Multiphase CFD Modeling of Trickle-Bed Reactor Hydrodynamics

Rodrigo J.G. Lopes and Rosa M. Quinta-Ferreira

***Abstract*—This study aims to incorporate most recent multiphase models in order to investigate the hydrodynamic behavior of a TBR in terms of pressure drop and liquid holdup. Taking into account transport phenomena such as mass and heat transfer, an Eulerian *k*-fluid model was developed resulting from the volume averaging of the continuity and momentum equations and solved for a 3D representation of the catalytic bed. Computational fluid dynamics (CFD) model predicts hydrodynamic parameters quite well if good closures for fluid/fluid and fluid/particle interactions are incorporated in the multiphase model. Moreover, catalytic performance is investigated with the catalytic wet oxidation of a phenolic pollutant.**

***Index Terms*—CFD, Euler-Euler model, Hydrodynamics, Multiphase Flow.**

I. Introduction

Multiphase flow systems are described by the cocurrently downward flow of gas and liquid through a packed bed and its commercial applications arises in processing of fuels and chemicals such as desulfurization, hydrotreating, hydrocracking, distillation and filtration. Over the last three decades, the research conducted for the design of such multiphase systems still relies on simplified empirical models rather than on a theoretical basis. The lack of knowledge about the detailed flow picture in packed beds relies in the complex mechanisms governing the fluid flow so that pilot scale experiments is often carried out to perform scale-up studies. Therefore, in reactor design, the coupling between different flow regimes as well as mass and heat transfer rates are directly linked with the hydrodynamics of multiphase reactors such as trickle-bed reactors (TBR). The success of the modeling of multiphase flow processes is virtually related with recent advances achieved in computational fluid dynamics (CFD) given that nowadays computers offer unprecedented numerical power to address complex chemical process operational and design issues. Our case study outlines an alternative CFD modeling method to investigate the hydrodynamic behavior of a TBR in terms of pressure drop, liquid holdup and catalyst wetting efficiency. After a brief review of modeling approaches, further details of an Eulerian two-fluid model is provided discussing velocity 3D maps and catalyst surface temperature profiles evaluated in unsteady state after performing the CFD validation.

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II. State of the Art

The large number of studies that have been reported in the literature on various hydrodynamic aspects of trickle-bed reactors rely on several correlations and models of pressure gradient and liquid holdup. The existing hydrodynamic models can be broadly classified into two different categories [1]-[9]. The first category uses an empirical approach based on dimensional analysis to produce explicit correlations for pressure drop and holdup. These correlations have several parameters for fitting the experimental results in which the predicted values of pressure gradient and liquid saturation vary considerably. The second category involves the development of models resulting from equations of motion and considers determination of drag forces of gas and liquid phases at various operating regimes. In this category it has been used three distinct approaches: the relative permeability model, the fundamental force balance model and the slit model [4]. More recently, the effort has been routed for advanced CFD models based on macroscopic mass and momentum conservation laws, in which the drag force has a contribution to both particle-liquid and gas-liquid interactions [5]. The present trend is to develop models based on the fundamental approach to exploit their wider range of applicability unlike the correlative models, which are system specific. Therefore, our model is based on the fundamental physics based approach containing the mechanistic details of the system coupled with reaction kinetics for the catalytic degradation of liquid pollutants performed elsewhere [10] and attempts to model pressure drop and liquid holdup at high-pressure operation for the trickle-bed reactor. The CFD model was then developed focusing a unified approach in modeling of the hydrodynamics with incidence for the downflow mode to present a more realistic picture of the complex hydrodynamics prevailing in the reactor.

