Abstract
In this paper we present a modified equation of state law for use within Smoothed Particle Hydrodynamics (SPH). We then compare this to existing solutions for convection problems, specifically those obtained using the Boussinesq approximation. These developments are required in order to accurately model complex and thermally driven problems, such as natural convection and other applications particularly seen in geophysics. In SPH, practical examples of heat conduction and energy are scarce, when compared with fluid flow formulations that determine pressure simply from density and an artificial sound speed. Previous work has involved the inclusion of temperature and energy effects into the calculation of pressure to solve for simple problems where thermal buoyancy is the only source of dynamics. While there are a number of heat transfer algorithms in use within SPH, it is uncommon in literature to couple the thermal energy of the system to the governing equations being used to determine the dynamics of the system. This work discusses conventional equations of state, previous work performed in this area in terms of introducing a thermal influence into the dynamics of the overall system and other approaches that have been identified to date in wider literature. The results produced from this new approach to the SPH equation of state are discussed and compared with traditional equations of state, as well as with other mechanisms for instigating thermally driven convective flow, such as the use of the Boussinesq approximation. The problem considered is that of a differentially heated cavity for a prescribed set of conditions. These developments facilitate future work towards a more overarching energy implementation of the governing equations to better represent the influence energy can have on a system when purely isothermal flows are no longer being considered for use in much more complex physical systems.

Introduction
Heat transfer in fluids and its effect upon motion is of interest in many areas within science and engineering including desalination plans, within reactor cores in power plants and in complex enhanced oil recovery techniques such as steam assisted gravity drainage. This is especially true when considering complex multi-fluid or multi-phase interactions that are seen in these cases. Natural convective flow is one particular type of flow where the thermal dynamics of a system are especially critical. One of the most commonly used methods to drive fluid flow in a natural convection model, also known as a buoyancy driven problem, is the use of the Boussinesq approximation. This approximation allows models to assume that a small change in temperature will have an appreciable effect upon the density of a substance in the case where there are no dominating forcing terms present. This assumption is used in a wide variety of different numerical schemes in literature. The major problem with the Boussinesq approximation is that it is only truly valid for small differences in temperature. In order to obtain a more encompassing numerical method, it is important to have a robust method capable of handling larger temperature gradients. In this work Smoothed Particle Hydrodynamics (SPH) is used to model natural convective flow utilising Boussinesq implementations as well as comparing some alternative approaches. For this work, the regime used will remain valid for the Boussinesq approximation to show agreement between methods before extending this to greater temperature gradients in future work. While the general foundation for problems involving thermal conductivity within SPH has been around for some time [3, 4], it has not been widely applied in literature. For problems more complex than straightforward solid conduction problems, it is necessary to consider what effect temperature will have upon the dynamics of a system.

SPH is a fully Lagrangian particle based method and has been widely used since its inception in the areas of momentum driven fluid flow to great success [8]. However, there has been limited investigation into areas of buoyancy driven flow. While there has been some modelling of buoyancy driven flows, such as modelling natural convection in a closed box and of the Rayleigh-Bénard instability [2, 3], this has been done using a modification to the standard SPH body force term via application of the Boussinesq approximation [11]. The use of SPH should allow for these phenomena to be modelled without the utilisation of ad hoc relations. Since SPH is a compressible fluid formulation that uses a rigid equation of state to approximate incompressibility, the Boussinesq approximation should not technically be applicable and this type of phenomenon should instead be more robustly handled through the use of a more physically correct equation of state. While there has been a number of examples of heat conduction in SPH [3, 4], there has been little agreement in literature in regards to how to connect energy and motion in the system, or if this is even possible. One of the first instances where this coupling could occur would be within the equation of state and in literature, there has been little work or discussion around this. There have been examples in wider literature of using energy to influence the governing dynamic equations in SPH [1], but this has mostly been used as diffusive tuning parameters and none have taken the temperature into account. Previous work in this area has been to include the source for motion for a thermally driven system to be within the equation of state [10]. With commonly used modifications to the basic SPH method such as the use of particle number density [6, 12, 13] this allows the application of thermal effects in ways other than directly modifying a body force. In this paper, it will be shown that it is possible to obtain thermally driven convective flow without modifying the body force component of the SPH governing equations. The source of this will come about from a modification to the density of the system, giving a buoyancy density and then comparing this to Boussinesq driven results as well as other work which has made similar modifications in the past with success [11].

SPH Formulation
In general SPH theory, a volume is discretized into a set of dis-
ordered particles (or integration points), all possessing a position vector of \( \mathbf{r}_i \). The SPH integral approximation for a given field quantity as a function of position, \( A(r) \), is given by

\[
A(r) = \int A(r') \delta(r - r') \, dr'
\]  

(1)

where \( \delta \) is the Dirac delta function.

In order to be able to evaluate this function a numerical approximation is taken

\[
A(r) = \int A(r') W(r - r', h) \, dr'
\]  

(2)

where \( W(r - r', h) \) is the kernel or smoothing function for the two interacting particles, \( r \) and \( r' \), and \( h \) is the smoothing length, which is the bounds of interaction distance for particles. As \( h \rightarrow 0 \), \( W(r - r', h) \rightarrow \delta(r - r') \) which gives the exact result of the interpolant \( A(r) \) above.

