

DNS for solid fuel flames

Miriam Rabacal^{1,2} and Nils Erland L. Haugen^{3,4}

¹University of Duisburg-Essen, Germany

²Instituto Superior Técnico, University of Lisbon, Portugal

³SINTEF Energy Research, Norway

⁴Norwegian University of Science and Technology (NTNU), Norway

Introduction

Here, a short review of literature on Direct Numerical Simulations (DNS) of solid fuel flames is presented. In this context, solid fuel flames refers to the chemical conversion, through oxidation or gasification reactions, of pulverized solid fuels. Traditional wood log combustion or forest fires are *not* included. The only fuels considered are coal and biomass within particle size intervals relevant for suspension combustion/gasification applications.

In traditional single phase flow simulations, the DNS approach is quite well defined as a solution of the Navier-Stokes equations where all scales are resolved. Here, "all scales" refer to all *fluid* scales down to the Kolmogorov scale of the turbulence. For multi-phase flows the definition of a DNS is not as clear. In this review, three distinct definitions of a multi-scale DNS are presented.

The first, and most strict definition, is the so called resolved particle approach (RP-DNS). In this approach both the particles themselves *and* all the turbulent scales are resolved on the simulation mesh.

In the point-particle DNS approach (PP-DNS), all the turbulent scales are resolved, but the embedded particles are treated as point particles. This requires that the particles are much smaller than the Kolmogorov scale, and hence that they are also much smaller than the mesh size. Since the boundary layer around the particles is not resolved, closure models are used to model the momentum, heat and mass transfer between the particles and the fluid.

The resolved single particle in a quiescent fluid (RP-QF) approach considers one single particle where the particle itself is resolved and the boundary layer may be resolved or modeled. It is assumed that the particle is immersed in a laminar flow and behaves as a perfect tracer.

These three approaches to DNS simulations will be discussed in the remaining sections, and while the main focus had been on coal, recently biomass has become a subject of interest.

The resolved particle DNS approach (RP-DNS)

The RP-DNS approach is the most accurate simulation approach, but also the most CPU intensive. The particles that are relevant for pulverized sold flames are typically significantly smaller than the Kolmogorov scale of the turbulence. Since the particles should be resolved by at least 10 mesh points

in each direction, this implies that the mesh resolution has to be much (typically several decades) finer than in the point particle approach. Due to this, there are currently no papers available in the literature describing the RP-DNS approach for solid fuel flames.

The most relevant work currently available is the work of Deen et al. (2014) [1], where the authors consider 663 stationary spheres that experience simplified exothermal catalytic surface reactions. The spheres considered are large and the fluid is assumed to be quiescent. The same group has also published a review on direct numerical simulation of fluid–particle mass, momentum and heat transfer in dense gas–solid flow [2].

In the RP-DNS approach, the mesh size has to be much smaller than the size of the particles, while in the PP-DNS approach, the mesh size must be much larger than the particles. It is interesting to note that no intermediate approach exist, which can handle particles of the same size as the mesh size.

The point particle DNS approach (PP-DNS)

In the PP-DNS approach, the fluid flow is solved in the same manner as for single-phase flows, but with additional source terms due to the momentum, mass and heat transfer between the phases. In this way, a relatively large number of particles can be handled while the domain size may be almost as large as the domains used for typical single phase reactive DNS'. The main contributions on this topic are from Zhejiang University in China [3] and Newcastle University in the UK [4,5]. Both of these groups have used similar models; for the volatiles they use the competing two-step devolatilization model of Kobayashi, together with a two-step global chemical reaction kinetics for the homogeneous combustion. For the heterogeneous reactions of the char, three global reactions accounting for oxidation and CO₂ gasification are used. In the work of Luo et al. [3], a pulverized coal jet flame is studied in order to provide statistical data for modelling of coal combustion. Brosh et al. [4,5], on the other hand, use the DNS simulations to study the ignition of pulverized coal and the influence of turbulent intensity, equivalence ratio and particle size.

The resolved single particle in a quiescent fluid (RP-QF)

Given its relative low computational cost, the RP-QF approach allows describing heterogeneous and homogeneous kinetics in detail. Therefore, the RP-QF approach is an interesting tool to study the effects of the oxidizing/gasifying environment on particle conversion. Major contributors in this topic have been the University of Sidney, University of Utah, Stanford University, Sandia National Labs, and more recently Politecnico di Milano [6-11]. In general, the modeling approaches are quite similar, but with some distinctive features between codes. The major differences lie in the complexity of the chemistry modeling. All approaches consider a 1-D spherical symmetric domain for simplicity. These groups have contributed with studies that give important insight into the complexity of the oxidation and gasification reactions, and help improve the understanding of experimentally measured gasification and oxy-fuel char combustion and burnout trends in the literature.

SKIPPY (Surface Kinetics in Porous Particles) is a code that describes a steady-state spherical, reacting porous particle and its reacting boundary layer [6-8]. It was originally developed by Prof. Haynes from the University of Sidney and has been further developed in collaboration with the University of Utah [6] and Sandia National Labs [7,8]. Relevant features of the code are as follows: particle

properties are assumed to be isotropic; internal mass transport is described by the Darcy law (assumes low Knudsen number); oxidation and gasification reactions are treated as adsorption-limited; and the particle morphology is modeled. This code has been used to study the effects of the bulk gas composition, particularly under coal oxy fuel conditions, on the char burning rate and to analyze boundary layer and intra particle temperature and species concentration distribution [6-8]. Furthermore, the effects of boundary layer chemistry have also been examined [7].

The Stanford in-house code, developed by Prof. Mitchell, describes a transient spherical porous particle and models film properties [9]. Relevant features of the code are as follows: the particle is described by concentric shells; the particle properties are assumed to be isotropic; the particle is assumed to be thermally thin; diffusion controlled internal mass transport (any Knudsen number) is assumed; oxidation reactions are treated with intrinsic reactivity; and the particle morphology is modeled. This code has been used to evaluate the applicability and efficiency of classical simplifying assumptions used for coal combustion modeling, such as the power law mode and the Thiele modulus relation, over the 3 char combustion zones.

More recently, Niu and Shaddix [10] presented a study where a transient code based on the concentric shells description of the particle was used to study the influence of the ash film and ash dilution on the char burning rate. In this first approach, ash chemistry is not considered.

Finally, Maffei et al. [11] have presented the only study that focuses on biomass conversion. The Milano in-house code describes a transient spherical biomass particle immersed in a perfectly mixed gas. Relevant features of the code are as follows: the particle is described by concentric shells; the particle properties are assumed to be isotropic; diffusion and flow controlled internal mass transport are employed (any Knudsen number); highly detailed in house kinetics is used; and the particle morphology is modeled. This code has been used to study the effects of the bulk gas composition, comparing conventional and oxy fuel conditions, on the char burning rate and to analyze intra particle temperature and species concentration distribution. Currently the group is developing the code to include the boundary layer description, have solid anisotropic properties and to use mobile meshing to take into account the depletion of the porous solid domain.

References

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