particulate matter emissions

Period when the underpinning research was undertaken: 2014–2020

Details of staff conducting the underpinning research from the submitting unit:

Name(s):	Role(s) (e.g. job title):	Period(s) employed by submitting HEI:
Fabrizio Bonatesta	Reader	[text removed for publication]
Denise Morrey	Professor	
Changho Yang	Senior Lecturer	
Edward Hopkins	Research Assistant	
Davide Sciortino	Research Assistant	
Federico Biagiotti	Research Assistant	

Period when the claimed impact occurred: 2019–2020

Is this case study continued from a case study submitted in 2014? No

1. Summary of the impact

Exposure to small particulate matter (PM) emitted by engines causes more than 4 million premature deaths worldwide every year. Modern gasoline direct injection (GDI) engines are used in road transportation and are particularly problematic because they produce large numbers of ultra-fine particles. New EU regulations strictly limiting PM emissions mean traditional engine manufacturers must now find ways to reduce them, and in turn reduce the global health risk.

The Engine Modelling Team (EMT) at Oxford Brookes University (OBU) has developed new knowledge about the way soot forms in GDI engines, along with novel 3D computational fluid dynamics (CFD) models of these engines. These have led to a shift in practice for one global engine manufacturer and the supporting industry. By proving the concept of 'Limiting Temperatures for the Retainment of Liquid Film' and innovative technical solutions, the EMT have enabled Ford Motor Company to appreciate the full extent to which fuel puddling over the piston crown affects soot generation, leading the company to investigate new piston technologies and control approaches. The EMT also developed the most accurate GDI engine modelling framework available through commercial engine modelling software platforms. Major companies Siemens DISW and Ricardo Software are now embedding this framework into their software releases.

2. Underpinning research

The growth of digital engineering is a priority, according to the latest UK Automotive Council roadmaps (2017). This is to reduce the need for hardware testing, and instead use multi-physics software simulation tools. Since 2014 the EMT at OBU, led by Dr Fabrizio Bonatesta, has been collaborating with the Ford Motor Company, Siemens DISW (formerly CD-adapco) and more recently Ricardo Software to support the further growth of modelling tools for the automotive industry. They have concentrated on developing models for the simulation of GDI engines within industry-standard Computer-Assisted Engineering (CAE) software environments **[R1 to R4]**, with a primary focus on improving understanding of the mechanisms leading to PM formation **[R1 to R6]**.

DynAMO (dynamic analysis modelling and optimisation of GDI engines) is a Ford-led collaborative R&D project involving OBU, Loughborough University, Bath University, Sheffield University, Siemens DISW, Ricardo, STFC Hartree Centre, Cambustion and HSSMI, co-sponsored by Advanced Propulsion Centre – APC6 Call (TSB Ref. 78938-506185, GBP11,026,753, 2017–2021, total project cost: GBP22,000,000 – 50% industry funded). As part of the first phase of the

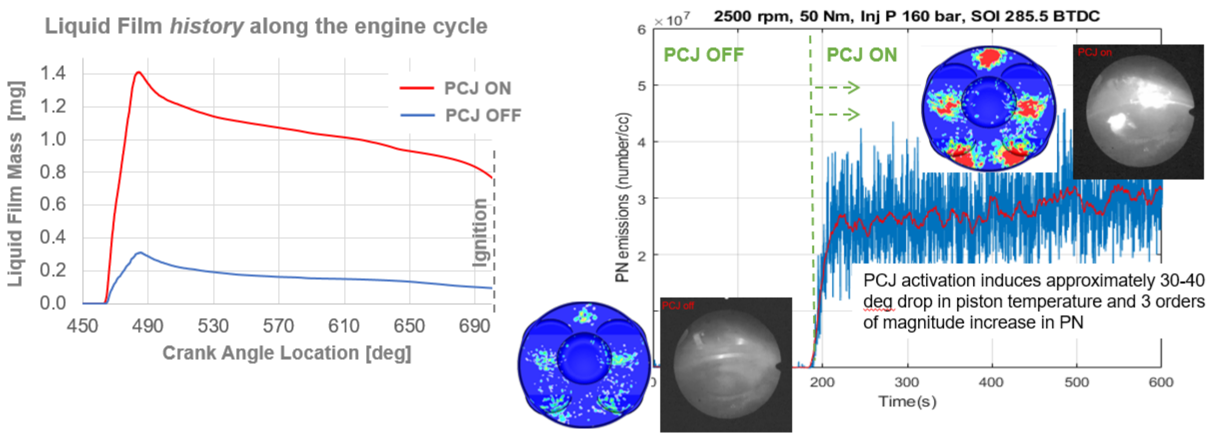
DynAMO project (2017–2019), the OBU team focused on CFD model development **[R3, R4]**. They proposed novel approaches for the calibration of spray and combustion models, based on design of experiment (DoE) and multi-objective optimisation techniques. They also proposed a new robust methodology to accurately model liquid film formation and evolution across wide ranges of engine operating conditions.

