Imperial College London

Mechanical Engineering Department

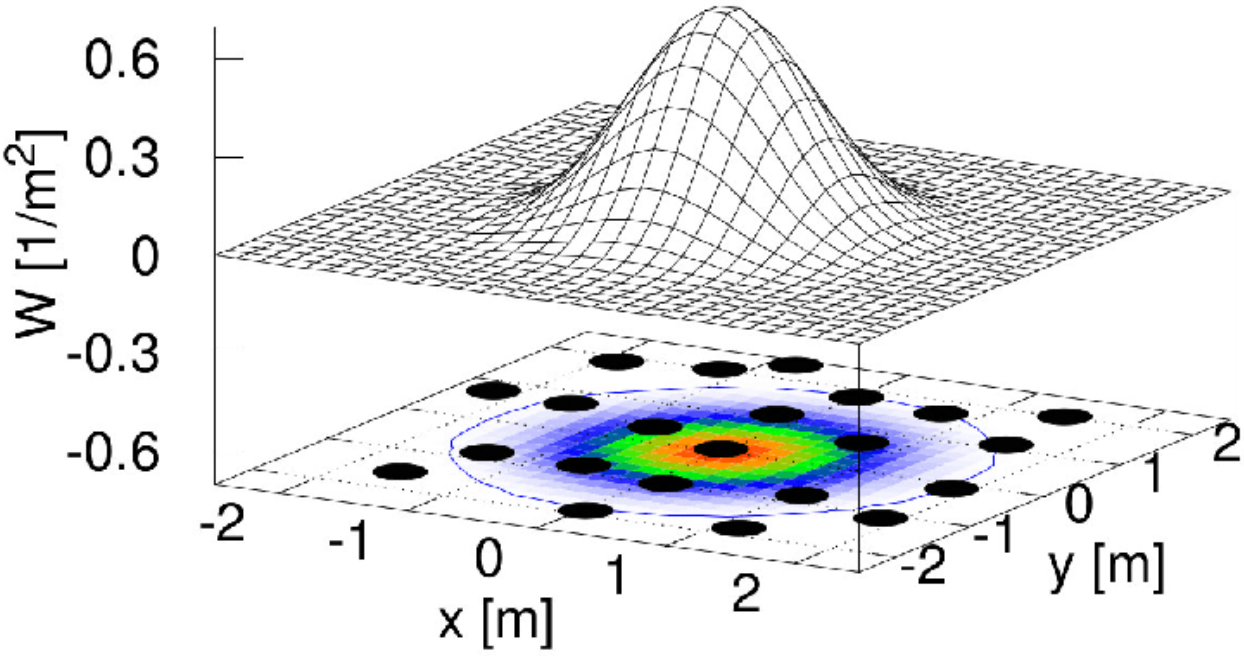

Fig 1 - Image taken from Chaussonnet et al. (1)

ME3 Literature Research Project
Smooth Particle Hydrodynamics

Author: H. R. Hart

CID Number: 01190775

Supervisor: Professor A. Taylor

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Abstract

The study of atomisation deals with the theory and analysis of sprays which is particularly important in all liquid fuel applications such as car and jet engines. Computational Fluid Dynamics (CFD) programs are the current workhorses for analysing the implications of any particular atomisation design within these engines. With an ever-present demand for computing time, much research has gone into finding an alternative approach to the standard Finite Volume (FV) and Finite Difference (FD) methods. One such alternative is Smooth Particle Hydrodynamics (SPH). This review will compare this new proposal against the current competitors and discuss how these methods are relevant to atomisation since CFD software tends to be application dependent in its efficacy.

This review will find that finding a globally superior computational method at this point is not straightforward since both SPH and CFD have advantages. SPH has the ability to utilise the computing power available more efficiently with one study demonstrating a 70% reduction in computing time. Conventional CFD however, given its long history and basis of research, has been shown to produce results very close to experimental data when appropriate theories are applied.

Contents

1. Aim & Objectives

1.1. Aim

The aim of this project is to compare the efficacy of Smooth Particle Hydrodynamics to that of 'standard' finite difference and finite volume Computational Fluid Dynamics given the following instruction from the end client: '*Currently, the detailed 'CFD' calculation of many important applications of sprays in Mechanical Engineering (e.g. cars, gas turbines) are mostly by 'brute force' techniques, the poor computer having to track of the liquid core in the atomiser through to the millions upon millions of droplets. SPH promises to reduce the computing power required by an order of magnitude or more. Is this possible or just more 'snake oil' peddled by academics keen to make a name for themselves? How is it supposed to work?*'.

1.2. Objectives

The aim of the project will be fulfilled by adhering to the numbered objectives given in this section. The outcome of these objectives will be summarised as conclusions in section 7.

1. Summarise standard CFD methodology. This is discussed in section 3.
2. Summarise Smooth Particle Hydrodynamics methodology. This is discussed in section 4.
3. Summarise atomisation and its challenges. This is discussed in section 5.
4. Compare the efficacy of SPH vs. 'standard' CFD in the context of atomisation. This is discussed in section 6.

2. Introduction

Computational Fluid Dynamics (CFD) is one of the most important areas for Mechanical Engineers. The Navier-Stokes equations are extraordinarily powerful and yet only fully solvable for the simplest of problems, excluding any turbulent flows (2) . CFD uses computational power to discretise the fluid in time and space in order to find an approximate solution. Unfortunately, fluid flows, especially those with turbulence, are very chaotic and therefore a high computational resolution is required in most cases to achieve an accurate solution (3) . At our current stage of technological development, this high demand for computing time severely limits the extent and accuracy of much important fluid dynamics research. Unless the fundamental physical understanding of fluid flows is improved (the Clay Mathematics Institute offers $1,000,000 for a smooth and globally defined solution to the Navier-Stokes equations (2)), it falls on engineering research to find ways to make CFD more efficient. One proposed solution is Smooth Particle Hydrodynamics (SPH) (1) .

3. Fundamentals of Computational Fluid Dynamics

Since the Navier-Stokes equations are usually impossible to solve (2) , particularly in the case of turbulent flow, an iterative estimate must be calculated to simulate the flow. The most effective way to do this is by Computational Fluid Dynamics (CFD) which uses computing power to execute these calculations quickly.