III. CFD Model

In the present work, the flow in the trickle-bed reactor was modeled using a multiphase CFD approach incorporated in the FLUENT 6.1 (FLUENT INC. USA) [11] software that is the Eulerian multiphase model. In the Eulerian two-fluid approach, the different phases are treated mathematically as interpenetrating continua. The derivation of the conservation equations for mass, momentum and energy for each of the individual phases is done by ensemble averaging the local instantaneous balances for each of the phases. The current model formulation specifies that the probability of occurrence of any one phase in multiple realizations of the flow is given by the instantaneous volume fraction of that phase at that point where the total sum of all volume fractions at a point is identically unity. Fluids, gas and liquid, are treated as incompressible, and a single pressure field is shared by all phases. In multiphase flows, the continuity (1), momentum (2) and species continuity equations (3) are solved for each phase and the momentum transfer between the phases is modeled through a drag term [12].

$$\frac{\partial U_x}{\partial x}+\frac{\partial U_y}{\partial y}+\frac{\partial U_z}{\partial z}=0 \tag{1}$$

$$\frac{\partial}{\partial t}(\alpha_i\rho_i\vec{U}_i)+\nabla\cdot(\alpha_i\rho_i\vec{U}_i\vec{U}_i)=-\alpha_i\nabla p+\nabla\cdot\hat{\tau}_i+ \alpha_i\rho_i\vec{g}+\sum_{p=1}^{n}(\vec{R}_{ij}+\dot{m}_{ij}\vec{U}_{ij}-\dot{m}_{ji}\vec{U}_{ji})+\vec{F}_{ij} \tag{2}$$

$$\frac{\partial\rho_i}{\partial t}+\nabla\cdot\rho_i\times\vec{U}+\nabla\cdot\vec{j}_i-w_i=0 \tag{3}$$

$$\vec{j}_i=-\rho\, D_i\,\nabla\cdot\alpha_i$$

ρ is density, U the mass average velocity, h is specific enthalpy and g is gravity; subscripts i and k represents different species. The arrow overbar signifies a vector, and ˆ is a second-order tensor. μ and b are the first and second coefficients of viscosity, respectively. κ is the thermal conductivity, and D_i is the multi-component diffusion coefficient and α_i is the mass fraction. In turbulent flows, the incompressible transport equations are given by (4)-(6).

$$\frac{\partial\rho k}{\partial t}+\sum_i\frac{\partial\rho U_i k}{\partial x_i}=\sum_j\frac{\partial}{\partial x_j}\left[(\mu+\mu_t)\frac{\partial k}{\partial x_j}\right]+\sum_i\sum_j\tau_t\frac{\partial U_i}{\partial x_j}-\rho\varepsilon \tag{4}$$

$$\frac{\partial\rho\varepsilon}{\partial t}+\sum_i\frac{\partial\rho U_i\varepsilon}{\partial x_i}=\sum_i\frac{\partial}{\partial x_j}\left[(\mu+0.77\mu_t)\frac{\partial\varepsilon}{\partial x_j}\right]+C_{\varepsilon1}\frac{\varepsilon}{k}+\sum_i\sum_j\tau_t\frac{\partial U_i}{\partial x_j}-\frac{C_{\varepsilon2}\rho\varepsilon^2}{k} \tag{5}$$

$$\tau_t=\mu_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\left(\rho k+\mu_t\frac{\partial U_k}{\partial x_k}\right) \tag{6}$$

δ_{ij} is Kronecker delta and k subscript indicates a summation over the x_k Cartesian coordinates. The thermal energy balance and the heat flux are expressed in (7) and (8), respectively.

$$\frac{\partial\rho h}{\partial t}+\sum_i\frac{\partial\rho U_i h}{\partial x_i}=\frac{\partial P}{\partial t}+\sum_i U_i\frac{\partial P}{\partial x_i}+\sum_i\left\langle U_i^{"}\frac{\partial P'}{\partial x_i}\right\rangle_m+\sum_i\frac{\partial q_i}{\partial x_i}-\sum_i\frac{\partial}{\partial x_i}\left\langle\rho U_i i^{"}\right\rangle_m-\sum_i\sum_j\left[\tau_{ij}\frac{\partial U_i}{\partial x_j}+\left\langle\tau_{ij}\frac{\partial U_i^{"}}{\partial x_j}\right\rangle_m\right] \tag{7}$$

$$q_j=-\kappa\frac{\partial T}{\partial x_j}-\sum_{j=1}^{n}\frac{\mu}{Sc}\left(h_i\frac{\partial\alpha_i}{\partial x_j}\right)=-C_p\frac{\mu}{\Pr}\frac{\partial T}{\partial x_j}-\sum_{j=1}^{n}\frac{\mu}{Sc}\left(h_i\frac{\partial\alpha_i}{\partial x_j}\right) \tag{8}$$

