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The effect of turbulent clustering on particle reactivity

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Abstract

The effect of turbulence on the heterogeneous (solid–fluid) reactions of solid particles is studied numerically with Direct Numerical Simulations (DNS). A simplified reaction system is used, where the solid–fluid reaction is represented by a single isothermal reaction step. It is found that, due to the clustering of particles by the isotropic turbulence, the overall reaction rate is entirely controlled by the turbulence for large Damköhler numbers. The particle clustering significantly slows down the reaction rate for increasing Damköhler numbers which reaches an asymptotic limit that can be analytically derived. This implies that the effect of turbulence on heterogeneously reacting particles should be included in models that are used in CFD simulations of e.g. char burnout in combustors or gasifiers. Such a model, based on the chemical and turbulent time scales, is here proposed for the heterogeneous reaction rate in the presence of turbulence.

Keywords: Turbulent reacting multiphase flow; Char oxidation; Clustering

1. Introduction

Particles that are exchanging mass with a surrounding turbulent flow are found in a wide range of situations, both in nature and industrial applications. Examples of these are pulverized coal combustion in large power plants and fluidized beds in the process industry. A general feature among all these systems is their multi-scale nature, where the smallest scale is typically the size of the particle, or even the internal structure of the particle, while the largest scale is the much larger size of the entire combustion chamber or reactor. In the intermediate range between these two extremes, one finds the scales of the turbulence, which go from the Kolmogorov scale to the energy containing scale (the integral scale). Another common feature is that the particles exchange mass with the surrounding fluid through chemical reactions on the surface of the particles, as e.g. during the oxidation or gasification of char.

The effect of turbulence on different large scale properties of the flow, such as turbulent viscosity, diffusivity and conductivity has been known for a long time. A relatively large number of models have been developed in order to account for these effects,

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such as e.g. the k-ε model [1] and different versions of the Reynolds Stress Model [2]. When homogeneous combustion is considered, relatively good models such as the Eddy Dissipation Model [3], different variants of Probability Density Function models [4] or models based on conditioned parameters such as Conditional Moment Closure models [5] are being used. Veynante and Vervisch [6] review the current state of homogeneous combustion modeling, where they link distinctive homogeneous combustion regimes to different Damköhler numbers, which is the ratio of turbulent and chemical timescales. A perfectly stirred reactor system is used for low Damköhler numbers while reactions take place in thin wrinkled reaction zones for high Damköhler numbers. In essence, the regimes differ in the degree of spatial separation of reactants; while in the homogeneous case all reactants are gaseous, the heterogeneous case contains solid particles embedded in a fluid. However, spatial separation and its effect persists, as inertial particles cluster in turbulence, leading to regions of high or low particle concentration. Experimental and numerical studies of this phenomenon are reviewed in the work of Eaton and Fessler [7]. A detailed numerical investigation can be found in the work of Squires and Eaton [8] and for photos and statistics of preferential concentration of particles in isotropic turbulence in an experiment, the reader is referred to the work of Wood et al. [9]. Annamalai and Ramalingam [10] investigated the combustion modes for particles in a frozen gas phase dependent on their concentration and found that for densely clustered particles, the combustion behavior deviates from individual particle combustion. The present study aims to extend this analysis to heterogeneous combustion regimes in turbulent flows with particles that are clustered by the flow.

A range of efforts to simulate heterogeneous conversion systems under turbulent conditions have been made. Among recent work one can mention that of Silaen and Wang [11] who simulated an existing gasifier with Reynolds-averaged Navier Stokes (RANS) using different turbulence models for the continuum phase and compared their results with measurements. The turbulence effect on particles was included using a stochastic tracking scheme for the particles position, hence turbulence was not taken into account for the heterogeneous reaction rate or transport of gas phase species to the particles. Vascellari et al. [12] ran 2D RANS simulations with kinetics calibrated to experiments and a detailed description of the heterogeneous reactions inside the particle via an effectiveness factor and solving directly for the species partial pressure at the particles surface by assuming local equilibrium. They compare their simulations with measurements from an industrial-scale gasifier and achieve good agreement. Yet, to the knowledge of the authors, only very few studies of combustion or gasification, where account is made for the effect of turbulence on the heterogeneous char conversion, are published, among these are the papers of Luo et al. [13], Brosh and Chakraborty [14] and Brosh et al. [15]. Here, the Direct Numerical Simulations (DNS) approach is utilized, where all turbulence scales are explicitly resolved on the computational grid, and hence the effect of the turbulence is implicitly accounted for.

Despite all the effort that has been put into the development of models for turbulent homogeneous combustion or gasification, no good model has been proposed for turbulent heterogeneous combustion or gasification. This means that when particles that react with the surrounding fluid, such as during char oxidation (i.e. gas phase species react with the solid part of the particle, not the volatile part) are embedded in a turbulent flow, the turbulence is typically never taken into account in the simulations. The goal of this paper is to highlight the effect of turbulence on solid particles using DNS, and to develop a simple model for the influence of turbulence on reactive particles.

2. Implementation

The direct numerical simulations are performed with the Pencil Code [16], a finite difference code for compressible reactive flows that is fully parallelizable and shows good weak scaling behavior. It uses a sixth-order finite difference scheme for spatial discretization and a memory-efficient third-order Runge–Kutta scheme [17] for temporal discretization. The particles are treated in a Lagrangian manner and a cloud-in-cell method [16] is used both to interpolate the fluid phase variables at the particles position and for the back reaction from the particles to the fluid. To achieve a system that is independent of direction, all boundaries are periodic and gravity forces are neglected for particles and fluid alike.

2.1. Fluid phase equations

In order to isolate the effect of turbulence on reactivity alone, we consider a simplified case with only one reactive species, which is treated as a scalar field advected and diffused by the carrier fluid. This reactant is passive for the fluid flow and is assumed to react only with the solid phase in a catalytic manner. As a result, the reactant is converted on the surface of the particle, but no mass and energy is exchanged with the particle. For simplicity, the reaction is further assumed to be neither endothermic nor exothermic. It proceeds at a constant rate λ, which only depends on the surface area of the solid phase. The equation describing the