CAMURE-11 11th International Symposium on Catalysis in Multiphase Reactors
ISMR-10 10th International Symposium on Multifunctional Reactors
MILANO, ITALY - 21-24 March, 2021

CFD investigation of hydrodynamics in an industrial preneutralizer chemical reactor for ammonium fertilizer production

Safae Elmisaoui[1,2]*, Lhachmi Khamar[1,3], Saad Benjelloun[1], Mohamed Khamar[2], Jean Michel Ghidaglia[1,4]

1 MSDA Modeling, simulation, and Data Analysis, Mohammed VI Polytechnic University, Benguerir, Morocco;
2 LGCE, Laboratoire du génie civil et environnement, Mohamed V University, Rabat, Morocco
3 LIPIM, Laboratoire d'ingéneirie des procédés, informatique et mathématiques, ENSA-Khouribga, Sultan Moulay Slimane University, Khouribga, Morocco
4 CMLA Centre des mathématiques et leurs applications, ENS Cachan, Paris Saclay University, Paris, France
**Corresponding author E-Mail: Safae.elmisaoui@um6p.ma*

1. Introduction

Stirred tank reactors have been used frequently in many chemical processes, these reactors represent the masterpiece affecting the product quality. In phosphate fertilizers manufacturing processes, they ensure the most important tasks in desirable properties of the produced slurry to be converted in granules by feeding the drum ammoniator-granulator [1][2]. Despite the common use of this chemical reactors, the understanding of mixing and hydrodynamic characteristics of these systems is still limited and the optimization of mixing conditions in this equipment has remained a challenging issue. The CFD approach is chosen as the modelling and simulation tool that proved its power and robustness in the study and the analysis of complex flows.

The physicochemical phenomenon called "preneutralization" is based on the reaction between ammonia bubbles and phosphoric acid liquid inside a continuous preneutralizer reactor; which is a non-standard stirred tank reactor. It is equipped by a pitched blades turbine agitator that promote mass and heat transfer, also it reduces foaming and improve ammonia absorption [1]. Mixing ensure a turbulence that enhance a smooth functioning of the chemical reaction [3].

The main goal of this work is to study the hydrodynamic of multiphase flow and the mixing quality within the preneutralizer in order to evaluate the effects of the process mastering operating parameters on the preneutralization reaction rate and on the fertilizer slurry physicochemical properties. Especially, rotational speed of the agitator, ammonia bubbles size and feeding inlets positions on the homogenisation of the flow[5].

2. Numerical method

The modelling and simulation work, in this paper, is performed using Computational Fluid Dynamics (CFD). This simulation, that allow to reduce the requested efforts for experimental and design data acquisition. In the current research study, we applicated the mixture multiphase flow approach for a three-dimensional geometry exploring the real dimensions of the existing unit operation wich make a challenging task to take.

The Reynolds-Averaged Navier Stokes (RANS) equations remain the most used approach for modelling and simulating turbulent flows in the engineering field. On the one hand, we adopted this approach in order to study the fast kinetic reaction between ammonia (gas) and phosphoric acid (liquid). On the other hand, we were able to focus on the phenomena of transport; in particular the mass transfer between phases, and to reduce the error between observed and calculated values Reynolds-Averaged Navier Stokes (RANS) equations remains the more used approach for studying flow flows turbulence in engineering field. In addition, we are simulating a reacting multiphase flow, in which the reaction between ammonia (gas) and phosphoric acid (liquid) accrues immediately, this condition needs the use of chosen model as the sophisticated on allowing to capture the different phenomena; especially mass transfer from phase to phase and reduce the observed error.

For the chemical species concentrations evolution in the reacting medium, we coupled Navier Stokes equations with species transport equations wich allow us to evaluate the homogenisation of the mixture phases and the reactants conversion in the preneutralizer. To simulate the motion of impellers, Multiple Reference Frame (MRF) method was employed due to its effectiveness and its huge impact on time consuming compared to the sliding mesh method.

The fluid domain investigated in this work, is shown in Figure 1a. Design modeler and ANSYS mesher are used as geometry and mesh generator, respectively. A mesh convergence study was carried out to chose the optimal one ($y^+<0$). The domain is discretized by an unstructured finite volume method with an upwind scheme.

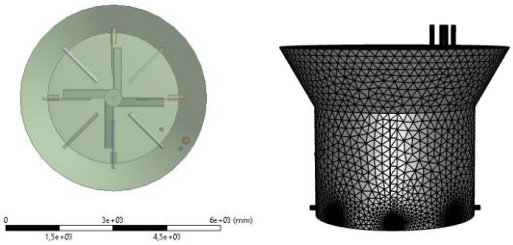

Figure 1. Geometry design (a) and mesh of the preneutralizer (b)

3. Results

The CFD results were in good agreement with experimental data, and with the available studied cases in the literature wich proves that the model is sufficiently accurate and significant. The obtained results revealed that the flow characteristics are extremely sensitive to the agitator rotational speed, to ammonia bubbles size, and reactants feeding positions. That explain the fluctuations in the chemical reaction rate related directly to this operating and geometrical conditions.

4. Conclusions

It appears that the tailored CFD model of a multiphase reacting flow within the preneutralizer can predict a wide range variety of transient phenomena and it was a successful tool for modeling the hydrodynamic behavior and effect on the chemical reaction rate. Detailed chemical kinetics modeling taking into account turbulent mixing is shown to provide accurate results when compared with the industrial measured data. The results revealed that the flow characteristics are extremely sensitive to the studied parameters controlling the distribution of the velocity, pressure, density fields. Indeed, the obtained results explain and give access to a complex industrial domain difficult to control. This study opens the door on different chemical engineering components to take into consideration to develop a robust and real representative simulation that can further used in the intensification of preneutralizer.

References

[1] J. Henry, “Operating manual of Di Ammonium Phosphate process,” (internal document) - TLS - Times Lit. Suppl., no. 5911, p. 29, 2016.

[2] UHL, Vincent (ed.). Mixing V1: Theory And Practice. Elsevier, 2012

[3] N. P. Cheremisinoff, N. P. Cheremisinoff, N. P. Cheremisinoff, and N. P. Cheremisinoff, “Chapter 7 – Mixing Equipment,” Handb. Chem. Process. Equip., no. 1, pp. 435–488, 2000.

[4] International Fertilizer Development Center. and United Nations Industrial Development Organization., *Fertilizer manual*. Kluwer Academic in cooperation with, 1998.

[5] M. Ebrahimi, M. Tamer, R. M. Villegas, A. Chiappetta, and F. Ein-moza, “Application of CFD to Analyze the Hydrodynamic Behaviour of a Bioreactor with a Double Impeller,” 2019.