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Modeling and Simulation of Thermal Transfer in Batch Reactor

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Abstract: Batch reactors are frequently used in chemical, petrochemical or biochemical industry, for the production of various quality products. Processes used are discontinuous and varied. Indeed, they are characterized by non stationary and non linear systems. An optimal control of the process; requires a modeling and a simulation of the thermal behaviors inside the agitated jacketed reactor in view of the improvement of a high product quality and conditions of security. In certain fields, where the cost and the difficulty of tests are limiting factors, it is advantageous to develop the numeric simulations of these chemical processes. Thus, this study concerns the modeling and simulation of the thermal transfer in an agitated jacketed batch reactor, it is based on a model developed from the global energy balance and empiric correlations which give relationships between thermal transfer coefficients and the stirrer speed. We have achieved the validation of the model by confronting model results with several sets of experiences; for two types of stirrers.

Key words: Batch reactor, thermal transfer, coefficients, modeling, simulation, transition flow, semi-empiric model

INTRODUCTION

The objective of this study is to provide a tool of prediction, of the agitated liquid temperature profile (Ta) in the reactor. Since, thermal transfer coefficients that characterize these mechanisms are only accessible from experimental measures; we have established empiric correlations between these coefficients and stirrer speed (N). Then, we have constructed mathematical model, witch is used for the simulation of the temperature profile.

MATERIALS AND METHODS

The used equipment, for the experimental study of heat exchanges consists in a mechanically agitated reactor, of a capacity of 2 L, provided of jacket of 0.5 L, hardback to a circuit of heating and cooling. The whole is connected to a microcomputer that enables the display of temperatures in the reactor and in the jacket by means of an acquirement power station. Temperatures are measured by the PT100 probes immersed in the agitated liquid and in the coolant liquid; the Fig. 1 shows the experimental installation.

The mechanical agitation is assured by a motor of RW20-IKA type that offers a range of speed from 60 to 2000 rpm, equipped with a stem made of stainless steel on which is fixed the mobile of agitation. We have two turbines; a turbine impeller with six flat blades (TPD) and a turbine impeller with three tilted blades (TPI). The values of temperature acquirements (Tje, Tjs, Ta1, Ta2) measured by probes present on the installation are recorded in entries files.

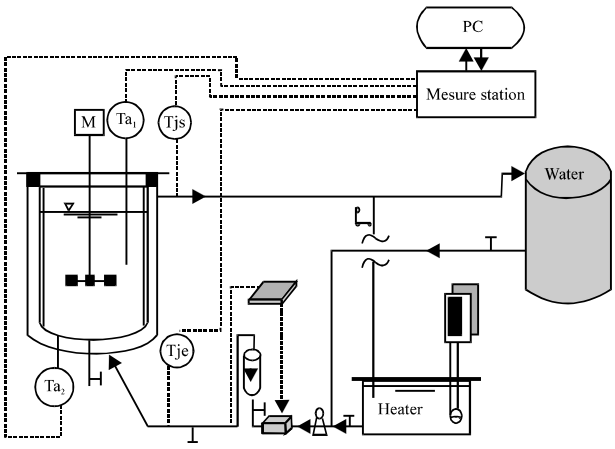

Fig. 1: Experimental installation
Ta_1 : Agitated liquid temperature at the middle (°C)
Ta_2 : Agitated liquid temperature at the bottom (°C).
Tje : Jacket entry temperature (°C)
Tjs : Jacket exit temperature (°C)

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The calculation of thermal transfer coefficients depends exclusively on the properties of the agitated liquid, the coolant liquid and the geometric features of the reactor and the agitation system. For this, we have estimated these transfer coefficients by the following methodology.

Local transfer coefficient in jacket-side: The local coefficient of heat exchange in jacket-side (hj) is a function of the coolant liquid flow rate (qv), by means of dimensional analysis from the Nuselt number and Reynolds number in jacket side. This coefficient is estimated according to the correlation given by Stein and Schmidt (1986). The results are presented on the Fig. 2.

$$Nuj = \left[3.65^3 + 1.61^3 Re_j Pr\left(\frac{Deq}{H}\right) + 0.664^3 Re_j^{1.5} Pr\left(\frac{Deq}{H}\right)^{1.5}\right]^{1/3} \quad (1)$$

Nuj: Jacket Nuselt number $Nuj = \frac{hj\ Deq}{\lambda j}$.

hj : Local transfer coefficient in jacket-side (W m^{-2} °C^{-1}).
Rej : Jacket Reynolds number.
Pr : Prandtl number.
H : Jacket height (m).
D_{eq} : Equivalent diameter of the jacket (m).
λj : Coolant liquid thermal conductivity (W m^{-1} °C^{-1})

