Computers and Chemical Engineering 60 (2014) 307–314

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Optimization of reagents injection in a stirred batch reactor by numerical simulation

P. Vite-Martínez[a], C. Durán-Valencia[b], J.A. Cruz-Maya[c], A. Ramírez-López[d], S. López-Ramírez[e],*

[a] Instituto Politécnico Nacional, ESIQIE, Departamento de Metalurgia y Materiales, Apdo. Postal 75-874, México, D.F., C.P. 07300, Mexico
[b] Instituto Mexicano del Petróleo, Avenida Eje central Lázaro Cárdenas No. 152, México, D.F., C.P. 07730, Mexico
[c] Instituto Politécnico Nacional, UPIITA, Av. IPN 2580, México, D.F., 07340, Mexico
[d] Universidad Autónoma Metropolitana, Departamento de Ingeniería Industrial, Av. San Pablo 180, México, D.F., C.P. 02200, Mexico
[e] Universidad Nacional Autónoma de México, Facultad de Química, Ciudad Universitaria, México, D.F., C.P. 04510, Mexico

A R T I C L E I N F O

Article history:
Received 29 October 2012
Received in revised form 29 May 2013
Accepted 9 September 2013
Available online 23 September 2013

Keywords:
Tracer
Concentration
Evolution
Curve
Batch reactor
CFD

A B S T R A C T

Computational fluids dynamic was used to analyze the mixing operation within a stirred batch reactor to distribute rapid and homogeneously reagents, used in the refining process of liquid lead. The flow pattern and distribution of the reagents inside the reactor were analyzed through tracer response curves obtained by numerical simulation.

The predominant mechanism of momentum and mass transfer for macro-mixing is convection for the mean and eddy flows. Based on the assumption that the tracer is distributed in the vessel by convection and diffusion, the dynamic distribution of the tracer concentration inside the stirred batch reactor was calculated by solving the Reynolds-averaged conservation equations and the Realizable κ–ε turbulence model. The mean and tracer flow was considered as incompressible, isothermal and single phase under turbulent conditions.

To optimize the injection point of reagents in the stirrer batch reactor, several simulated tracer concentration curves were obtained from monitoring points located at different radial and axial positions.

1. Introduction

During the lead refining process, copper and silver are removed by adding sulfur and zinc, as consequence, insoluble products such as Cu_2S and Ag_2Zn_5 are generated according to reactions (1) and (2), respectively, floating toward the interface to be part of the dross.

$$S + 2\underline{Cu} \Rightarrow (Cu_2S) \tag{1}$$

$$5Zn + 2\underline{Ag} \Rightarrow (Ag_2Zn_5) \tag{2}$$

In the reactor, the reagents can be injected on the surface or within the liquid lead, such decision impacts on the homogenization time. Injecting the reagents into the metallic bath, the time of the chemical reactions can be reduced (Plascencia-Barrera, Romero-Serrano, Morales, Hallen-Lopez, & Chavez-Alcala, 2001). Inspired on that, basically, the aim of this work is to optimize the mixed process in a batch reactor through the appropriate selection of injection point of the reagents.

Stirred tanks are widely used in different types of processing industries for mixing operations, reactions, crystallizations, etc. either in a batch or continuous mode. Mixing has a significant effect on economy due to the time involved in the process and the final quality of products. Poor mixing or improper flow pattern within a stirred tank may be the reason for insufficient homogenization, process disturbance, and excess of chemical costs due to insufficient reaction time or poor mixing.

Computational fluids dynamic (CFD) is a mathematical technique widely used, that offer an alternative to traditional experimental method, to fluid flow analyze, equipment design, and optimization. It has been successfully used in system associates with metallurgical processes (Bailey et al., 1999; Kumar, Bailey, Patel, Piper, & Forsdick, 1999; Ohguchi & ORobertson, 1984; Pinelli & Magelli, 2000; Sawada & Ohashi, 1987; Szalai, Muzzio, & Bittorf, 2002). The use of CFD in stirrer bath reactor has been mainly applied in the chemical industry to identify optimal process conditions. Tracer concentration evolution (TCE) curves have been widely used too, in the search of new shape and velocity of stirrers (Wang, Mao, & Shen, 2006). The quality of mixing depends on the

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* Corresponding author. Tel.: +52 55 53 63 29 97.
E-mail addresses: slr@unam.mx, simon.lopez.ramirez@gmail.com (S. López-Ramírez).

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http://dx.doi.org/10.1016/j.compchemeng.2013.09.005

Nomenclature

n	number of data
N	number of reactor working in series
P	pressure
t	time
u	mean velocity

Greek symbols

ε	dissipation rate of the turbulent kinetic energy
κ	turbulent kinetic energy
μ	viscosity
μ_{eff}	effective viscosity
μ_t	turbulent viscosity
ρ	density
v	kinematic viscosity

Table 1
Coordinates of the Injection point of tracer in the reactor.

