Fuel Processing Technology 156 (2017) 43–53

Contents lists available at ScienceDirect

Fuel Processing Technology

journal homepage: www.elsevier.com/locate/fuproc

Research article

Numerical investigation of heavy fuel droplet-particle collisions in the injection zone of a Fluid Catalytic Cracking reactor, part II: 3D simulations

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ARTICLE INFO

Article history:
Received 8 June 2016
Received in revised form 31 August 2016
Accepted 12 September 2016
Available online 5 October 2016

Keywords:
VOF
FCC
Droplet
Particle
Cluster
Collisions

ABSTRACT

This study investigates the collisions between heavy gasoil droplets and solid catalytic particles taking place at conditions realized in Fluid Catalytic Cracking reactors (FCC). The computational model utilizes the Navier-Stokes equations along with the energy conservation and transport of species equations. The VOF methodology is used in order to track the liquid-gas interface, coupled with a dynamic local grid refinement technique in order to minimize the computational cost. Phase-change phenomena, as well as catalytic cracking surface reactions (2-lump scheme) are taken into account. In this paper, the numerical model is extended to investigate the droplet-particle collision process in three dimensions. In order to save computational resources, only half of the droplet is investigated, by imposing symmetry conditions. Firstly, single droplet-catalyst collisions are simulated and compared against the corresponding ones provided by 2D axisymmetric simulations and afterwards, the model is applied for the characterization of the collision dynamics between a single droplet and a particle cluster, i.e. a realistic 3D particle configuration. As the droplet flows through the space between the catalytic particles, important phenomena are observed, such as a) drop levitation due to the formed vapour layer and b) a thin liquid sheet formation, both of which affect the rate of gasoline production, as well as predictions for liquid pore blocking mechanism; a phenomenon frequently observed industrially. Results indicate that gasoline production decreases when the collision target is a particle cluster, instead of same number (as many as in the cluster) single catalysts, as the corresponding contact area decreases.

1. Introduction

The collision of liquid droplets with spherical particles appear in many engineering applications such as particle spray coating, spray drying, as well as inside industrial fluidized bed reactors. An example of the latter, are the FCC (Fluid Catalytic Cracking) reactors, which are an integral part of modern refineries and act as the main focus of the current work. In the FCC reactors, the contact between atomized heavy fuel droplets and solid catalytic particles results in the "cracking" of the long chain heavy petroleum molecules (gasoil) to shorter chain ones (gasoline, LPG), that are industrially more useful.

The "cracking" reactions take place between the vapour produced by the hot evaporating heavy fuel droplets and the catalysts' surface [1]. These reactions occur throughout the whole length of the reactor. However, as pointed out by [2–4], there is a need to interpret in a better way the phenomena that take place in the injection zone of such reactors, as the "pre-cracking" happening in this region affects product yield selectivity [4], while also, as it is observed industrially, the non-evaporated liquid originating from the injected droplets hitting the particles may end up blocking their pores and thus result in their deactivation [5].

Experimental studies (selective studies include [6–10]) have been used in the past in order to investigate this zone, as well as the whole reactor, however, only general observations are made concerning droplet sizes, temperatures, break-up locations and evaporation, due to the difficulty that lies in liquid spray behaviour characterization in this complex mixing zone. Moreover, in Computational Fluid Dynamics simulations [2,3,11–14], the injection zone is investigated from a large-scale perspective, meaning that the level of detail used cannot capture the complex and violent phenomena that happen when cold droplets are injected in the hot injection zone.

Interface tracking methods can provide the advanced level of detail needed for such investigations. In [15–17], the first efforts to involve single droplet dynamics to the FCC industry were recorded, however, to the authors' best of knowledge, the conditions investigated were never close to the real FCC ones. In Part I of the present study, a first try was reported to simulate single droplet-particle collisions at realistic FCC operating conditions, taking into account both droplet evaporation as well as cracking reactions at micro-scale. In Part I, the numerical

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http://dx.doi.org/10.1016/j.fuproc.2016.09.012
0378-3820/

Nomenclature

Acronyms

CFD	Computational Fluid Dynamics
cpR	cells per Radius
DTP	Droplet To Particle size ratio
FCC	Fluid Catalytic Cracking
LPG	Liquefied Petroleum Gas
UDF	User Defined Function
VOF	Volume of Fluid Method

Symbols

D	diameter (m)
$Re = \rho_l u_0 D_0/\mu_l$	Reynolds number (−)
RR	reaction rate (kmol/g_{cat}s)
SSA	specific surface area (m^2/g)
t	time (s)
T	temperature (K)
$\vec{u}$ (u,v,w)	velocity (its components) (m/s)
V	volume (m^3)
$We = \rho_{liq} u_0^2 D_0/\sigma$	Weber number (−)
Y	mass fraction (kg-specie/kg-gas)

Greek letters

α	liquid volume fraction (−)
θ	contact angle (°)
μ	dynamic viscosity (kg/ms)
ρ	density (kg/m^3)
σ	surface tension coefficient (N/m)
τ	non-dimensional time ($=tu_o/D_o$)

Subscripts

g	gas
l	liquid
o	initial condition
p	particle

framework was presented, followed by a parametric investigation of single droplet-particle collisions on a two-dimensional axisymmetric framework.