We also set the condition of normalization so that

\[
\int W(r - r', h) \, dr' = 1
\]  

(3)

and generally approximates a Guassian.

The next stage of the SPH method is to discretise (2) in order to implement a numerical procedure for it. This is done by approximating the function by a summation interpolant over the particles, \( N \), that are present in the system. This as seen for an arbitrary particle, \( i \), as follows

\[
A(r_i) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} A(r_j) W(r_i - r_j, h)
\]  

(4)

where \( m_j \) and \( \rho_j \) are the mass and density of particle \( j \) at a position \( r_j \). Equation (4) suggests that this summation is performed over every \( j \) particle present within the problem space but in practice this translates into only the particles contained within, generally, \( 2h \) due to the rate at which the value of the smoothing function deteriorates with respect to particle separation distance. The value of \( h \) is constant and generally set as the initial particle spacing.

The ratio of \( m_j/\rho_j \) represents the approximate volume of space that each particle takes up and this maintains the consistency between the continuous and discrete forms of the field equation being used. It follows on from equation (4) that the gradient of our field value is

\[
\nabla A(r_i) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} A(r_j) \nabla W(r_i - r_j, h)
\]  

(5)

Using this we have our general field equations used in our implementation of SPH

\[
A(r_i) = \sum_{j=1}^{N} \frac{A(r_j)}{n_j} W(r_i - r_j, h)
\]  

(8)

\[
\nabla A(r_i) = \sum_{j=1}^{N} \frac{A(r_j)}{n_j} \nabla W(r_i - r_j, h)
\]  

(9)

**Governing equations**

The governing equations for SPH are those for the Navier-Stokes equation for incompressible viscous flow

\[
\frac{dv}{dt} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 v + g
\]  

(10)

where \( v \) is the velocity vector, \( t \) is time, \( \rho \) is pressure \( v \) is kinematic viscosity and \( g \) is gravitational acceleration. It is also noted that for SPH implementations, due to its particle based nature, advective terms are handled intrinsically through the movement of the particles.

Breaking the general equation for motion into its components and applying the SPH discretization methods we get the pressure component as

\[
-\frac{1}{\rho} \nabla p = \frac{1}{m_i} \sum_{j} \left( \frac{p_i}{n_i} + \frac{p_j}{n_j} \right) \nabla W_{ij}
\]  

(11)

and the viscous component as

\[
\nu \nabla^2 v = \frac{1}{m_i} \sum_{j} \frac{n_i n_j}{n_i n_j} \frac{\nabla W_{ij}}{|r_{ij}|^2}
\]  

(12)

where \( \mu \) is the dynamic viscosity.

The rate of change in internal energy due to conduction and with spatially or thermally varying conductivity and without any generation being present is

\[
\frac{dU}{dt} = -\frac{1}{\rho} \nabla (k \nabla T)
\]  

(13)

where \( U \) is internal energy, \( k \) is thermal conductivity and \( T \) is temperature. Once again, SPH discretization methods are applied and the final expression as a function of particle number density as follows

\[
\frac{dU}{dt} = \frac{1}{m_i} \sum_{j} \frac{4k_i k_j}{n_i n_j} \frac{T_i - T_j}{|r_{ij}|^2} \nabla W_{ij}
\]  

(14)

Since energy exchange is always balanced between a given pair of particles that are interacting, it is ensured that thermal energy conservation is maintained and that heat will flow from a higher temperature to a lower temperature inherently. This particular formulation is modified from a straight forward result in order to account for potential discontinuous thermal conductivities [4] and is shown in further detail in previous work [10].

Instead of determining the temperature of a particle during the time stepping portion of a simulation, we choose to calculate it as a part of the scope of the equation of state and to instead iterate internal energy during the time stepping phase, as per
The equation of state used for this method is that put forward governing mechanics. It is not possible to modify the density without breaking other density of the fluid but for numerical reasons in most methods, this variation to the body force is justified under the assumption in temperature and the ambient temperature.

Modified Equation of State

The Boussinesq Approximation

The simplest implementation of the Boussinesq approximation is done by substituting a term onto the body force component into equation (10). This takes the form of \( -\beta g \Delta T \) yielding

\[
\frac{\partial w}{\partial t} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 v - g\beta \Delta T
\]

where \( \beta \) is the thermal diffusivity and \( \Delta T = T - T_0 \) is the difference in temperature and the ambient temperature.

This variation to the body force is justified under the assumption that the effects of temperature difference is sufficient to alter the density of the fluid but for numerical reasons in most methods, it is not possible to modify the density without breaking other governing mechanics.

The equation of state used for this method is that put forward by Morris [9]

\[
p = c_0^2 (\rho - \rho_0)
\]

where \( c_0 \) is the artificial speed of sound and \( \rho_0 \) is a reference density. The artificial speed of sound is estimated from the parameters of a system and is usually tuned until a converging result is obtained and it is through this that the quasi incompressibility seen in SPH is achieved.