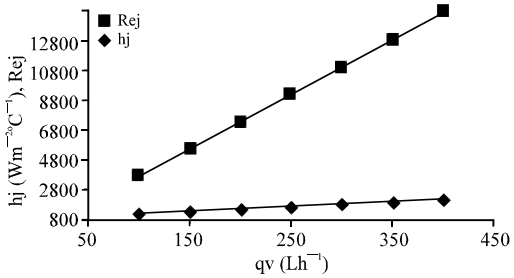

Fig. 2: The coolant liquid flowrate influence on Reynolds number and on the local heat exchange coefficient in jacket side

Global transfer coefficient: The global transfer coefficient (Ui) through the heat exchange area (A) is got by the equation of the global heat balance in the agitated reactor:

$$\rho a.Va.\ Cpa\ \frac{dTa}{dt} = Ui\ A(Tj - Ta) - Qp + P \quad (2)$$

A : Global heat transfer area of reactor (m^2).
Cpa : Agitated liquid specific heat (W kg^{-1} °C^{-1}).
dt : Time interval (s)
P : Power dissipated by the agitator (W).
Qp : Heat losses (W).
Ta : Agitated liquid temperature (°C).
Tj : Jacket average temperature (°C).
Ui : Global transfer coefficient (W m^{-2} °C^{-1}).
Va : Agitated liquid volume (m^3).
ρa : Agitated liquid density (kg m^{-3}).

In this equation the sum of the term (Qp) and the term (P) is negligible in front of the thermal flux given up by the coolant fluid. Therefore, the global transfer coefficient is estimated by the following relation resulting after adjustment:

$$Ui = \frac{\rho a.Va.\ Cpa(T_{af} - T_{ai})}{A.\Delta t.(T_j - T_{am})} \quad (3)$$

T_{ai} : Agitated liquid temperature at initial time (°C).
T_{af} : Agitated liquid temperature at final time (°C).
T_{am} : Agitated liquid average temperature (°C).

The physical properties of the agitated liquid are calculated by relations given by Streck and Poland (1967), valid for a temperature from 0 to 125°C.

The average values of the global transfer coefficient estimated for the two agitation mobiles studied are represented on the Fig. 3 according to Reynolds Number.

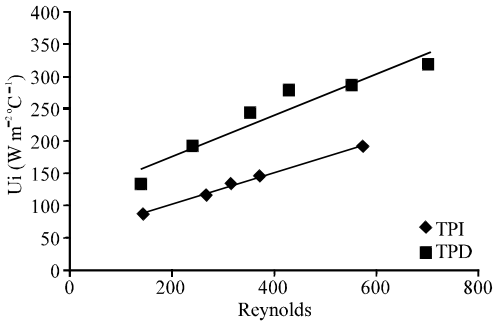

Fig. 3: Evolution of the global transfer coefficient for the two agitation mobiles with the Reynolds number

Re: Reynolds number $Re = \frac{\rho a N d^2}{\mu}$.

N : stirrer speed (rpm).
d : stirrer diameter (m).
μ : agitated liquid viscosity (m^2/s).

Local transfer coefficient in reactor-side: In agitated reactor, Brown *et al.* (1947), Chilton *et al.* (1944) and Uhl (1955), give the local transfer coefficient (hi) according to the stirrer speed (N). Actually, for a given system, stirrer speed is the only parameter that influences this coefficient. These authors write for a number of Reynolds lower than 400, the following correlation:

$$hi = C.N^{2/3} \quad (4)$$

hi: local transfer coefficient in reactor-side($Wm^{-2}\,°C^{-1}$).

The expression of the resistance to the thermal transfer becomes under the shape:

$$Ui^{-1} = \frac{1}{C}.N^{-2/3} + C_1 \quad (5)$$

1/C: slope of the straight line in Wilson's method.
C1: ordinate to the origin in Wilson's method.

While applying Wilson's (1915) graphic method, we have drawn the Fig. 4, which represents Ui^{-1} according to $N^{-2/3}$ and then we have determined the constant 1/C and C1, as well as the values of the local transfer coefficient in reactor-side.