IV. Numerical Method

The numerical simulation was performed on a cylindrical grid (L – 1m, ID – 0.05m) and the mesh adopted in the TBR reactor is tetrahedral around and over the catalyst particles and hexahedral elsewhere with 800,000 cells with the first ten catalytic layers shown in Fig. 1. Catalytic bed grid generation for the trickle-bed reactor was created using the integrated solid modeling and meshing program Gambit (Fluent Inc., USA) [14]. The approach consists in dividing the domain in subdomains, each of which is represented by a boundary-fitted coordinate mapping to a specific region in which a uniform grid is generated. In order to manage with the geometric complexity of the catalytic bed, the subdomain decomposition was unstructured, leading to multiblock block-structured grids. The local grids for a sample catalyst particle are structured and the flexibility of this kind of grid was covered for trickle flow in which boundary parts move relatively to each other. Furthermore, this is a way to include adaptivity in the structured grid context. The discretization takes place on boundary-fitted structured grid and the flow is governed by the incompressible *Navier-Stokes* equations. The discretized continuity equation serves as an algebraic constraint and often a semi-heuristic turbulence model is used to predict time-averaged flow variables based on a compromise between accuracy, memory requirements and computing time. The local refinement and coarsening of unstructured tetrahedral meshes in our case study require local grid modifications to efficiently resolve solution features for computing three-dimensional problems that arises in TBR. However, repeated anisotropic subdivision can significantly deteriorate the quality of a tetrahedral mesh demonstrating that isotropic subdivision is mandatory if mesh quality is to be controlled effectively for arbitrary refinement levels in tetrahedral meshes, without resorting to local mesh regeneration. Experimentally, it is observed that trickle-bed reactors present random directional flow fields imposing serious limitations to tetrahedral meshes that could

lead to an inefficient distribution of grid points in the final mesh. The momentum equations are solved with the coupling SIMPLE algorithm and the second upwind discretization scheme. The pressure is computed by means of the PRESTO scheme. Model equations were solved in a transient fashion with a time step of 1 s for the Eulerian simulations and a number of sub-iterations were performed within each time step to ensure continuity. The residuals convergence was accelerated by under-relaxation parameters, 0.4 for pressure and 0.8 for velocity vector field. Inlet boundary conditions are assigned at the top distributor and outlet conditions at the free surface.

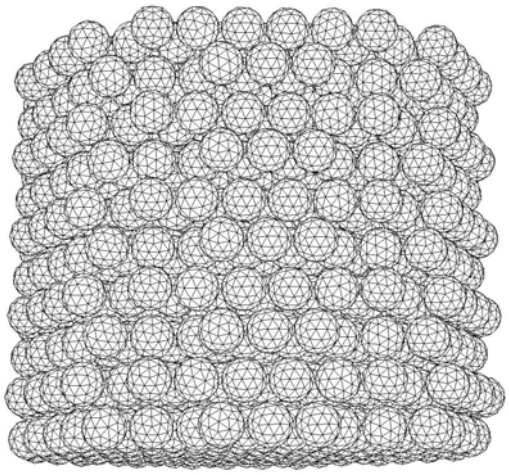

Fig. 1 – Trickle-bed reactor computational mesh

The turbulent flow is modeled through a set of modified k-ε equations with terms that include interphase turbulent momentum derived from the instantaneous equation of the continuous phase and involves the velocity covariance. The equations discussed above are solved using an extension of the SIMPLE algorithm. The momentum equations are decoupled using the full elimination algorithm available in FLUENT in which the variables for each phase are eliminated from the momentum equations for all other phases. The pressure correction equation is obtained by summing the continuity equations for each of the phases. The equations are then solved in a segregated, iterative fashion and are advanced in time. At each time step, with an initial guess for the pressure field, the primary- and secondary-phase velocities are computed. These are used in the pressure correction equation and based on the discrepancy between the guessed pressure field and the computed field, the velocities, L/G holdups and fluxes are suitably modified to obtain convergence in an iterative manner. In the first stage, several runs were computed with sufficiently fine meshes to evaluate this dependency. At this point, it was possible to check the near-wall mesh in the post-processing treatment. The solution independency was then established after several assays with the definition of turbulence boundary conditions available in k-ε model. The boundary conditions at the walls are internally taken care by FLUENT, which obviates the need for boundary condition inputs for k and ε supplied by inlet boundaries, specifically velocity inlet. Pressure inlet was also tested but the results seem to be well described by the first which specify more realistic boundary conditions at the inlet. It should be pointed that inlet turbulence can significantly affect the downstream flow as observed in high pressure trickle-bed reactor [15]. In the trickle-bed simulations performed, the fidelity of the results for turbulent flows is largely determined by the turbulence model being used and in order to enhance the quality of turbulent flow simulations, the mesh generation accounts for wall-bounded flow, at least on catalyst particle, since the wall is expected to significantly affect the flow.

