Numerical Simulation of a Steel Converter Using Smoothed Particle Hydronamics

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Abstract

In the steel making process, high carbon content liquid pig iron is poured into a basic oxygen converter. Oxygen is top blown onto the fluid surface at high velocities to reduce the content of carbon and other impurities within the liquid metal to desired levels. The behaviour within the converter cannot be observed because of the extremely high temperatures, so to gain insight into the activity within in the converter numerical simulation methods are required. A smoothed particle hydronamics (SPH) methodology method has be implemented to model the multi fluid behaviour of this system. SPH is a Lagrangian particle based method of discretizing the Navier-Stokes (NS) Equations which are used to describe fluid flow. The contents of this paper will describe the SPH methodology in detail as well as discuss its application in simulation of the oxygen converter.

Contents

Chapter 1

The Navier-Stokes (NS) Equations

1.1 History

The Navier-Stokes (NS) Equations, are a set of partial differential equations named after Claude-Louis Navier and George Gabriel Stokes which are used to model the behaviour of Incompressible Newtonian Fluids. The set of equations were originally derived in the 1840s through fundamental conservations laws (momentum, mass, continuity and energy) in addition to first order approximations. Later is was shown that the NS Equations could also be derived from molecular dynamics in the early 1900s as well as through cellular automata in the 1980s. The equations are considered to be some of the most important equations ever formulated, despite this fact a unique three dimensional solution (or anti- solution) has yet to be found. The search for a solution to the Navier-Stokes Equations have led them to be included in the Clay Mathematics's seven Millennium Prize Problems which offers a million dollars to the first person to provide a valid or prove the existence of a solution of one of the seven problems. Even without a unique solution the equations can be usefully utilized through discretization and approximation techniques so that these set of equations can be used to understand fluid behaviour accurately.

Chapter 2

Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) is the utilization of computers to help solve the NS Equations for fluid problems. Since the 1960s computers have been strong enough to be used on the NS Equations to model high Reynolds number fluids. CFD methods are broken up into two general categories;Eulerian CFD and Lagrangian CFD .

2.1 Eulerian Methods

Eulerian methods, the more common of the two, are methods that are based off analysing specific locations in space at which a fluid passes through in time. These locations are defined by a "grid" or a "mesh". At the cross sections of the mesh, values such as velocity, pressure etc. can be determined. Naturally the tighter knit the mesh the more accurate results a simulation can return.

2.2 Lagrangian Methods

Lagrangian methods on the other hand do not require a mesh, and as such are often referred to simply as grid-less or mesh-less methods. Instead of analysing locations in space in which the fluid body passes through, the fluid body is broken up into a finite number of fluid parcels or particles which follow the motion of the fluid. At these particles locations fluid values can be determined. It may be useful to think of particles as moving grid points that

displace along with the fluid. Eulerian methods can generally produce more accurate results than Lagrangian methods, however this is heavily at the expense of computational time and power required. Lagrangian methods though, not as accurate are much faster and simpler for the computer to process. One reason for this is that usually in Lagrangian methods mass of is assigned to each particle which greatly simplifies mass conservation.

Chapter 3

Smoothed Particle Hydronamics (SPH)

SPH is a Lagrangian CFD method initially developed for astrophysical simulations by Gingold, Monaghan and Lucy in 1997. Since its original formulation SPH has been adapted and modified to fit a variety of physical problems including multi fluid flow and compressible solid mechanics problems. SPH is an interpolation method which determines field values such density, pressure and viscosity based on the influence of neighbouring particles.

3.1 Pros

- Pressure terms are calculated based on a particle's relative densities. Unlike grid-based methods that require computationally exhausting solving of linear systems of equations, SPH relies on the neighbouring particles to determine the pressure term.
- Mass conservation is guaranteed .Each particle carries a set mass which eliminates the need to solve for mass.
- Fluid boundaries do not need to be expressed explicitly. Multi density systems will naturally separate and create free surfaces.
- Computationally cheaper compared to Eulerian methods. SPH is so much faster that is can be used for real time and even interactive simulation (albeit at the cost of accuracy).