Nano-size particles are liable to form in large quantities especially during engine warm-up and transient operation (such as acceleration). The EMT work has shown that pooling of liquid within the combustion chamber is responsible for the emission of nano-size carbon particles in these phases. It also identified the cylinder wall/piston temperature as the factor most likely to lead to the build-up of liquid fuel ‘film’ in small-capacity spray-guided GDI engines operating in stoichiometric mode **[R4]**.

The OBU team used sophisticated spray, surrogate fuel and heat transfer models to establish how the piston surface temperature affects the spray-to-wall impingement and evaporation regimes. These result in variable levels of liquid film being present at the beginning of the combustion process. The modelling has shown that under mid to high engine load, with common gasoline fuel, surface temperatures above 230°C ensure there is little liquid film before combustion. However, the practice of piston cooling, operated through Piston Cooling Jets (PCJ) with the sole concern of material safety, may prevent the piston surface from operating at or above this safe temperature threshold.

The OBU team introduced the concept of ‘Limiting Temperatures for the Retainment of Liquid Film’ **[R4]**, which also explains the surge in particle number (PN) emissions typically seen while operating a modern GDI engine in transient mode – for example during acceleration. Due to the relatively long thermal transient of the piston top surface, a sudden increase in engine load can result in piston temperatures being too low, leading to large deposits of liquid film. In turn, the burning of this liquid (pool-fire) generates vast PN emissions. Model validation laboratory tests, instigated by the OBU results, have shown how even relatively small reductions in piston temperature of 30–40°C, as a result of PCJ activation, lead to increases in PN of up to four orders of magnitude.

The figure below shows the influence of PCJ activation, at an engine speed of 2500 rpm and a torque of 50 Nm. As shown by the OBU modelled liquid film profiles and corresponding images at spark timing, PCJ activation decreases piston surface temperature by about 30–40°C, generating large puddles of liquid in the spray-to-wall impact regions. The DynAMO project also acquired borescope images, which show vast luminescent regions indicating pool-fire and diffusive flames towards the end of combustion. In this case, PN emissions increase by approximately three orders of magnitude. The effects of a sudden acceleration (sudden increase of engine load) are very similar.



Parallel project work carried out in collaboration with Ricardo Software, at a later stage of the

DynAMO project, concentrated on improving a number of fundamental models for incorporation into Ricardo's 0D/1D engine modelling platform WAVE. A new advanced turbulence model, which more accurately reflects the in-cylinder flow characteristics of a modern GDI engine, was integrated into their newly released spark-ignition (SI) predictive combustion model. Software environment work was also carried out by the OBU team, expanding the platform receptivity for the integration of the novel PN functional models under development at OBU.