3.1. Discretisation

Since the calculation is not a continuous solution, the space being considered must be discretised. There are 4 main ways in which the space can be discretised (4) (5) :

1. Finite Elements
2. Finite Volumes
3. Finite Difference
4. Spectral

This discretisation gives rise to a grid onto which fluid properties must be mapped (6) . Much CFD research is concerned primarily with how to estimate fluid properties at relevant nodal points. Many of these methods can be as simple as described in the Imperial College Mechanical Engineering 2nd Year Mathematics module (7) . The Navier-Stokes equations must be written in discretised form so that iterative time stepping methods can be used to output a solution. The mass conservation equation is simply a statement of the empirical observation that mass cannot be created or destroyed. The continuous Einsteinian differential form is given in equation 1 where symbols have their usual meaning.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}$$

Equation 2 shows the momentum equation in the same form.

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} + \varrho g_i \tag{2}$$

Naturally, these equations are continuous and so require discretisation. In general, this can be simply done by simply replacing differentials with a difference between grid values. In addition to satisfying the Navier-Stokes equations, various other quantities must be conserved by the fluid. This is a particular inconvenience for grid based CFD as the system will not automatically know

that mass, for example, should be conserved. This is one advantage that SPH has over grid-based algorithms (8) and will be discussed further in section 6. In order to estimate values of velocity, pressure, density (in the case of compressible flow), stress tensor and body force at grid points, there are various simple estimation methods. These include interpolation, extrapolation and quadratic upwind interpolation (4).

Quadratic upwind interpolation requires two points 'upwind' from the point of interest, and one 'downwind' giving 3 points which is sufficient for quadratic curve fitting and interpolating. Imagine that the two upwind points are at x_1 and x_2 and the downwind point is at x_3. We wish to know the value of a quantity at some point x_i and take it to be a function of space, f(x). The value of this quantity can be found by using equation 3.

$$f(x_i) = f(x_2) + \frac{(x_i - x_2)(x_i - x_1)}{(x_3 - x_2)(x_3 - x_1)}[f(x_3) - f(x_1)] + \frac{(x_i - x_2)(x_3 - x_i)}{(x_2 - x_1)(x_3 - x_1)}[f(x_1) - f(x_2)] \quad (3)$$

These 'lower order' methods are considered very robust (9) and require less computing power in general. However, as research in CFD has continued, higher order methods have become more commonplace. Various propositions include the discontinuous Galerkin (10) and Runge-Kutta Discontinuous Galerkin (11) which uses higher order Runge-Kutta differential equation solutions as given in the aforementioned course notes (7).

The Galerkin method is essentially a way of optimising a discrete field estimate of values so that errors are minimised. Suppose that we seek an estimate for the value ϕ in the field v. The value ϕ is then estimated with a polynomial series as a function of position, and errors (= e) at known points are calculated. The algorithm then attempts to satisfy the expression given in equation 4.

$$\oint_v w(\vec{r}) \cdot e(\vec{r}) dv = 0 \quad (4)$$

w is a weighting function which also depend on position. In theory w can be anything and the algorithm will attempt to satisfy the above relation for any value of w. Clearly then, this is now an

optimisation problem involving the polynomial coefficients and a variety of weighting functions. A computer can solve this, like all optimisation problems, with matrix manipulation.

According to results given by Bassi and Rebay (1996) (12), lift and drag coefficients can be calculated with varying results depending on the order of element solution used in the proposed higher order approach. In addition, Bassi and Rebay found in their earlier paper (13) that the use of the higher order discontinuous Galerkin method was generally very successful both in terms of accuracy and efficiency.

In addition to the important issue of spacial discretisation, the CFD algorithm must implement temporal discretisation. Again, this can be as simple as implementing implicit or explicit Euler time stepping which are both first-order accurate at their simplest. For higher orders of accuracy, some algorithms will use the second order accurate Crank-Nicholson scheme (14)(15). The benefit of using this scheme is that the differential governing the time dependant change of a value is evaluated halfway between 'now' and one time-step into the future. In this sense, this time stepping procedure is very similar to a Runge-Kutta second order scheme. Equation 5 shows the governing estimation relation of the Crank-Nicholson scheme.

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \dot{\phi}\left(x, t_{n+\frac{1}{2}}\right) = \frac{1}{2}\left(\dot{\phi}(x, t_{n+1}) - \dot{\phi}(x, t_n)\right) + \mathcal{O}(\Delta t^2) \tag{5}$$

3.2. Turbulence Modelling

There is nothing particularly special about the physics underlying turbulent flow. At the molecular level, the particles continue to act like small, hard spheres. At the continuous scale, the Navier-Stokes equations continue to describe the flow if it is Newtonian. However, the Navier-Stokes equations do not necessarily yield a simple solution, and it just happens to be that above a certain Reynolds number (effectively the ratio between kinetic and viscous effects), there is a marked change in behaviour in the fluid which makes its behaviour much less predictable (16).
In order to more accurately and concisely model turbulence in the Navier-Stokes equations, Reynolds proposed what is commonly known as a Reynolds decomposition (17) and this is given in equation 6.

$$u_i = \bar{u_i} + u_i' \tag{6}$$

In this equation, the averaging bar ($\bar{}$) indicates the time averaged quantity beneath the bar as expressed in equation 7. The turbulent term which is a function of time with average zero is denoted with a superscript prime (‘).

$$\bar{\varphi} = \lim_{T\to\infty} \int_{t}^{t+T} \varphi(t)dt \tag{7}$$

The Reynolds decomposition gives rise to a new form of the governing equations known as the Reynolds Averaged Navier-Stokes whose momentum component is given in equation 8 in Einsteinian form.

$$\rho\overline{u_\iota}\frac{\partial\overline{u_j}}{\partial\overline{u_\iota}} = -\frac{\partial\bar{p}}{\partial x_j} + \mu\frac{\partial^2\overline{u_j}}{\partial x_i\partial x_i} - \frac{\partial\rho\overline{u_\iota' u_j'}}{\partial x_j} \tag{8}$$

The most important part of equation 8 is the final term, known as the Reynolds stress term. Including all directions, this term adds 6 independent unknowns to the governing system of equations. The simplest way of dealing with this term if to find the spatial and temporal average for implementation into the simulation (18) . This is certainly not an ideal simplification to use when there are fluctuations in the magnitude of turbulence caused by an unsteady flow (19). While methods of dealing with this issue have been proposed, for example the use of Favre-averaged equations (20) , the favoured method within the realm of traditional CFD has shifted to Large Eddy Simulation (21).