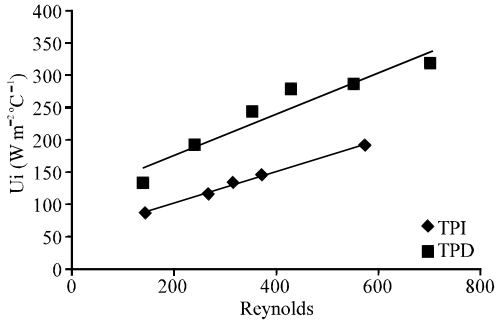

Fig. 4: Wilson's graphic method for the determination of the local transfer coefficient in reactor-side

Empiric correlations: In the end of the experimental study (Baghli, 2003), it appears that global and local transfer coefficients (Ui) and (hi) depend strongly on the geometric and hydrodynamic features of the agitation mobile, as well as on its speed. From these experimental results we have got; for a Reynolds lower than 400, correlations which are shown in the Table 1.

Table 1: Experimental results

	Type of mobile	
	TPD	TPI
hj	hj = 3.355.qv +841.83	hj = 3.355.qv +841.83
Ui	$Ui^{-1} = 0.2765.N^{-2/3} + 0.0007$	$Ui^{-1} = 0.4571.N^{-2/3} + 0.0006$
hi	$hi = 3.6973.N^{2/3}$	$hi = 2.1584.N^{2/3}$

While analyzing the results of the thermal transfer and in particular the evolution of the side-reactor local transfer coefficient; we noted that the turbine impeller with six flat blades (TPD) is much more efficient than the turbine impeller with three tilted blades (TPI), (Baghli *et al*., 2002). Our correlations are reliable for the calculation of the thermal transfer coefficients. Actually, the results give by these correlations are in agreement with Brook and Su (1959) for a turbine impeller with six flat blades.

Semi-empiric modeling: We consider the mixture process in a laboratory scale batch reactor mechanically agitated; the agitated liquid in the reactor is the oil 20W50 and the coolant liquid in the jacket is water. This system is inert (without chemical reaction).

Fundamental equations: The mathematical formulation of the system requires a detailed analysis of the process. It is based on the fundamental equations of the heat transfer.

Equation of the energy balance in the reactor:

$$\rho_a VaCpa\frac{dTa}{dt} = -UiA\left[Ta(t) - Tj(t)\right] - Qp + P \quad (6)$$

Equation of the energy balance in the jacket:

$$\rho jVjCpj\frac{dTj}{dt} = UiA[Ta(t) - Tj(t)] - \rho jCpj\ qj[Tj(t)-Tje(t)] \quad (7)$$

Cpj : Coolant liquid specific heat ($W\,kg^{-1}\,°C^{-1}$).
qj : Coolant liquid (water) flow rate ($l\,h^{-1}$).
Vj : Coolant liquid volume (m^3).
ρj : Coolant liquid density ($kg\,m^{-3}$).

With the following initial conditions:

$$Tj(t) = Tj(0)$$
and $$Ta(t) = Ta(0).$$

After reorganization, a differential equation of 2nd order in term of Tj(t) is gotten (Kumpinskey, 1995):

$$\frac{d^2Tj}{dt^2} + \left[\frac{UiA}{\rho jCpjVj} + \frac{UiA}{\rho aCpaVa} + \frac{qj}{Vj}\right]\frac{dTj}{dt} + \frac{UiA}{\rho aCpaVa}\frac{qj}{Vj}Tj = \frac{qj}{Vj}\frac{dTje}{dt} + \frac{UiA}{\rho aCpaVa}\frac{qj}{Vj}Tje \quad (8)$$

We have solved this equation numerically by the method of RUNGE-KUTTA, with the initial conditions indicated higher. The variation of the coolant liquid temperature (Tj) is used for the resolution of the Eq. (6) that gives the temperature of the agitated liquid (Ta) according to time (Baghli, 2003).

Semi-empiric thermal model: This model is based, first on the empiric correlations, for the calculation of the global transfer coefficient (Ui). Second, it is based on the numeric resolution of Eq. (8) and (6). So this semi-empiric model enables the prediction of the agitated liquid temperature (Ta), according to the evolution of the temperature in the jacket. Indeed, the physical properties of fluids, volumes of the reactor and the jacket and the total surface of heat transfer are known.

We have elaborated a computer program in Fortran 90 that allows the numeric calculation and the display of the temperature profile in the reactor according to time, following the type and the speed of the mobile of agitation chosen. Thus, this model enables the calculation of local and global transfer coefficients (hi, Ui). The initial temperatures in the reactor and in the jacket, as well as, the stirrer speed are the entry data of this model. The temperature (Ta), the average values of the global and local coefficients (Ui, hi) are exit data of the model.

RESULTS AND DISCUSSION

We have applied this model to our system, for different speeds of agitation. Figure 5 and 6; representing the prediction of temperature profiles for the agitated liquid, respectively for the turbine impeller with three tilted blades (TPI) and the turbine impeller with six flat blades (TPD).