V. Hydrodynamic Validation

Since the CFD methodology is not specifically designed for application in constrained geometries, such as particle packed beds, it is necessary to verify if the simulated results are valid. Although the CFD code is based on fundamental principles of flow and heat transfer, some of the boundary issues are modeled using empirical data not necessarily appropriate for fixed bed applications. Validation of CFD flow field calculations has generally taken one of the two forms. In the first, noninvasive velocity measurements inside the packed bed have been made, and compared to velocities computed from a model of either the entire experimental bed or a representative part of it. In the second form, computed pressure drops have been compared to either measured values or established correlations for pressure drop in fixed beds, such as the Ergun equation. The present case study employed the last method to assess the Eulerian model. Therefore, the numerical methodology is validated against experimental data available from literature related to the hydrodynamic information for TBR operation. Indeed, the actual strategy is to compare CFD results in terms of well known parameters such as liquid holdup and pressure drop that are the two most employed characteristics in TBR development study. The experimental conditions and the parameters commonly measured in high pressure TBRs are evaluated extensively in topics such as: pressure effect on physicochemical properties, phenomenological analysis of two-phase flow, flow regime transition, single-phase pressure drop, two-phase pressure drop, liquid holdup, gas-liquid interfacial area and mass transfer, catalyst wetting efficiency as well as catalyst dilution with inert fines in laboratory scale TBRs. In this context, the mesh was validated by checking the mesh sensitivity and by comparing the numerical results against the single-phase and two-phase experimental data. The validation of CFD codes using pressure drop is most reliable when actual experimental data are taken in equipment identical to the situation that is being simulated. Existing literature correlations such as the Ergun equation are known to have shortcomings with respect to wall effects, particle shape effects, application to ordered beds and validity at high Reynolds numbers (Re). The applicability of literature correlations to typical CFD simulation geometries needs to be examined critically before fruitful comparisons can be made because pressure drop

measurements can provide an indirect means of checking on the computations at higher flows, although most comparisons have been made at relatively low flow rates. Therefore, pressure gradient and liquid holdup was the two fundamental hydrodynamic parameters evaluated for the design, scale-up, and performance studies of TBR. Pressure drop is an important parameter in the design of two-phase concurrent reactors because if affects the energy supply and it has been use to correlate the gas-liquid and solid-liquid mass transfer whereas liquid holdup is the liquid volume contained in a unit column volume. It should be pointed that in the model validation it was taken into consideration that almost all the holdup data available in open literature refers to laboratory columns [15].