Large Eddy Simulation (LES) offers an approach to turbulence modelling which is still simplified, and yet captures most of the information in the flow. Like the RANS approach, the eddy simplification imagines a flow as the sum of two distinct components: a steady flow modelled as the time averaged component, and an unsteady flow caused by superimposed circular motions at a variety of different scales. The key to the LES method is filtering information based on significance and separating between large, medium and small-scale eddy effects which are treated differently according to properties (i.e. viscosity, body force). These can be discounted in order to find a sensible balance between computational resources and accuracy (22)(23). One significant advantage of this method is the ability to tune the resolution of the effective scale filter used by the algorithm in order to find a solution that is appropriate for the situation. The governing form of the Navier-Stokes momentum used in LES is given in equation 9.

$$\frac{\partial\bar{\rho}\widetilde{u_\iota}}{\partial t} + \frac{\partial\bar{\rho}\widetilde{u_\iota}\widetilde{u_j}}{\partial x_j} = \frac{\partial\overline{\tau_{\iota j}}}{\partial x_j} - \frac{\partial\bar{\tau}_{ij}^{s}}{\partial x_j} - \frac{\partial\bar{p}}{\partial x_i} + \varrho g_i \tag{9}$$

In equation 9, the overbar tilde (∼) indicates that the value has been filtered according to the scheme given in equation 10.

$$\tilde{\varphi} \equiv \frac{\overline{\rho\varphi}}{\bar{\varphi}} \tag{10}$$

It is clear from equation 9 that the stress term has been separated into two components: steady and sub-grid scale stress, $\partial\bar{\tau}_{ij}^{s}$, which is conceptually similar to the addition of a Reynolds stress when using the RANS equation. Determining the value of this stress term(s) is the subject of much research, including Smagorinsky in the 60s (24) and others subsequently(25)(26).

In summary, the concepts behind CFD have been around for some time now and much work has gone into finding computational refinements that aim to achieve the correct compromise between accuracy and simplicity. The context of the situation matters more now as a result of the extensive specialisation of various regimes. Rodi has completed a comprehensive study (27) comparing RANS and LES outputs to experimental data. Since the experiments performed were mostly concerned with the flow around a cube, the most important part of the flow was the separation of the flow from the back face, and therefore with the large scale turbulent eddies associated with this flow. Because LES is much better equipped to deal with the modelling of large scale eddies, its output better predicted the experimental data which can be visualised in figure 2.

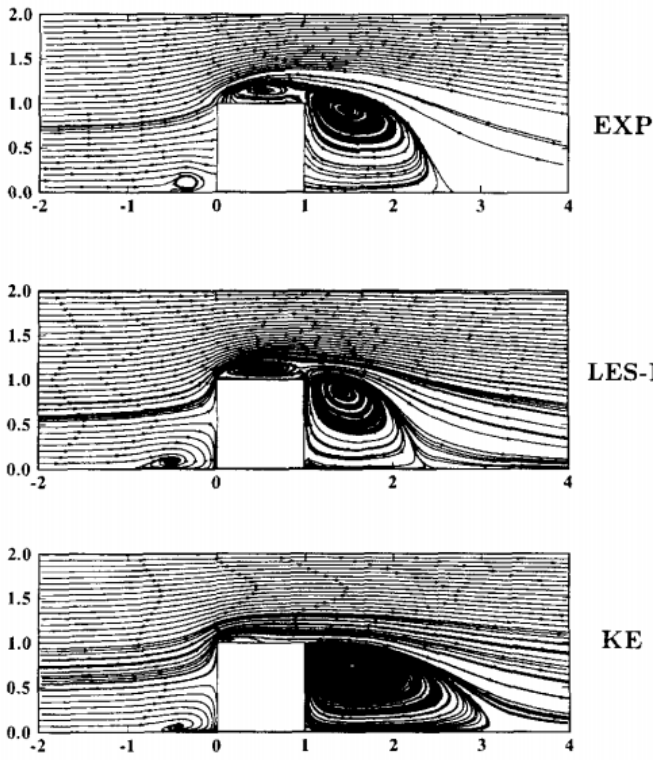

Fig. 2 – Experimental (EXP), LES (LES) and RANS (KE) flows compared. Taken from Rodi (1997)(27)

While LES clearly has the upper hand on accuracy and suitability to model large scale turbulent flows, it is significantly more expensive. Rodi (27) cites a computing time for LES of 160 hours when the equivalent RANS calculations took 6 hours.

4. Fundamentals of Smooth Particle Hydrodynamics

For many years, conventional CFD has dominated the business of flow prediction (28) . Because of its long life and computational demand, CPH has recruited many additional complexities to make it more accurate and efficient. Subsequently, Smooth Particle Hydrodynamics (SPH) has been developed as a completely novel approach and promises to be an all-round solution for many situations from its origins in interstellar physics (29) , to fracture mechanics (30) , and finally to conventional fluid mechanics (1). The common feature of conventional CFD methods is the incorporation of some kind of grid which allows flow derivatives to be estimated at convenient resolutions. In most circumstances, the grid does not deform (although there are cases where deformable grids can be used (31)) and so the method is distinctly Eulerian. Smooth Particle Hydrodynamics is mesh-free and so the reference frame is Lagrangian. As there is no grid, common issues such as mesh distortion can be avoided (32).

The first paper on Smooth Particle Hydrodynamics was a report by Lucy in 1977 (33). This was shortly followed up on by Gingold and Monaghan later that year (34). Initially, the field was applied only to astrophysics which is rather different to conventional studies of fluid flow.

The idea behind SPH is basic. The program brings a number of ‘particles’ into being (although far fewer than in reality) and gives each one an area of influence, as indicated by figure 1 on the cover page of this report. This is done through the mathematical overlaying of a ‘kernel’ which in most cases roughly resembles a bell curve. This gives the particle an appropriately diminishing influence as distance from it increases. A kernel is necessary to transform the problem from a Newtonian balls-bouncing-off-each-other problem into a quasi-continuous problem that can be solved with the differential form of the Navier-Stokes equations, which is more appropriate for ‘particles’ that are far larger than the molecules they represent. Without the particles’ properties being smoothed, the field would be useless for calculation since the density would be extremely high at a particle’s location and zero in the free space surrounding. The same argument pertains to

pressure and differential velocity. The fundamental mathematical properties of a kernel, ω, are given in equation 11 and 12.

$$\int \omega(r,h)dr = 1 \tag{11}$$

$$\lim_{h\to 0} \omega(r,h) = \delta(r) \tag{12}$$

In equation 12, $\delta(r)$ is the Dirac delta function whose definition is given in equation 13. The parameter h is defined as the width of the kernel and usually gives a good estimate of the significant bounds of the particle's influence, although the function does usually have a very small influence far away like any Gaussian distribution. The Dirac delta is otherwise known as a sifting function as one can integrate its product with a function to obtain the value of that function at a point. As implied by equation 11 and 12, the integral of the Dirac delta everywhere is defined as 1.