3.2 Cons

3.3 The SPH Equations

The key feature of SPH is it's interpolation of field values based on the weighted sum of neighbouring particles. To determine a scalar field value A, at the location of a particle, the particle will take in weighted contributions from surrounding particles that fall within its range of influence. This range of influence is called the "smoothing radius", which is extended radially outwards from the particle. The amount of contribution that a neighbour particle is dictated by the "smoothing function" which is a function that takes into account the smoothing radius h as well as Δr, the distance to the neighbouring particle. More details about the smoothing functions will be provided later.

$$A_s(r) = \Sigma_j m_j \frac{A_j}{\rho_j} W(r - r_j, h) \tag{3.1}$$

Where $A_s(r)$ is the field value, m_j is a neighbour particle's mass, A_j is the neighbour particle's field value, ρ is the neighbour particle density, $W(r - r_j, h)$ is the smoothing function that takes in the distance between particles $r - r_j$ and the smoothing radius h in as parameters. Intuitively this equation should be easy to understand, what it states is this: To determine the value of a specific field value at a particle location (eg. density, viscosity etc) take the sum of of each neighbouring particle as j iterates from the first neighbour to the last and multiply it by the smoothing functions which determines the neighbours contribution based on the distance of separation. The smoothing radius has compact support, meaning that if the distance between the particles is greater than the smoothing radius then the contribution of the neighbour particles will be zero. The closer the neighbour the larger the affect on the centred particle.

$$\nabla A_s(r) = \Sigma_j m_j \frac{A_j}{\rho_j} \nabla W(r - r_j, h) \tag{3.2}$$

$$\nabla^2 A_s(r) = \Sigma_j m_j \frac{A_j}{\rho_j} \nabla^2 W(r - r_j, h) \tag{3.3}$$

similarly the gradient and the Laplacian can be expressed as above. A nice property of the SPH formulation is that when taking field derivatives only the derivative of the smoothing function needs to be considered.

Let's look at an example at how the field value ρ density can be obtained through the SPH formulation.

$$\rho(r) = \Sigma_j m_j \frac{\rho_j}{\rho_j} W(r - r_j, h) \tag{3.4}$$

Plugging ρ density into the SPH equation gives us the following, which can later be used to calculate the pressure acting on particle.

$$\rho(r) = \Sigma_j m_j W(r - r_j, h) \tag{3.5}$$

Chapter 4

Internal Forces

4.1 Pressure

The pressure is linked to the density through the ideal gas equation. An alternative to using the ideal gas equation is to use Tait's Equation.

$$p = k(\rho - \rho_0) \tag{4.1}$$

Where p is the pressure, k is the gas stiffness, ρ is the calculated density and ρ_0 is the rest density.The stability of the fluid system is dependant on the the pressure term and the viscosity term. The pressure force is a spring type force, while the viscosity acts as a damping force. Each particle is given a rest density ρ_0, if the calculated density varies from the the rest density then a pressure force will act on the particle to restore it to ρ_0. Realistically liquid densities should not be very compressible , however maintaining incompressibility with SPH can be difficult. Ideally k should be the real world number however in simulations large values of k can result in extreme numerical instability. The best that can be done is the assign a value for k that is as large as possible.

4.2 Viscosity

Chapter 5

External Forces

5.1 Gravity

5.2 Surface Tension

5.3 Buoyancy

Chapter 6

The Steel Converter

6.1 System Specific Challenges

The modelling of a steel converter with SPH presents a few challenges that generally are tricky to handle with SPH. First off the the system is a multiphase system containing liquid steel and oxygen which can be hard to model because of large density differences. In this case the density ratio is extremely large with the liquid steel's density being over seven thousand times denser than the oxygens. The stability of the SPH fluid is controlled by the pressure term which works to restore a fluid body to its rest density when it is compressed. The pressure term is controlled by the calculated density which is the weighted summation of a neighbouring particle densities. As such, as an oxygen particle approaches the surface of the liquid steel, it will experience a large sudden increase in calculated density as it takes the steel neighbour particles into account. Conversely the steel particles will not experience a large pressure force do to the air particles unless there is an extremely large number of them.

The second difficulty with this system is the high velocities. The oxygen that exits the lances is travelling at high a velocity which can present problems if the time step is not sufficiently small enough. At the steel-oxygen interface if an oxygen particle is travelling too fast, it can pass through the steel boundary before the steel even interacts with it. The problem is the combination of the high velocity and the low density makes it difficult for the air particles to properly interact with the liquid steel surface. The time step cannot be realistically reduced further without requiring significantly more computation time. To deal with this issue modifications can be made

to the SPH code.

6.2 Pseudo code

6.2.1 Initialize Parameters

6.2.2 Neighbour Search

6.2.3 Density

6.2.4 Pressure

6.2.5 Forces

6.2.6 Acceleration

6.2.7 Output

6.3 Particle Types

6.3.1 Water/Steel

6.3.2 Air/O2

6.3.3 Boundary

6.4 Geometry

6.5 Visualization

6.5.1 Paraview

6.6 Stability

6.7 Modifications

6.7.1 Element Method Coupled SPH

6.8 Results

6.8.1 Dam Break

6.8.2 Surface Tension Test