Several runs simulating operating pressures in the range 10 to 30 bar runs were carried out for the vector field of liquid and gas velocity and for liquid hold up and pressure drop using spherical catalysts with 2 mm diameter. Simulated CFD liquid holdup and pressure drop are represented in Figs. 2 and 3 by lines as a function of liquid mass flux water when the reactor operates with air as the gas phase at different gas flow rates. The experimental data plotted were obtained with one reactor with dimensions described by Nemec and Levec [15]. In the high interaction regime modeled for the gas and liquid phases, the predictions are in good agreement with experimental values which enables the validation of our CFD model. In fact, the computational fluid dynamic model validation was carried out first in single-phase pressure drop simulations with only the gas phase flowing downward the bed; afterwards, two-phase flow is simulated to perform the final comparison between predicted hydrodynamic parameters and experimental data. In the whole range of Re numbers for gas phase, pressure drop predictions are within 10% error when comparing with the literature measurements. The resulting pressure drop is given by the addition of laminar flow local losses with frictional losses. At very low velocities, exclusively laminar or viscous contributions to pressure drop are observed but at higher velocities the laminar term from *Blake-Kozeny-Carman* equation and the inertial term from *Burke-Plummer* equation are additive. This mutual contribution that represents the ratio between the static pressure and the hydrostatic pressure is plotted in Fig. 2. The operational region of flow rates ($10<Re_G<400$) is that of particular interest to TBR and in this ambit Eulerian model fits the pressure drop data as well as liquid holdup quite well within acceptable limits of 10%. Furthermore, taking into account that the detailed knowledge of liquid holdup is essential for safe processing to prevent hot-spot formations and possible runaways that could have significant influence on the liquid residence time distribution, mass- and heat-transfer processes as well as wetting efficiency, our results in terms of liquid holdup were also successfully validated in Fig. 3 avoiding many correlations that have been published in multiphase reactors.

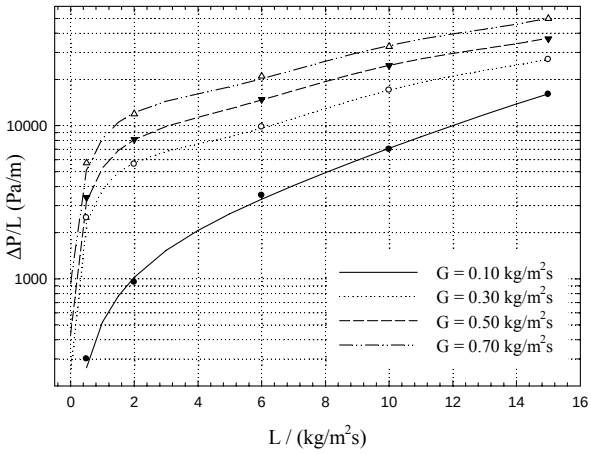

Fig. 2 – Comparison of simulated pressure drop as a function of liquid mass flux at constant gas flow rates with experimental data [15]

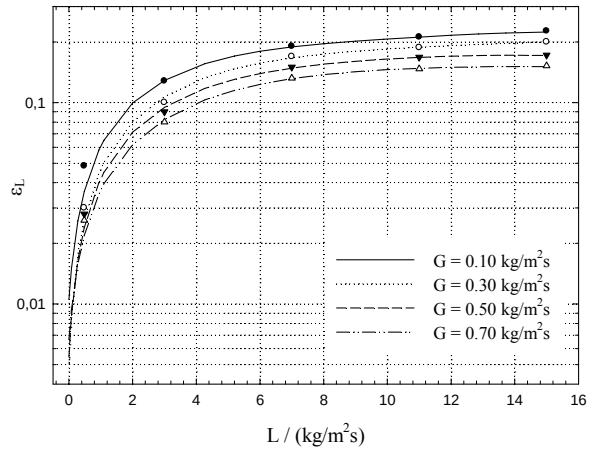

Fig. 3 – Comparison of simulated liquid holdup as a function of liquid mass flux at constant gas flow rates with experimental data [15]

According to Fig. 3, liquid holdup decrease when the pressure was increased for given gas and liquid superficial velocities. This decrease is interpreted as due to a shift in the reactor fluid dynamics from a state predominantly controlled by gravity to a state controlled by gas-liquid shear stress or pressure drop. Comparing Figs. 2 and 3, where the pressure gradient per unit reactor length has been plotted as a function of liquid mass flux, we see that for very low values of pressure drop the liquid holdup are equally small. With the increase of pressure drop due to higher reactor pressures, the total driving force enlarges noticeably and, hence, the liquid holdup growth rate reduces when the liquid mass flux increases. On the other hand, the investigation of liquid distribution in the cocurrently gas/liquid system at elevated pressures could also be related to the results plotted in Figs. 2 and 3, in which it can be seen that liquid holdup values at elevated gas flow rates are much lower in comparison with those accounted in lower gas flow rates conditions. This effect can be explained by means of the ratio between the driving forces, shear and gravitational forces, and the retarding viscous force. As the viscosity of liquid increases