$$\delta(r) = \begin{cases} \infty, & r = 0 \\ 0, & r \neq 0 \end{cases} \tag{13}$$

In theory, the kernel could be any function that conforms to the rules as set out above. In practice however, it does help if the particle has the most influence at r=0, the location of the particle. Gaussian probability functions and axially-symmetric exponential decay make for good kernels. Implementing the kernel solution begins by integrating a property, φ, with the kernel to obtain an estimate, φ', as shown in equation 14 where $\vec{r}$ is the position and $\vec{R}$ is a dummy variable for the integration.

$$\varphi'(\vec{r}) = \int \varphi(\vec{R}) \cdot \omega(\vec{r} - \vec{R}) d\vec{R} \tag{14}$$

The estimate is then multiplied by density/density and summed over all the particles to give the estimate of the value pertaining to the field, rather than a single particle (b), as shown in equation 15.

$$\varphi'_{total}(\vec{r}) = \sum_{b} \frac{\varphi_b \cdot \omega(\vec{r} - \vec{r}_b)}{\rho_b} \tag{15}$$

The value φ can, in principle, be any fluid property. For example, equation 16 shows the SPH formulation for the density field, as follows from equation 15 (35).

$$\rho_{total}(\vec{r}) = \sum_{b} m_b \cdot \omega(\vec{r} - \vec{r}_b) \tag{16}$$

The same can then be repeated for pressure, velocity and body force as appropriate. Because the kernel overlay causes the field to be continuous, the differentiation of properties is trivial and does not require a finite difference grid calculation.

One major advantage of SPH is that because the code maintains a constant number of particles of known mass, there is no scope for mass not being conserved which can be an issue in conventional CFD (36). However, momentum is not automatically conserved by this estimation since one particle doesn't automatically generate the same force on other particles as other particles impart on the first particle.

According to Monaghan (35) , there are ways that one can express the Navier-Stokes equations such that momentum is guaranteed to be conserved. Naturally, then, this method has already acquired its own patches to deal with inadequacies in the base idea. In time, it is to be expected that SPH will acquire as many different variants as CFD seems to have up to this point, and so it is not an advantage that SPH is revolutionary.

As with most computational flows, it is useful to be able to insert boundaries since the solids in a problem mostly define the way that a fluid will flow. There are a number of ways that boundaries can be defined, depending on the properties that are desired at that boundary. If, for example, boundary energy losses (heat transfer) are unimportant, then a boundary can be defined in SPH as a surface along which the particles will experience reflection as if they were Newtonian hard-shell billiard balls bouncing off a perfect cushion (37). This method is ideal for simple, purely flow based (i.e. not concerned with thermal effects) problems as the programming is very simple to implement. In more precise and heat sensitive applications however, other methods are more

appropriate. For example, the boundary can be represented as a field of forces which act to repel particles that come near, either with or without the particle kernel overlaid (38). This method is better for simulating the real-life situation where the wall does essentially act like a short-range force repelling the incident particles. The final, and most precise method, is implementing a layer of fixed particles (39) into the flow so that momentum and energy transfer can be modelled between particles as in real life. One problem that arises with this approach is that the fixed fluid particles at the boundary will be attracted to fluid particles that are moving away from the boundary because density will decrease in the void. Despite this, Monaghan and Kajtar have shown that fixed particles accurately model reality when implemented alongside SPH (39).

As with standard CFD, it is important to consider time stepping. For the initial astrophysical applications, the method of time stepping used was leapfrog. This method essentially controls movement of particles according to the conditions present midway between the time steps (40). While as computationally efficient as Eulerian time stepping, it is second order accurate compared to the Euler method's first order. Since the initial implementations however, second order Runge-Kutta has become a more popular approach and has been shown by Benz to be very precise (41).

One application of SPH which was originally problematic was interaction of supersonic clouds. Gingold and Monaghan found that the clouds simply streamed through each other without interacting (42). In this and other applications, a superimposed viscosity term was introduced to cause the particles to interact when passing too quickly for the computation (43).

5. Atomisation

Atomisation is an important physical phenomenon which is crucial to understand and implement in a number of commercial and industrial processes. The foremost application, for now, is in the chamber of an internal combustion engine where fuel is injected at high pressure to be mixed with the air. Other applications include industrial spray painting and crop insecticide spraying. In all of these applications, the primary quality to be maximised is fineness of the droplets. In the case of internal combustion engines, smaller droplets allow a greater contact area for oxygen to react with the hydrocarbon fuel and therefore a quicker and more efficient combustion is achieved (44) . A more efficient combustion generally implies a clean combustion because complete combustion produces more energy per mole of fuel and produces only carbon dioxide and water (and NOx particles strictly speaking). This is less harmful than when soot, unburnt hydrocarbons and carbon monoxide are also produced.

Early studies of atomisation were very limited due to the microscopic and unstable nature of the process. Since the advent of advanced computing power and high-speed cameras, experimental research has accelerated (45). When designing any atomisation mechanism, for example a new internal combustion engine, it is important to have a mathematical model beyond the experimental data from video footage. Fortunately enough, since the end of the second world war, there has been much research in the pursuit of mathematically modelling droplets. This literature review will begin by looking at the mechanism used to atomise the fluid and then move on to look at how the droplets behave when interacting at high speed with a secondary fluid of different density (often air in the case of IC engines).

5.1. Atomisers

The simplest type of atomiser in an IC engine is a simple nozzle (44). This type of atomiser relies on a high pressure drop across a flow element, usually some form of inverted cone or constricted hole, which acts to break up the fluid as it passes this boundary. A more advanced version of the single-fluid pressure atomiser is the twin-fluid atomiser. This acts to separate the primary fluid, usually combustible fuel, by injecting it through a nozzle while being impinged on at high velocity by the secondary fluid, usually air, in order to disperse the droplets. Figure 3 shows the layout of a typical twin-fluid atomiser, known as ‘flow-blurring’, and how air is directed near the point of primary injection.