Axial		Radial	
Point	Coordinates (m) (x, y, z)	Point	Coordinates (m) (x, y, z)
A	0.125, 0.095, 0.095	1	0.225, 0.045, 0.045
B	0.175, 0.095, 0.095	2	0.225, 0.055, 0.055
C(4)	0.225, 0.095, 0.095	3	0.225, 0.075, 0.075
D	0.255, 0.095, 0.095	4(*C*)	0.225, 0.095, 0.095
E	0.325, 0.095, 0.095	5	0.225, 0.125, 0.125
F	0.425, 0.095, 0.095	6	0.225, 0.145, 0.145

Table 2
Physical properties of the liquid lead.

Property	Value
Viscosity (m $\text{Kg}^{-1}\,\text{s}^{-1}$)	0.01939
Density ($\text{Kg}\,\text{m}^{-3}$)	10515.96
Molecular weight ($\text{Kg}\,\text{Kgmol}^{-1}$)	207.2

ability to distribute homogenously reagents in the whole reactor in a short time, reducing reagents consumption and the time required for the operation. Previous researches have shown good agreement between experimental data and CFD numerical results in the case of the mixing tanks (Chiu, Naser, Ngian, & Pratt, 2008; Chiu, Naser, Ngian, & Pratt, 2009; Micale, Brucato, Grisafi, & Ciofalo, 1999; Rahimi & Parvareh, 2005; Rutherford, Lee, Mahmoudi, & Yianneskis, 1996; Zadghaffari, Moghaddas, & Revstedt, 2009).

In this work, conventional CFD simulation was used to analyze the injection of reagents and to select the feeding point in a stirred batch reactor (kettle) used to refine liquid lead, optimizing the mixing time. Transient TCE curves were used to select the feeding point. The velocity and concentration profiles were used to analyze the fluid flow pattern to detect dead zones or non-mixed zones. The mixing process was analyzed under steady and unsteady state condition, single phase and two species (lead and tracer).

Those TCE curves obtained by simulation exhibited an oscillatory response and, in order to be analyzed, they were split into individual curves, whose statistical dispersions were obtained conventionally. The inverse of the dispersion of the tracer concentration curve is the number of reactors connected in series and, the optimal arrangement has more reactors working in this manner (Levenspiel, 1989, 1999). In the better reagent injection point, the mixing time was lower, and the number of equivalent reactor working in series was higher.

2. Numerical setup

This study was carried out in a 0.98 ton vertical reactor with a paddle impeller with four flat vertical blades (Fig. 1). The impeller was operated at 200 rpm in turbulent regimen, with rotational Reynolds number ($\text{Re} = \rho ND^2/\mu$) of 35246. The length of the reactor was 0.55 m, with a reactor length-to-diameter ratio of 1.26. The coordinates of the injection points of tracer in the reactor are defined in Table 1. Injection and monitoring points were placed in the same angular plane (Fig. 2), but at different axial and radial positions. For each injection point (Fig. 2(a)), a transient TCE curve was obtained from the average of the 10 monitoring points (Fig. 2(b)).

The mean and tracer flow were considered as incompressible, isothermal, single phase, and fully turbulent. The tracer properties (Table 2) were created with identical properties of lead, so that it affects neither reactor hydrodynamics nor the material balance.

In order to modeled the mean flow behavior and predict the tracer concentration evolution curve within the batch reactor, a

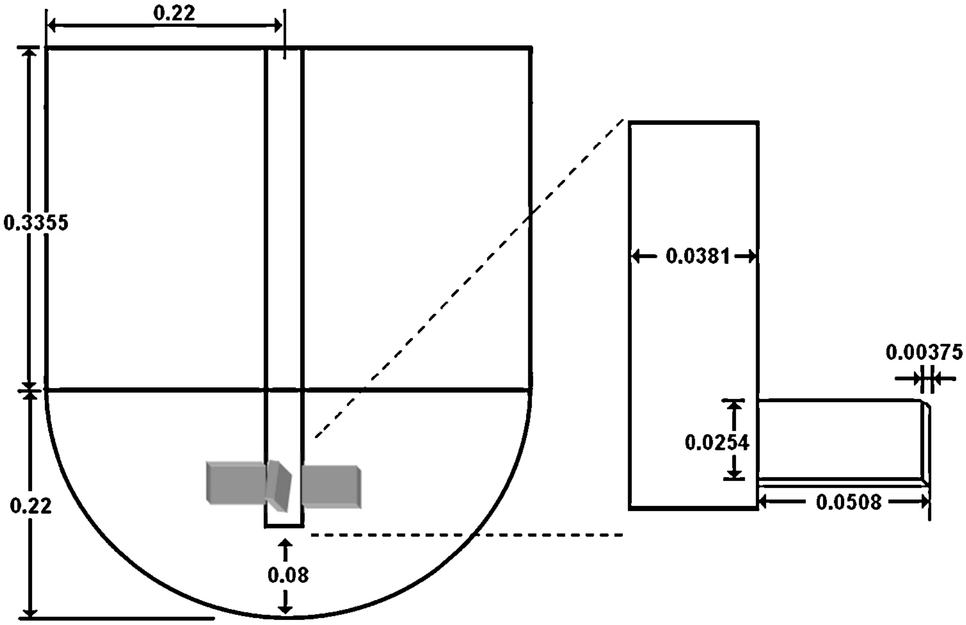

Fig. 1. Geometrical dimensions of the reactor analyzed in this study (m).