exponentially with increasing pressure, the ratio of driving forces and viscous force increases also. This causes a gradual reduction of the liquid saturation in the packed bed. Moreover, the comparison between the hydrodynamic parameters determined at 10 and 40 bar shows that the effect of the reactor pressure has greater influence on the pressure drop than it has on the liquid holdup, as expected. Furthermore, CFD model results state that liquid holdup is slight insensitive to low gas flow rates. This fact could be interpreted by the evolution of liquid holdup as a function of gas density by plotting liquid holdup as a function of superficial mass liquid velocity demonstrating that the theoretical model is able to predict quite well the significant influence of the gas flow rate on the hydrodynamic parameters when comparing the theoretical results with the experimental data sets. It should be also emphasized that the fixed-bed modeled in this work had the tube to particle diameter ratio higher than 10 so the available geometry and data taken from literature should not be affected by the reactor column wall. In accordance to Fig. 3, when the liquid mass flux increases, the liquid holdup also increases for L higher than 8 kg/m^{2}s being the growth rate smaller for the same total pressure value whereas an increase of the total pressure results in a considerable decrease of liquid holdup. The influence of the gas flow determined by a different operating pressure on the liquid holdup is less pronounced at low values of liquid mass fluxes. For example, in case the reactor operates with a gas flow rate at 0.7 kg/m^{2}s, the liquid holdup is substantially lower when compared with the case it operates at 0.1 kg/m^{2}s. These higher differences at higher liquid flow rates result from the fact that a further increase of the reactor pressure at a constant gas velocity corresponds to a higher driving force. The theoretical predictions from the model correctly account for the strong influence of the gas flow on the hydrodynamic behavior of the trickle-bed reactors, as stated by several authors [1]-[4]. The important influence of the gas flow is attributed to the interactions phenomena exerted by the gas phase on the liquid phase. These interactions clearly appear to be significant at high superficial gas mass velocities.

Finally, in order to address CFD flow streamlines, the 3D map taken with a vertical catalyst layer illustrated in Fig. 4 indicate that the velocity is higher at points where the flow is processed downward in axial direction. In accordance to these results, the maximum gas velocity is about 0.5 cm/s (whereas the liquid velocity is about 0.005 cm/s) which is in the range of well accepted trickle flow maps reviewed in the literature [1]. In fact, the TBR hydrodynamics are affected differently in each flow regime and the operating conditions that are of particular interest in the industry is the extensively used trickle flow encountered at low gas and liquid superficial velocities. In the 3D map, it is shown the uniformity in packing structure with spherical particles, but the gas/liquid distribution depends not only on the superficial gas and liquid velocities but also in particle shape and particle equivalent diameters in order to study the effect of particle geometry. Spheres were used by virtue of their unique shape and are incapable of influencing the structure of the bed by their orientation. Some additional differences between the porosities of beds, despite the same packing procedures were due to wall effect, which as mentioned before did not affect the overall pressure drop. With regards to the porosity dependence within the inertial regime, it should be reported in the basis of theoretical simulations of flow through random arrays of spheres that the porosity function is also well taken into account as long as the porosity is around 0.4 as is indeed the case for packed bed reactors when made up of spheres. The values of porosity distribution function for the present CFD Eulerian model were applied in the range from 0.38 to 0.40. It should be also pointed that when the superficial velocity of gas is sufficient to interact comparatively with that of liquid, liquid distribution improves significantly and the pressure drop arises as described elsewhere [13]. In our simulation activities, it was assumed that the trickle-bed reactor has a uniform distributor at the top and we can state that liquid distribution do not depends on the design of the distributor.