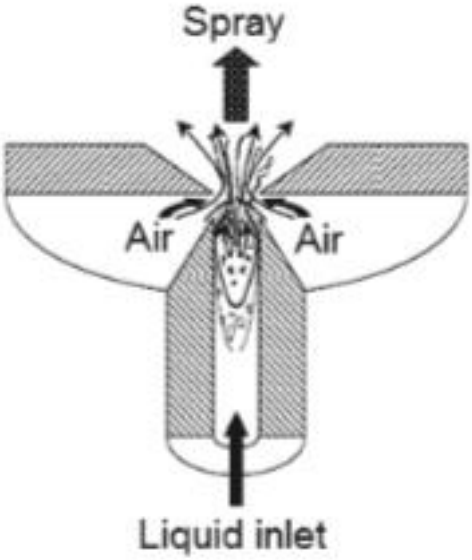

Fig. 3 – Schematic of flow-blurring atomiser. Taken from Panchesara et al. (2009)(46)

Azevedo *et al.* (44) showed that there is a compromise to be considered when selecting nozzle geometry. When considering three different nozzle geometries: cylindrical, conical and conical-cylindrical it was shown that conical atomisers most effectively product fine droplets but have the disadvantage of having a lower discharge coefficient which measures the extent to which the fluid is flowing effectively across the given area of injection. The expression used to calculate discharge coefficient is given in equation 17.

$$c_d = \frac{\dot{m}}{A\sqrt{2\rho \cdot \Delta P}} \tag{17}$$

The symbols in equation 17 have the following meaning: c_d is the discharge coefficient, A is the injection area, ρ is the primary fluid density, $\dot{m}$ is the mass flow rate and ΔP is the pressure drop across the atomiser.

Another popular type of atomiser is the rotary atomiser. These rely on the centrifugal effect to fling fluid droplets radially at high speed and in doing so break up the fluid with a combination of centrifugal separation and complex ligament instability, to be discussed later. It is commonly observed that the fluid, injected initially at the axis of the rotating disc or cup, flows to the extremes of the surface and then forms thin threads of fluid called ligaments (47). Figure 4 shows how ligaments are formed on the edge of a spinning disc.

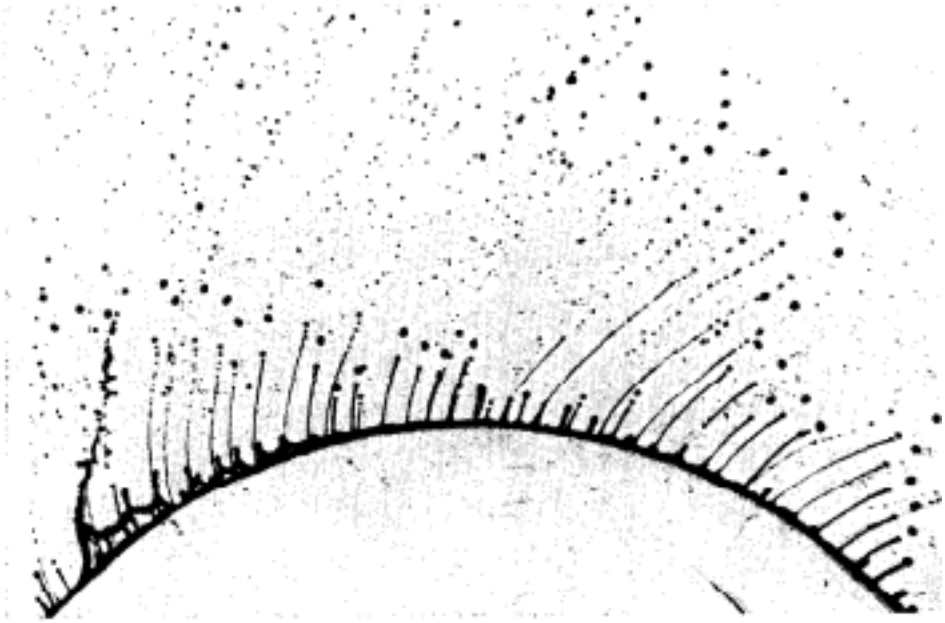

Fig 4. – Ligament formation on a rotary atomiser. Taken from Frost (1981)(48)

Also shown in figure 4 is the propensity for the fluid ligaments to become unstable and fracture. One feature, sometimes an advantage depending on the application, of rotary atomisation is that the particle droplets often have a relatively uniform size distribution when compared to twin-fluid atomisation (49). The instability is difficult to model accurately, and two notable explanations have been proposed to explain it. The first is Kelvin-Helmholtz instability. William Thompson, Lord Kelvin, and Hermann von Helmholtz proposed their theories in an attempt to model the instability of a fluid when in contact with a secondary fluid (50) (51). The underlying rationale behind instability of the ligaments in air begins with waves being created on the ligament surface, like waves formed on the surface of the sea when high winds sweep over it. This phenomenon is similar in nature to, indeed even the same as, the onset of turbulence. From this it is obvious to state that Kelvin-Helmholtz (KH) instabilities are a consequence of high Reynolds numbers (16). A simple way of thinking about Kelvin-Helmholtz instabilities is to consider two fluids moving over one another. Naturally, there will be fluctuations in the height of the boundary as shown in figure 5, even if the fluctuations are microscopic. The question that now must be considered is whether that fluctuation is likely to grow or return to its datum height, similar to predicting whether a ball is stable on the top of a hill or in a valley. Kelvin-Helmholtz theory invokes the Bernoulli effect to argue that beneath a depression in the fluid interface, the constricted fluid will be required to accelerate to conserve mass flow rate and so pressure will decrease. The converse occurs where the fluid channel is bloated. This causes the fluid boundary to move in the direction of its initial displacement and so the natural fluctuations are indeed unstable. The rising primary fluid is then

caught in the higher velocity region of the secondary fluid's boundary layer and so is swept in a way that causes hook or wave like shapes to form as seen in clouds, gas giant planet surfaces and oceans.