3. References to the research

1. Sciortino, D. D., Bonatesta, F., Hopkins, E., Yang, C., Morrey, D., A Combined Experimental and Computational Fluid Dynamics Investigation of Particulate Matter Emissions from a Wall-Guided Gasoline Direct Injection Engine, Energies, 10(9), 1408, 2017. DOI: 10.3390/en10091408

2. Tan, J. Y., Bonatesta, F., Ng, H. K., Gan, S., Numerical Investigation of Particulate Matter Processes in Gasoline Direct Injection Engines through Integrated Computational Fluid Dynamics–Chemical Kinetic Modeling, Energy & Fuels, ACS, 2020. DOI: 10.1021/acs.energyfuels.9b03945

3. *Biagiotti, F., Bonatesta, F. et al. Modelling Liquid Film in Modern GDI Engines and the impact on Particulate Matter Emissions – Part 1. Article draft at December 2020, it has been submitted to International Journal of Engine Research at the time of writing.

4. *Bonatesta, F. et al. Confidential DYNAMO Project Reports for Quarter 7, May 2019, Slides 20-25.

5. Bonatesta, F., Chiappetta, E., La Rocca, A., Part-Load Particulate Matter from a GDI Engine and the Connection with Combustion Characteristics, Applied Energy, Elsevier, 124: 366–376, 2014. DOI: 10.1016/j.apenergy.2014.03.030

6. Bokor, C., Rohani, B., Humphries, C., Morrey, D., Bonatesta, F. Investigating the Impact of Gasoline Composition on PN in GDI Engines Using an Improved Measurement Method, International Journal of Engine Research, 2020. DOI: 10.1177/1468087420970374

*can be supplied by OBU Research Business & Development Office on request.

4. Details of the impact

In 2016 the World Health Organization (WHO) estimated that more than 4 million people die prematurely every year as a result of exposure to PM. Road transportation is responsible for the release of up to 20% of atmospheric carbon matter, or soot. Modern GDI engines are especially problematic because they produce large numbers of ultra-fine particles.

Soot formation in GDI engines is normally associated with imperfect mixing between air and fuel, and with liquid film of fuel being deposited on piston and cylinder walls during fuel injection. Exhaust filters are currently used by most manufacturers to comply with EU6b and US emission regulations. However, the most dangerous particles with a size of less than 23 Nm are not currently regulated, and cannot be removed effectively by filtration. As the forthcoming EU7 regulations will impose much stricter limits on PN emissions, for the GDI engine to remain viable for use in passenger vehicles, improved understanding and disruptive solutions are essential.

The impact generated by the OBU team as part of the DynAMO project has four main strands:

- It has fundamentally transformed Ford's knowledge around the mechanisms of PM formation and the link with limiting piston temperatures. This is playing a significant part in Ford's planning to comply with the new, stricter emission regulations.
- It has enabled Ford to begin the shift to less costly digital engineering tools (to replace hardware testing), as part of future engine development.
- It is enabling Siemens DISW, another DynAMO partner, to integrate the 3D CFD modelling approaches developed by OBU into beta versions of its market-leading software, STAR-CD and STAR-CCM+.
- It is enabling Ricardo, another DynAMO partner, to integrate significantly improved turbulence and combustion models into its 0D/1D WAVE software, and these are planned

for release as future add-ons/options.

Ford had a market share of automotive sales of approximately 14% worldwide and 10% in the UK in 2019. New knowledge and tools being established and embedded within the engineering teams on the Ford UK, Dunton Campus (and extended to Ford North America) are key to Ford's future economic, environmental and societal impact, globally. This is as a direct result of OBU's CFD modelling work.

Ford's technical expert for the DynAMO project explains in a support letter how the OBU modelling work has 'completely revolutionised' the understanding of particulate formation mechanisms within Ford. The theory advanced by OBU 'was a revelation … For the first time I could appreciate how … to explain transient PN behaviour'. Importantly, 'this new knowledge may assist Ford, and other automotive OEMs, to comply with the increasingly stringent legal PN emission regulations, ensuring the sustainability of GDI engine technology, even in hybrid applications' **[S1]**. A key factor in this is understanding the need to maintain high-enough piston temperatures at all stages of vehicle operation, which could ensure compliance with EU6 limits (6.0E+11 particle/km), and possibly beyond, without the use of costly filtering devices.