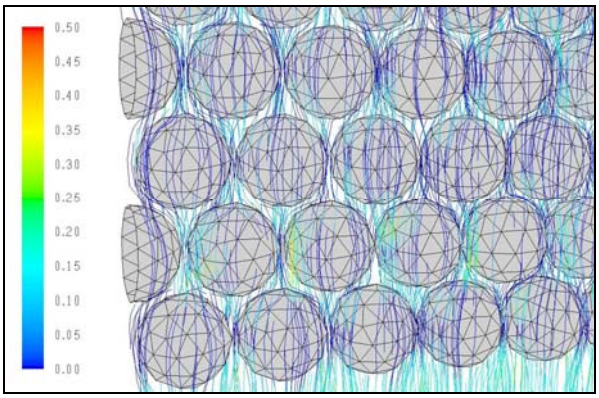

Fig. 4 – Gas streamlines colored by axial velocity (*cm/s*)

VI. Reaction Studies

Aiming to assess the TBR reaction behavior, the catalytic wet oxidation of a model phenolic acid solution was simulated in continuous mode by means of CFD codes. The kinetic expressions of a mixture of six phenolic acids previously calculated [10] were then integrated in the TBR computational model where it was assumed that chemical reaction occurs namely on the catalyst surface. This assumption is expected to be mostly reasonable because of the hydrodynamic interaction regime achieved by the Eulerian model. The CFD model has also taken into account external mass transfer limitations which is the most suitable when operating at large scale pilot plant units. According to Fig. 5, a temperature color map was taken with a flow time of two hours. As the operation is modeled in unsteady state, after evaluating successive temporal temperature color maps it is possible to conclude that steady state of TBR unit is achieved in this time.

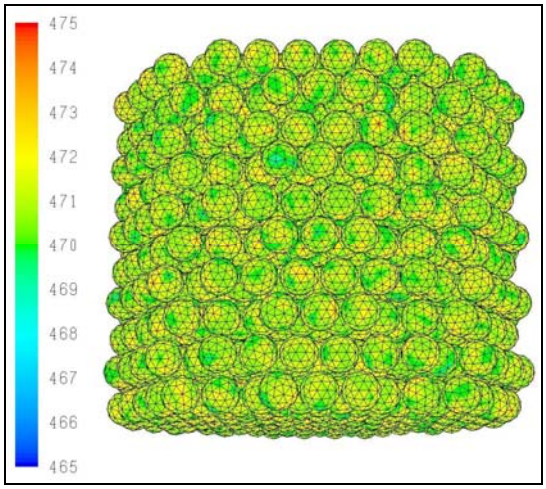

Fig. 5 – Catalyst surface temperature (*K*)

Furthermore, as the liquid holdup is directly related to the catalyst wetting efficiency that also might affect the reaction yield, in accordance to Fig. 5, the different temperatures ranging from 470 to 474 K attained in different locations of the catalyst particles indicate different reaction rates. These results in terms of catalyst surface temperature for the exothermic oxidation process of the pollutants reflect different wetting levels of the solid by the liquid effluent. Therefore, in the TBR design and scale-up studies external catalyst wetting efficiency is also a hydrodynamic parameter that indicates the utilization degree of catalyst surface area. However, the coupling nature of transport phenomena and kinetics in TBR is far from being completely understood so that general scale-up and scale-down rules for the quantitative description of multiphase flows depends on how phenomenological analysis is correlated with available numerical power to address complex chemical process operational and design issues.

VII. Conclusion

A unique physics-based model has been proposed for modeling trickle-bed reactors at elevated pressures aiming to predict the hydrodynamic parameters. The unified approach includes fundamental point force balance and takes into account the influence of gravity in the force balance. The model consists in an Euler-Euler treatment for the fluid phases coupled with the energy equation. The numerical simulations are compared against experimental data to validate the predicted pressure drop and liquid holdup. Operating conditions were simulated with 10-30 bar of reactor pressure while gas and liquid mass flow rate were in the range 0.10 – 0.70 and 0.05 – 15 kg/m^{2}s, respectively. The novel hydrodynamic model has been found to predict with a reasonable accuracy the experimental data, pointing out that the liquid holdup increases as the liquid mass flux increases and decreases for higher operating pressure values. At low values of pressure drop the liquid holdup is small but with an increasing value of pressure drop due to an increase of the reactor pressure, the liquid holdup growth rate reduces when the liquid mass flux increases. The influence of operating pressure on liquid holdup is less pronounced than in pressure drop. Finally, CFD runs performed in unsteady state for the catalytic wet air oxidation of one phenolic solution demonstrated the effect of temperature illustrated by catalyst surface temperature 3D map.

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