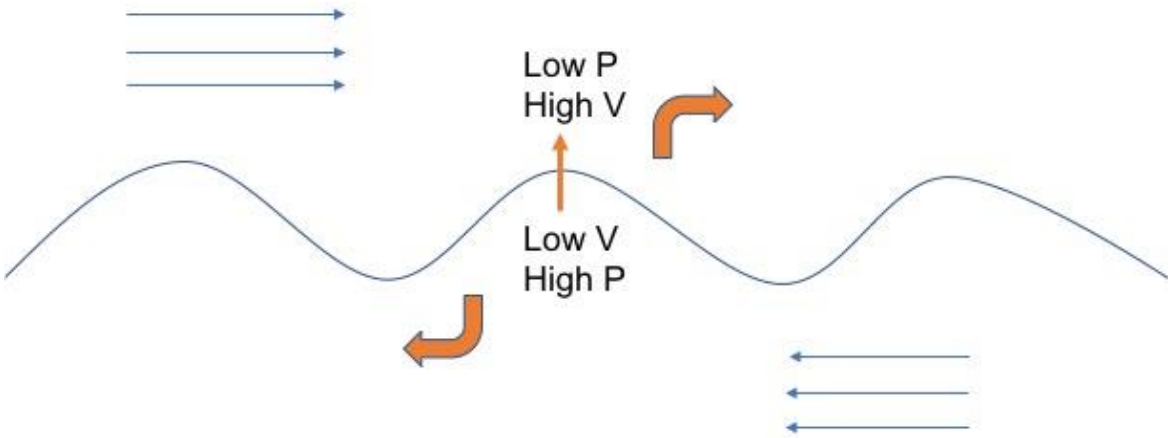

Fig. 5 – Kelvin-Helmholtz instability

Once the initial waves on the surface of the ligaments have been formed by Kelvin-Helmholtz instability, a secondary instability effect is thought to take over. Rayleigh-Taylor instability (52) is an effect commonly observed when two fluids with different densities are forced to interact. The typical topological form of this interaction is a mushroom cloud, most obviously observed when high temperature low density explosive gas is trapped under a blanket of atmosphere and forms a mushroom shape in response to the pressure of the higher density fluid outside. Other examples include formation of sub-water air droplets when the water is suddenly penetrated by an object at high speed such as a stone. As can be seen in the more developed fluid in figure 4, the Rayleigh-Taylor instability tends to result in fluid that clusters into small droplets due to the inherent relative immiscibility of the two fluid phases because of surface tension. This is the basis behind the observation that rotary atomisers produce a more uniform particle distribution.

5.2. Dynamics of Primary Fluid Droplets

Once the primary fluid has been broken up into relatively large droplets either by pressure atomisers, twin-fluid atomisers or rotary atomisers, the droplets experience further degradation when interacting and impinging freely on high relative velocity secondary fluid within the combustion chamber (in the case of IC engines).

The most basic model that is encountered when attempting to predict the relevant forces governing the dynamics of atomised droplets is that of a solid sphere in a free flow. This is a

reasonable model with which to begin basic analysis since the viscosity of atomised fluid, commonly water or oil, is significantly higher than that of the secondary fluid, commonly air, and so lower velocity gradients will be observed in the secondary fluids and these will broadly govern the behaviour of the dynamics. A simple mathematical way to model flow around a sphere is to apply the non-viscous Navier-Stokes equations, known as the Euler form, to a long cylinder in 2-dimensional 'potential' flow. This model will be accurate if one assumes that the planes of 2-dimensional flow around infinitesimally tall cylinders that make up a sphere do not interact, and that we focus only on flow far from the boundary layer where the Reynolds number is higher and so viscous effects do not play a role. The complex potential, F(z) for this flow is given in equation 18 (28).

$$F(z) = U\left(z + \frac{R^2}{z}\right) \tag{18}$$

This flow is the superposition of a free stream (first term) and a doublet, defined as the differential of a source flow. If the streamlines are plotted for this flow, given by the lines of constant real velocity potential, it clearly models simple potential flow around a cylinder with stagnation points on the front and rear and no flow separation. There is a streamline which forms the outline of a cylinder and since flow cannot ever cross a streamline, one can take this to represent a solid body, ignoring for a minute the no slip condition (which could be reasonable in an inviscid world). We will see later in this review that this may be a closer approximation to the truth than the no slip condition.

Beyond this basic mathematical model for flow around a sphere or cylinder, various experiments have shown that this model is far from accurate. Firstly, it has been shown that at Reynolds numbers above 20 the flow will separate from the downwind surface of the sphere and so create a wake (53). Additionally, Taneda showed as early as 1956 that above Reynolds numbers of 24, a vortex ring forms in the wake of a solid sphere (54). These experimental findings make the flow far more complicated to model with purely mathematical reasoning and so must be modelled with some form of CFD.

Up to this point, the only discussion of droplet dynamics in this review has been concerned with free flow around a solid sphere. Of course, an oil or water droplet is not solid and will, to some extent, act dynamically. This first and most significant diversion from the solid sphere model is

that the no-slip condition is not valid since the surface of the droplet begins to circulate with the flow, reducing the relative velocity of the secondary fluid and the primary surface. This is known as a Hill vortex (55). Clearly this has the potential to significantly change the nature of the boundary layer of a secondary fluid on the surface of the droplet. The final modelled divergence from the solid sphere model that will be discussed here is that droplets are not always spherical. Meteorologists and others have shown that very small droplets can maintain a spherical form, while larger droplets deform into a flattened shape (56).

When discussing experimental droplet dynamics, it is important to consider some dimensional numbers other than the Reynolds, given in table 1.

Table 1 – Relevant non-dimensional Parameters for Droplet Dynamics

Oh (Ohnesorge) =	$\frac{\mu_l}{\sqrt{\rho_l \sigma d}}$	(19)
Bo (Bond) =	$\frac{\rho_l g d}{\sigma}$	(20)
We (Weber) =	$\frac{\rho_g u^2 d}{\sigma}$	(21)
Ca (Capillary) =	$\frac{\mu_l u}{\sigma}$	(22)

In equations 19 to 22, subscript l refers to the primary fluid, subscript g refers to the secondary fluid, σ is the surface tension, u is the relative velocity of the fluids and d is the droplet diameter. All other symbols have their usual meaning. Bergeles, Hardalupas and Taylor found that with We = 0.14, Re = 141, Bo = 2.4 and a range of Ca and Oh numbers that the existing models for droplet dynamics broadly lined up with experimental results using oil droplets, excepting for the instant shortly after injection into the secondary fluid (31). They implemented the existing theory in the literature using the Volume of Fluid (57) methodology within the OpenFOAM CFD software. These results are encouraging for the field of atomisation droplet modelling, even without the need for the radical adoption of SPH.

6. Discussion of Computational Methods

The review will now move onto the fundamental question behind this research: which is 'better', traditional CFD or SPH? It will be shown that it is not necessarily helpful to label one as better than the other, rather to say that each has its place. There is a healthy degree of scepticism surrounding

the issue of SPH arising understandably from the assumption that those who are the prominent proponents of the approach are often those who will profit from its adoption. In this section, the relative strengths and weaknesses of SPH will be assessed and discussed in relation to their applicability, particularly with regard to atomisation.