Additionally, there are two relevant dimensionless numbers that are used in literature when describing regimes of flows being examined. These are the Prandtl number

\[
Pr = \frac{\nu}{a}
\]

where \( a \) is the thermal diffusivity of a fluid, which describes the ratio of momentum to thermal diffusivity within a fluid and the Rayleigh number

\[
Ra = \frac{g \beta L^4 \Delta T}{\nu a}
\]

where \( L \) is the characteristic length scale, which describes the ratio between buoyancy and viscosity within a fluid.

Modified Equation of State

The equation of state is used in SPH to determine the pressure a given particle exerts on its surroundings. For standard incompressible flow problems, using a truly physical equation of state will result in prohibitively small time steps. As such, fluids are modelled as quasi-incompressible. This also leads to most equation of states being modified on a case by case basis. The simplest example of an equation of state is the ideal gas law, which while used for weakly polar gases at low pressures and moderate temperatures, is indicative that temperature and energy play an important part in the dynamics of a system. Energy is not typically considered in standard SPH formulations and thus the more standard equation of states used, as seen in Equation (17), is based on a the speed of sound within the fluid being modelled, as well as its density [7].

Previous work [10] demonstrated the first steps towards developing a more encompassing equation of state for buoyancy driven flow within SPH. Since SPH is a compressible fluid formulation that uses a rigid equation of state to approximate incompressibility, the Boussinesq approximation should not technically be applicable and this type of phenomena should instead be more robustly handled through the use of a more physically correct equation of state.

As a result, the equation of state for the alternative implementation for thermally driven flow is

\[
p = c_0^2 (\rho - \rho_0) (1 + \beta \Delta T)
\]

Unlike previous equations, in this instance \( \beta \) is used as an artificial tuning parameter much like the use of the artificial speed of sound, \( c_0 \), in the more standard equation of state. This modification comes about from examining other work such as Szewc et al. [11]. This has to date produced the most effective implementation of a non Boussinesq approximation method for natural convection within the realm of SPH in literature. A drawback is the utilization of a background grid in order to assist with the calculation of a hydrostatic force, used to compliment the use of a buoyancy density. The way in which the density has been modified in this previous work has been drawn upon for use in modifying the equation of state in a similar fashion as shown in equation (20).Whilst the density in this work has not been modified, results have shown that it will require refinement in the future to increase robustness.

Comparison of Methods

Temperature and velocity visualisations are presented for a differentially heated cavity in Figure (1). The cavity is 1m x 1m in size with the left and right boundaries being isothermal with a maintained temperature of \( T_L = 1^\circ C \), \( T_R = 0^\circ C \) and the remaining fluid at an initial temperature of \( T_0 = 0.5^\circ C \). The fluid is modelled with \( \rho = 998 \text{ kg/m}^3 \), \( \mu = 0.001 \text{ kg/m.s} \), \( Pr = 0.71 \) and \( Ra = 10^5 \). The problem space was discretized into approximately 5000 particles (with some non-interactive boundary particles removed at initialization for efficiency reasons) and the problems were run until steady state was satisfied.

Figure (1) shows temperature, velocity in the x direction and velocity in the y direction for the Boussinesq formulation along the top row and analogous results for the modified equation of state formulations along the bottom row.

These results show good agreement between the two formulations. Notably, the overall profiles matched very well for the temperature visualisations. There appeared to be some smoothing issues within the modified equation of state formulation results for velocities but again, the overall shape was well matched. The other issue with the modified equation of state formulation is the excessive amount of compressibility seen in the fluid. This is a result of the equation of state being more easily driven by the gravitational body force present due to the wider range of pressures exhibited during the simulation because of the thermal influence.

From this, further work will involve refining the tuning parameters to alleviate these effects. This will include a further examination of the coefficients of the equation of state. These components include the unmodified speed of sound parameter as well as the density itself that is being used. As a part of this, a buoyancy density will be investigated in the future [11]. In addition, this formulation will be further improved by including the energy of the system more directly as a correcting parameter to alleviate any increased artificial effects seen due to the wider range of pressures experienced. Relating to the problem set up
itself, while the height is the only dimension that defines the Rayleigh number, the overall aspect ratio of the problem space may influence results. Though an increased in width is not expected to alter results significantly, it is something that will be investigated in further work.

Conclusions

The Boussinesq approximation has wide use throughout literature for buoyancy driven fluid flow. However, it is only valid for a relatively narrow range of thermal problem configurations. As such, it is desired that it be possible to formulate an approach which can handle a greater range of temperature gradients and still yield accurate results. In this work we have demonstrated a standard Boussinesq approximation implementation for a prescribed set up. This was then compared to results obtained for a modified equation of state approach for the same set up. Whilst there was some smoothing errors in the velocity profiles and extra compressibility effects seen, there was overall good agreement between the results in order to justify further work in this line with the intention of deriving a more physically robust equation of state for use in both buoyancy driven problems and more traditional momentum driven problems.

References


