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The direction decoupled Quiet Direct Simulation method for rapid simulation of axisymmetric inviscid unsteady flow in pulsed pressure chemical vapour deposition

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ABSTRACT

Pulsed Pressure–Chemical Vapour Deposition (PP–CVD) is a thin film deposition process which employs a highly unsteady flow with wide dynamic range of pressure. The large, time-varying density gradient during a PP–CVD process cycle produces a flow field in which the Knudsen number varies from the near-continuum to the rarefied regimes, making Direct Simulation Monte Carlo (DSMC) prohibitively expensive. The present directional decoupled Quiet Direct Simulation (DD-QDS) method is a novel kinetic-based flux scheme that computes fluxes of mass, momentum and energy at the interface of computational cells in a highly computationally efficient manner. The Maxwell–Boltzmann equilibrium distribution is enforced locally at each computational cell at each time step. In this paper, an axisymmetric second order directional decoupled QDS scheme is used to simulate highly unsteady flows encountered in PP–CVD reactor. Two simulations were conducted to investigate the PP–CVD reactor flow field at 1 Pa and 1 kPa reactor base pressures. The assumption of the local Maxwell–Boltzmann equilibrium distribution used in the QDS scheme is verified by examining the gradient length local Knudsen number based on the density, and by estimating the average number of molecular collisions within each computational cell in one computational time step. The validity of the local equilibrium assumption is found satisfactory at 1 kPa reactor based pressure but not at 1 Pa. The limitation of the QDS scheme in modelling PP–CVD flow was also investigated. The time required to establish the quasi-steady under-expanded jet is found to be ~4 ms, and the jet dissipates within 0.5 ms of the end of injection. This important information is required to set up PP–CVD operating conditions which give uniform film deposition.

1. Introduction

1.1. Development of the direction decoupled Quiet Direct Simulation method

There are a number of approaches for the simulation of gas flows and a large variety of solution methods depending on the nature and level of rarefaction of the flow. In the conventional Computational Fluid Dynamics (CFD) approach, finite volume methods have been used extensively to solve the Euler or Navier–Stokes equations. Due to the complexity of the governing equations, computational cost is high in the conventional CFD methods particularly if a turbulence model, for which extra equations must be solved, is required in the simulation. There is also usually the need of extra care in meshing of the computational domain in order to ensure accurate results, convergence and stability of the simulation. In addition, in unsteady flow simulation, it would be difficult to generate a fixed computational mesh suitable for the constantly changing flow field. An adaptive mesh may be used in order to ensure the grid alignment with the flow but this requires extra computational resources which may reduce the computational efficiency.

An alternative is a kinetic-theory based approach that takes into account the particle-based nature of gases in simulating the flow field. The most widely-accepted particle-based direct simulation method is the Direct Simulation Monte Carlo (DSMC) technique developed in the 1960s by Bird [1]. The DSMC algorithm requires the use of random numbers and is thus subject to statistical scatter and requires averaging over a large number of time steps to reduce the scatter in the sampled macroscopic properties. Another particle-based kinetic-theory approach is Pullin's Equilibrium Particle Simulation Method (EPSM) [2]. EPSM simplified the collision phase

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computation in DSMC in which simulated particles are assigned new velocities from the local Maxwell–Boltzmann velocity distribution. However, since the velocities are drawn randomly from the distribution, EPSM also exhibits statistical scatter in the results and as such requires averaging over a large number of time steps in the same way as DSMC.

Another kinetic theory-based approach is the flux-based simulation method. An example of the flux-based kinetic-theory approach is Pullin's Equilibrium Flux Method (EFM) [2]. This method employs split fluxes which are calculated across the interface of two cells by taking the moments of the equilibrium velocity probability function at the interface location. The technique is not subject to the statistical scatter inherent in particle-based methods, however, it involves the use of error function extensively which is computationally complex and expensive to evaluate.

The Quiet Direct Simulation (QDS) method was originally termed Quiet Direct Simulation Monte Carlo (QDSMC) when developed by Albright et al. as a method for modelling plasmas [3] and Eulerian fluids [4]. Smith et al. [5] then reformulated QDSMC to be a conservative finite volume scheme and implemented to second order accuracy. The reformulated QDSMC scheme was renamed QDS due to the lack of stochastic processes. The QDS method is a flux-based kinetic-theory approach which the continuous distribution function employed in previous kinetic-theory based methods is replaced by a discrete mass probability distribution function. The QDS method assumes a sufficiently high collision rate in each computational cell such that the velocity distribution relaxes completely to the Maxwell–Boltzmann local equilibrium distribution during the time step. A Gaussian quadrature (or Gauss–Hermite quadrature) is used to approximate the Maxwell–Boltzmann equilibrium condition. It has been shown that the application of Gauss–Hermite quadrature to the computation of the discrete mass probability distribution function requires only a low number ($\leqslant 4$ in general) of discrete velocities to obtain results virtually indistinguishable from the equivalent continuum results obtained from EFM [5].