6.1. Strengths of SPH

The primary strength of SPH arises not solely from experimental comparisons, but from the very way in which it is set up. Since it is a Lagrangian method, the particles themselves are tracked and so no grid is required onto which fluid transport properties must be mapped. This means that pre-processing time is significantly reduced (58). This also means that there is no possibility of encountering grid entanglement issues which can be a significant problem when the mesh attempts to track fluid surfaces, as detailed by Bergeles, Hardalupas & Taylor (31).

Another inherent, non-experimentally derived benefit of using SPH is that mass is always conserved because the software will initiate with a given number of 'particles' and track them until the simulation is completed. There is no possibility of simulated mass going astray. This is not necessarily the case with all CFD simulations since mass isn't pinpointed, rather estimated at points on a grid. Nonetheless, in one application of atomisation, mass was found to be conserved to within 0.09% using the Volume of Fluid Eulerian method (31). While with SPH one can certainly be more confident of conserving mass, Eulerian methods should not be dismissed since they can produce the same advantage quite easily.

It is often claimed that SPH has the advantage of being very scalable in comparison to grid based CFD methods. One strong piece of evidence for this is that, being a particle-based method, the number of calculations (per time step), C, will scale with the number of particles, N, as shown in equation 23 (59).

$$C \sim N \cdot log(N) \tag{23}$$

This means that initial, low resolution runs of SPH simulations will often accurately predict the computational strain of increasing the resolution by adding more particles. This notion is backed by significant research into the computational benefits of using SPH. As shown in figure 6, the SPH method scales remarkably well with the number of cores used in the simulation when compared with OpenFOAM and another commercial offering (60).

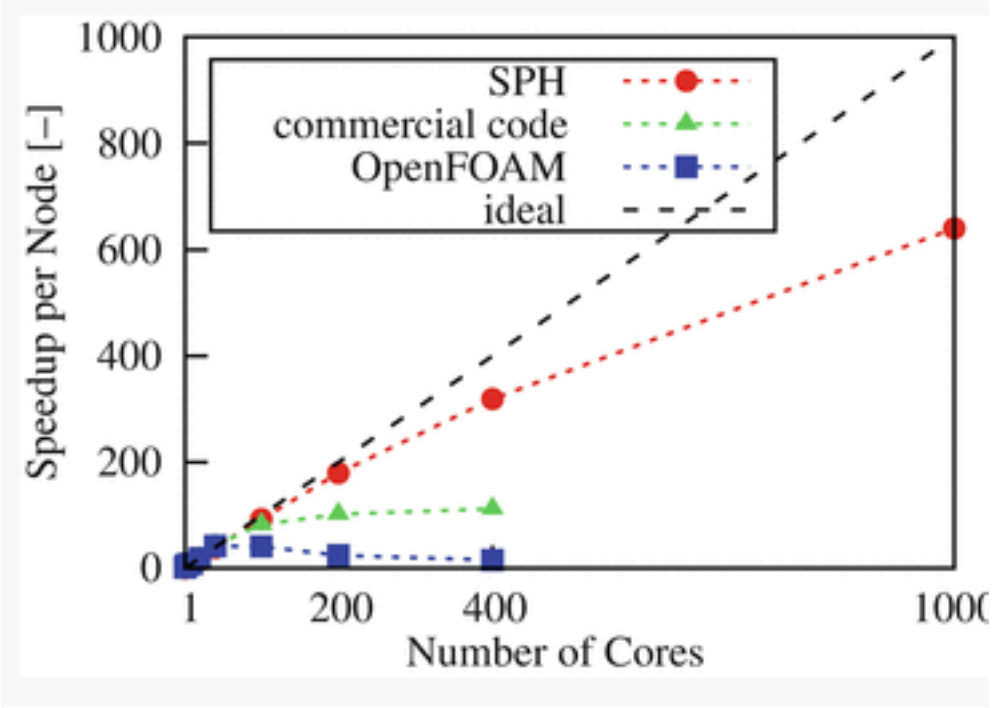

Fig. 6 – Scalability of SPH and other CFD methods. Taken from Braun et al. (2016) (60)

The vertical axis in figure 6 is labelled 'Speedup'. This is simply a quantity which indicates the relative performance of various algorithms. It is inversely proportional to the time taken to complete a task (61). It is the pure simplicity of SPH that allows implementations to achieve such scalability. The tasks are separable to the extent that cores can efficiently distribute calculations without having to constantly communicate. When the added complexity of grid tracking and ensuring conservation are overlaid this is not so simple. Indeed, the above-mentioned research is carried out in the application of primary air-blast atomisation and concludes that SPH is adequate for this task. The authors use the experimental comparison shown in figure 7 as evidence of accurate simulation. From figure 7 it can be seen that although initial formation of ligaments looks to be modelled accurately, the subsequent instability and breakup of those ligaments appears to be lacking in accuracy. This leads on to a critical point that must be emphasised: one cannot simply state the superiority of SPH on the basis of more efficient computational resource usage. The accuracy of the results is also important, and in that regard the desired output quality is highly relevant.

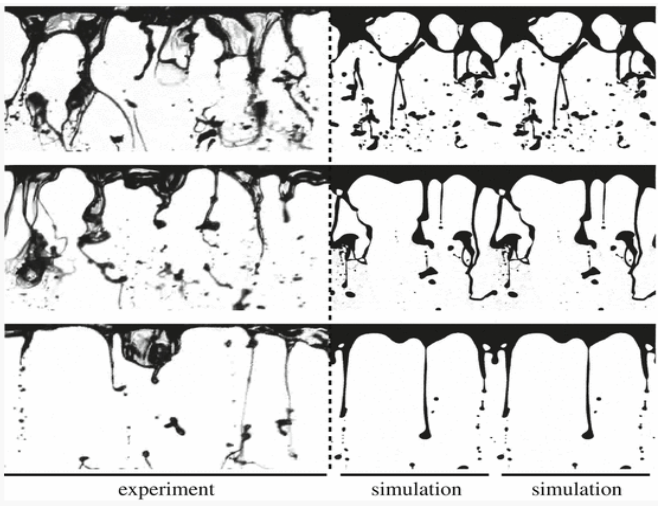

Fig. 7 – SPH simulation of primary atomisation. Taken from Braun et el. (2016) (60)

One promising avenue which is currently being developed in France at the Universities of Rouen and Havre is combining SPH with Eulerian methods within the open source platform, OpenFOAM (62) . When testing two phase injection scenarios against fine mesh pure Eulerian techniques, calculation time was 70% lower. When tested for injection in a turbulent second phase fluid, the calculation time was reduced by 55%. The researchers claim that the results found were very good and evidence visual similarity, however little numerical evidence is given for similarity for the more computationally efficient simulations. The team cites a paper from Italy (63) which demonstrates the accuracy of an SPH model for Ocean jets as an example of a high-fidelity solution, with velocity variations between SPH and icoFOAM (a pure Eulerian method) being limited to under 0.5%. The report from Rouen and Havre also charitably mentions a number of areas for improvement which will be discussed in the next section.