A further support letter produced by Ford echoes the first one, confirming current as well as future impacts generated by the OBU work, in terms of new understanding and development opportunities: 'The concepts and theories proposed by OBU have effectively changed the perception of these issues [the mechanisms of PM formation, and the influence of piston temperature on liquid film formation] within the Ford Technical Team, and open new areas of opportunity, including new piston design and novel calibration approaches such as the piston cooling strategy, which directly consider the trade-off between component durability and PM emissions*'* **[S2]**. The OBU team proposed a dual-fuel engine simulation that offers unprecedented accuracy. This enables reliable prediction of fuel distribution and liquid film, and how these start forming soot during combustion. The Ford support letter remarks on how the OBU work is contributing to the present shift in practice within the organisation, which is the second strand of impact claimed in this case study: 'The modelling work carried out by the team at OBU has been … impactful to Ford especially. Compared to common approaches … at Ford, the OBU modelling framework offers increased robustness, accuracy and functionality, and as such will assist the gradual but necessary transition … to cost-effective digital engineering … The tools are being established … within the engineering teams on the Ford Dunton UK Campus and extended to Ford North America, where development of new gasoline and hybrid powertrain platforms will continue to be strong for the foreseeable future' **[S2]**.

A further strand of OBU's impact relates to development by Siemens DISW, another DynAMO partner, which has a major share in the 3D CFD engine modelling market. Siemens will be rolling out the novel modelling framework to the wider CFD user community. The director of powertrain at Siemens DISW gives evidence of the OBU impact, which improved both understanding and practice within the organisation: 'To my knowledge, this is the most accurate GDI engine modelling framework available through a commercial CFD software platform. The methodologies proposed … are also of high significance to Siemens DISW because OBU unveiled shortcomings in the current offered … approach, which now Siemens DISW is addressing. The novel … methodologies will feed into future releases of … STAR-CD … and also support the new platform Simcenter STAR-CCM+ in-cylinder solution' **[S3]**. The OBU work has so far directly contributed to three releases of the STAR-CD software, which now offers a direct calculation of engine charge homogeneity, improved numerical stability for the modelling of liquid film and improved calculations of PM characteristics. The DynAMO project also provided experimental data, acquired for, processed and validated through the OBU models, and this is acknowledged in a Siemens blog describing its latest release of in-cylinder combustion modelling in STAR-CCM+ **[S5]**.

The models developed by OBU will be further integrated into the 0D-1D Ricardo WAVE platform. This has even more users than engine CFD software, which is mostly used by specialist departments. Ricardo's technology manager (software) gives a clear indication of the impact of this work on the Ricardo organisation, through the release of add-ons for future software and therefore the ability to more accurately model the generation of PN emissions: 'Oxford Brookes … have been able to identify flaws in the initial 0D turbulence model implementation … and validate the improved combustion model … The OBU team have proven to have a unique blend of excellent capability with relevant experience and the results of this work will be feeding into future releases of Ricardo WAVE via add-ons and best practice guidelines' **[S4]**.

Ford's confidence in the direction indicated by OBU's work also led to it investing £100,000 to significantly enhance the engine testing capabilities at OBU. OBU's specific contribution to the DynAMO project has been fundamental in enabling one of the world's biggest engine manufacturers to begin to successfully address the challenge of reducing PM in line with new EU regulations. It has also enabled leading software companies to create new products that may be transformative for their businesses. This paves the way for reducing the major health risk associated with PM in the future.

5. Sources to corroborate the impact

1. Evidence Letter from Mark Cary, former Technical Specialist, Ford Motor Company UK

2. Evidence Letter from Dennis Witt, Supervisor, UK Innovation & Outreach, Ford Motor Company

3. Evidence Letter from Robert Norris, Software Development Manager, Ricardo UK

4. Evidence Letter from Warren Seeley, Director – Powertrain, Siemens Digital Industries Software

5. Siemens, 'Simcenter STAR-CCM+ 2019.3: Simulate In-Cylinder Combustion', October 2019, https://blogs.sw.siemens.com/simcenter/simcenter-star-ccm-2019-3-simulate-in-cylinder-combustion/