In the present paper, that forms the second part of this two-part study, the attention is turned towards the collision between droplets and realistic particle configurations, as that of a particle cluster. After a thorough examination of the available open source literature and to the best of authors' knowledge, limited material exist (both experimental and numerical) concerning the investigation of the physical phenomenon of a droplet impacting onto a particle cluster. Only one numerical work was traced that included the deformation of a single droplet resulting by the motion of two particles [18]. In this work, the authors use the Level-Set function in order to track the liquid-gas interface motion, while they use a distributed-Lagrange-multiplier based method in order to account for the presence of particles. Initially, two particles are placed off-centre from each other, while a liquid droplet is placed in between. The particles start moving in opposite direction, which results in the squeezing, deformation and breakup of the liquid droplet. However, the operating conditions of this work fall out of the scope of FCC units.

Based on the scarce material found, this work tries to fill the identified gap and focuses on the phenomenon of droplet impingement onto particle clusters under realistic FCC conditions. The purpose of the present paper is to extend previous 2-D investigation made in Part I to three-dimensions. Model verification against the 2D predictions is performed, since no experimental results can be found. To the best of the author's knowledge, the evaporation of the droplet, as well surface cracking reactions were taken into account for the first time. In the next section, a brief description of the numerical model is initially given. The simulation of single droplet-particle collisions on a 3D framework is then described, followed by the impact of a single droplet on a particle cluster.

2. Numerical methodology

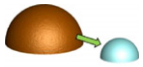
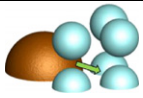
The CFD numerical model presented in Part I is utilized in order to simulate the cases of interest. The model solves the Navier-Stokes equations for the prediction of fluid flow, along with the energy conservation equation and transport of species equations. The Volume of Fluid Method (VOF) is used for interface tracking. The equations are solved in the commercial software ANSYS FLUENT [19], where User Defined Functions (UFDs) have been defined for the implementation of a phase change model (based on kinetic theory of gases [20] for gasoil droplet evaporation), surface cracking reaction rate, as well as a dynamic local grid refinement technique. This technique is applied so that the refined region of the grid follows liquid motion dynamically and thus computational cost is decreased compared to a uniform grid having the same resolution at the liquid-gas interface. A 2-lump scheme represents the catalytic cracking reactions (kinetics taken from [21]), while the material properties of petroleum gasoil and gasoline are represented by those of single species n-pentacosane ($C_{25}H_{52}$) and n-heptane (C_7H_{16}) respectively (Carl L. Yaws properties [22–24]). The "cracking" pathway begins on the gasoil droplet that evaporates in order to form gasoil vapour, which subsequently, in the presence of the catalytic particle surface, reacts to produce gasoline. Surface porosity is taken into account by a Specific Surface Area (SSA) variable for the catalyst. The extension of the models presented in Part I to three dimensions is straightforward.

3. Results and discussion

3.1. Cases examined

Firstly, the three-dimensional numerical model is verified against the results of the 2D single-droplet particle collisions presented in Part I; then it is utilized to investigate the droplet collision with a particle cluster. The comparison of the current cases with the 2D axisymmetric results is dictated by the lack of similar works in literature, while additionally, it offers a way to evaluate the efficiency of the 3D model and probably spot any effects of three dimensional flow details on the evolution of the phenomenon. The enumeration of the cases is in correspondence to the ones having the same operating conditions in Part I, using the multiplication symbol (example, Case2, Case2*). The three cases selected to serve for this verification are presented in Table 1; they represent two cases of DTP = 1, where the effect of impact velocity is examined (Case2* to Case4*, 15 m/s to 30 m/s) and one of DTP = 2 for the evaluation of droplet to particle size ratio effect on the phenomenon evolution. Cases2* and 7* represent the best/worst case scenario in

Table 1
Cases investigated for droplet-particle/particle cluster collisions in FCC reactor injection zone.

Case No.	DTP	U_o	T_p	We	Re	Refinement levels	
3–D Single droplet–particle collision							
2*	1	**15**	1000	4266	2272	3	
4*	1	**30**	1000	17,062	4544	3	
7*	2	30	**800**	34,124	9088	2	
3–D Single droplet–particle cluster collision							
9	2	30	**1000**	34,124	9088	2	