6.2. Weaknesses of SPH

The aforementioned French research (62) identifies two structural issues with the SPH approach that they have been looking into. The primary frustration is based on SPH's particle focussed nature. Since each particle is considered individually, it is more difficult to implement boundary conditions where the user may wish to define a set flow in or out of a chamber, for example. In a purely Eulerian model, the boundary condition can simply be implemented by forcing the velocity term at various grid points and allowing the other Navier-Stokes terms to correct accordingly, whereas ordering 'particles' to accelerate infinitely quickly in the other direction when encountering a boundary is plainly not physically sensible.

The second, more empirical problem encountered was the observation that SPH tends to suffer when faced with large shear stresses. This is not surprising to encounter since viscosity was a key weakness identified by Gingold and Monaghan in the 80s when SPH was mostly confined to astrophysics (42). A discussion of this research can be found in section 4. The issue of viscosity inaccuracy frequently appears and is definitely an issue that the advocates will need to solve before SPH can hope to become a mainstream, all-round package. In the astrophysics field, the issue was solved by imposing artificial viscosity onto the system and it seems that it may be sensible for the French researchers to incorporate such an approach into the coupled SPH/Euler model.

7. Conclusions

As described in section 1.2, the conclusions of this research project will aim to circle around to the original numbered objectives. Each of the four objectives will be concluded briefly, with significant emphasis on the last which delivers the overall conclusion of the report on the question of whether SPH is more effective than conventional CFD, particularly for atomisation. There are a number of recommendations that may guide software choice.

7.1. CFD Methodology Summary

Conventional computational fluid dynamics employs a grid based Eulerian approach to numerically estimating the consequences of the Navier-Stokes equations on a flow, given certain boundary conditions such as a solid surface, inlet pressures and flows. It is now an established field into which much attention and funding has been directed, meaning that the many underlying flaws have been resolved and complexities have been layered on top to improve fidelity and usability. OpenFOAM is the industry standard for computing flows as it is open source and allows plenty of flexibility for implementation.

While conventional CFD is a robust and tested method, computing time is a very precious resource in today's high demand environment and so pressures on CFD research to improve radically the computing demands of available software are as high as ever. Various papers, as discussed in section 3 have shown CFD to be very adequate when computing time is not as much as a factor.

7.2. SPH Methodology Summary

Smooth Particle Hydrodynamics is a radical innovation in the field of CFD in that it disposes with the idea of looking at flows in an Eulerian, frame-of-reference manner, and instead follows the Lagrangian approach of tracking individual fluid packets. These oversized fluid 'particles' act as if they have a sphere of diminishing influence surrounding them, mathematically represented by a 'kernel' which allows direct integration of transport properties to be done theoretically much faster. While originally developed by physicists looking to understand inter-stellar dynamics, SPH is now making a name for itself in the world of atomisation and arguably further real-world applications.

7.3. Atomisation Summary

With applications from crop management to engine fuel dispersion, atomisation is an area of crucial importance to the way of life that humans have become accustomed to, and more importantly atomisation is a huge part of our future. As such, it is important that academics and commercial entities alike gain as solid an understanding of this microscopic phenomenon as possible.

The methods used to enact the primary atomisation of fluids, including formation of ligaments and subsequent breakup through exploitation of Kelvin-Helmholtz and Rayleigh-Taylor instabilities, are relatively well understood. The area that now needs further work is asking how the atomised droplets then proceed to break up further as a result of interacting with the secondary fluid, commonly air. Some research is pursuing the path of attempting to merge existing two-phase droplet theory with hard-sphere fluid interaction in a conventional CFD framework, while other research is focussed on developing the new field of SPH with the intention of eliminating current inadequacies of analysis.

7.4. Relative Efficacy of SPH, particularly for atomisation

SPH is a remarkably effective technique when used in favourable situations. In many examples, computing time for fluid analyses have been shown to be dramatically reduce computing time. Additionally, SPH is a more intuitive method for modelling fluid flows because the idea is to use quasi-particles to model actual molecular particles, albeit on a much larger scale and so SPH is often far simpler to implement. This advantage also helps to make SPH a much more scalable computational problem than most conventional CFD software packages. Therefore, when

considering which software to choose for a study, it may be worth considering whether huge multi-core machines or computer networks are being used, as these will almost certainly be more suited to performing SPH analyses.

SPH is suited to scalable computer systems.

The issue that faces SPH is similar to the early problems that will have been experienced when implementing conventional CFD packages. There are some scenarios where SPH just does not perform as well. For example, viscosity has always seemed to be an issue for SPH packages, ever since the 80s when physicists observed issues with cloud interaction to now when at the cutting edge of SPH research, advocates are admitting that high viscosity scenarios are still an issue for their software.

SPH does not handle viscosity-dominant situations well.

While SPH is certainly promising in the long term as a clean and simple alternative to the established CFD model, it does not have a proven track record across a range of engineering applications. Current CFD methods are very effective and ultimately are clearly adequate so as to stimulate a huge demand for them. While computing time is very precious, even a potential all-round method like SPH would not solve this. Computing power would still be in demand because more resolution would be demanded. Significant advances in the field of atomisation have been made accurately without the need for SPH implementation by developing and building on the work in place to back Eulerian CFD, for example overlaying empirical data into a simplified CFD model.

SPH is a great prospect for the future, however at this point the current methods are adequate in most scenarios and have a proven track record which can be built on. SPH should be funded for research but does not yet constitute a reliable all-round method.

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Imperial College
London

DEPARTMENT OF
MECHANICAL ENGINEERING

2018-2019 ME3 LITERATURE RESEARCH PROJECT

Meeting Log

STUDENT:	H. R. Hart	SUPERVISOR:	A. Taylor
TITLE:	Smooth Particle Hydrodynamics.		

Meeting	Date	Student Signature	Supervisor Signature
Week 2	11/10/2018	H Hart	A Taylor
Week 5	2/11/2018	H Hart	A Taylor
Week 7	22/11/2018	H Hart	A Taylor
Week 9	7/12/2018	H Hart	A Taylor