The QDS method described in [5] is advantageous for its simplicity, its computational efficiency requiring no evaluation of computationally expensive functions, its deterministic approach eliminating statistical scatter inherent in the DSMC solvers, its localised computation with only the nearest neighbour information required for second order spatial accuracy allowing easy implementation for parallel computation, it is easily extended to multiple spatial dimensions and multiple gas species, and it is unconditionally stable. Yet, it is numerically diffusive and due to the assumption of perfect local equilibrium is capable of solving only inviscid flows at present.

For application to cylindrical or spherically axisymmetric flows, the traditional implementation of QDS would require consideration of volumetric effects on the flux computation. This can become involved when (i) extended to multiple dimensions, or (ii) fluxes are extended to higher order spatial accuracy. Hence, in this paper, the basic QDS scheme [5] is recast as an approximation to the EFM to extend its application to axisymmetric flows, in a manner familiar in conventional CFD, and named as directional decoupled QDS (DD-QDS). It is tested against standard test cases and applied the simulation of the unsteady complex flow encountered in Pulsed Pressure Chemical Vapour Deposition (PP–CVD) process.

1.2. Pulsed pressure chemical vapour deposition process

PP–CVD is a novel manufacturing technique developed by Versteeg et al. [6] to deposit thin films of solid material onto a substrate through a chemical process in repeated pulses. It has shown improved performance over conventional Chemical Vapour Deposition (CVD) methods including high precursor conversion efficiency, film quality and substrate conformity [7–9]. The operating cycle of the PP–CVD process consists of an injection and pump-down phase. During the injection phase, a controlled volume of precursor solution at high supply pressure is injected into a continuously evacuated reactor volume via an ultrasonic atomizer or choked orifice. The injection of precursor mixture is carried out rapidly in the partially evacuated reactor volume, increasing reactor pressure to a maximum. The process is followed by a pump-down phase when the reactor inlet valve is closed while the reactor volume is continuously evacuated by a vacuum pump to achieve a set minimum pressure before the next pulse cycle begins. The rapid injection of precursor solution leads to a high vapour concentration near the reactor inlet during the injection phase while the continuously evacuated reactor chamber causes the fluid density to reduce significantly with time after the end of the injection phase, and with the distance from the inlet. This pulsed process cycle causes a highly unsteady flow field with large density gradients throughout the reactor volume.

Previous numerical modelling of the PP–CVD flow field by Cave [10] using the unsteady DSMC modelling technique developed by Bird [11] found that the highly unsteady nature of the flow makes DSMC simulations extremely computationally expensive. The unsteady flow phenomena coupled with significant density gradient over the flow field also challenges conventional Navier–Stokes CFD solvers. Obtaining converged solutions at an acceptable computational expense using either DSMC or conventional Navier–Stokes solver is particularly difficult for such unsteady flow fields. For these reasons, in this paper, QDS has been investigated as a candidate method for rapid approximation of the PP–CVD flow field with acceptable accuracy. A speedy solution is essential particularly in the customisation of the PP–CVD reactor design and operational conditions selection in meeting a specific application of the thin film deposition technique. The limitations, arising from the assumption of local thermal eqauilibrium, on the accuracy of the QDS solution are explored.

2. Method

The Maxwell–Boltzmann equilibrium velocity distribution function has the form of:

$$p(v) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(v-u)^2}{2\sigma^2}\right) \tag{2.1}$$

where $p(v)dv$ is the probability of finding a molecule with a velocity in the range $v \rightarrow v + dv$, u is the bulk velocity and the velocity variance $\sigma = \sqrt{RT}$. The integration of moments of Eq. (2.1) over infinite velocity range can be represented by introducing the Heaviside step function H_s. This permits the fluxes splitting to approximate the EFM flux expressions given in Eq. (2.2) as:

$$\int_{-\infty}^{\infty} \frac{e^{-(v-u)^2/2\sigma^2}}{\sqrt{2\pi}\sigma} f(v)dv \approx \sum_{j=1}^{N} H_s(-q_j) w_j f(q_j) + \sum_{j=1}^{N} H_s(q_j) w_j f(q_j) \tag{2.2}$$

where $f(v)$ takes the value 1 if the mass flux is to be computed, the value v if the momentum flux is computed, and v^2 if the energy flux is computed. $H_s(x) = 1$ if $x > 0$, else $H_s(x) = 0$ while w_j and q_j are the weights and abscissas of the Gauss–Hermite parameters. The abscissas are the roots of the Hermite polynomials which can be defined by:

$$H_{n+1}(q) = 2qH_n - 2nH_{n-1} \tag{2.3}$$