Figure 5 and 6 show that during the heating of the agitated liquid, the temperature (Ta) evolves in non-linear way. The asymptotic value corresponds to the temperature of the heater. The initial slope of the temperature curve depends on the speed of agitation and of the type of mobile used.

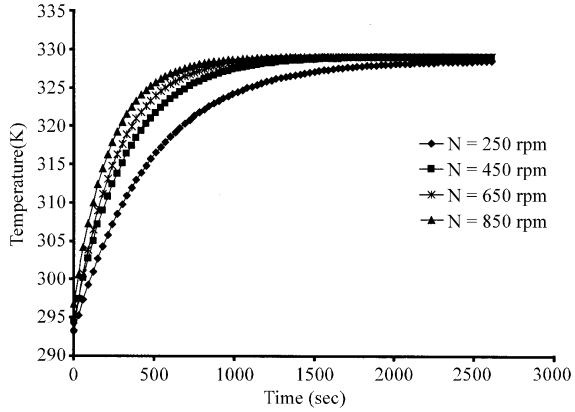

Fig. 5: Prediction of the agitated liquid temperature profiles for different stirrer speed (TPI)

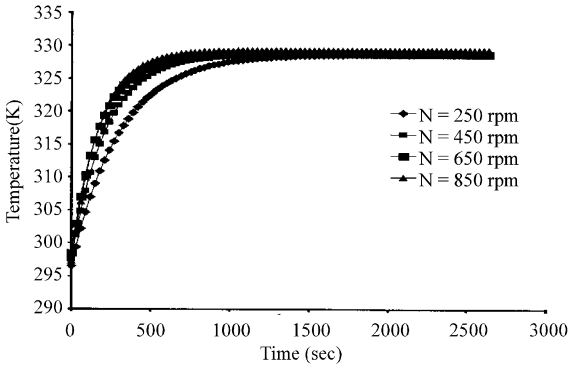

Fig. 6: Prediction of the agitated liquid temperature profiles for different stirrer speed (TPD)

Experimental validation: To validate our model we confronted results given by simulation, utilizing semi-empiric model, to the experimental results and we have defined its domain of validity. The Fig. 6 and 7 shows examples of temperature profile in the reactor, giving both by the model and by experimentation, for the two mobiles studied at stirrer speeds of 650 rpm.

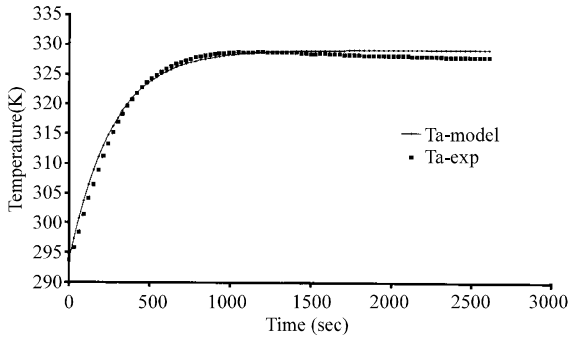

Fig. 7: Temperature profiles of the agitated liquid, (TPI) N = 650

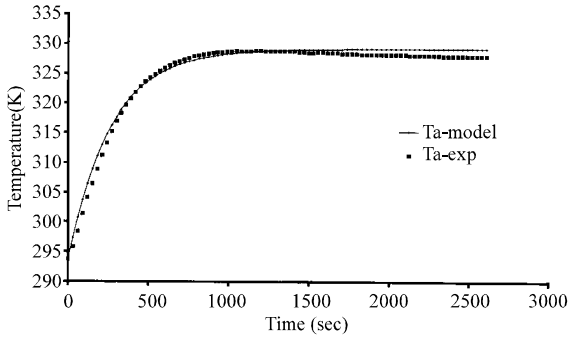

Fig. 8: Temperature profiles for the agitated liquid, (TPD) N = 650 rpm

While examining all representations for all stirrer speed experimented, we noticed that the proposed model described the same pace as the experimental values. The

Table 2: Statistic parameters

(TPI)			(TPD)	
N (rpm)	R	Var. (%)	R	Var. (%)
250	0.99583	99.167	0.9977	99.554
450	0.99348	98.701	0.98723	97.462
650	0.99441	98.886	0.99375	98.755
850	0.99393	98.789	0.98704	97.424

maximal gap between the two is equal to 2% in the majority of cases. In addition, statistical parameter calculations confirm this result.

Indeed, the analysis of the variance shows that 98% of the experimental points can be explained by our model (Table 2). In this case the maximal mistake is about 0.02 K. This value is comparable to the one committed by the experimentation which is about 0.01 K.

Application of the model to an exothermic reaction: In this part we have applied our model, to a reactive system with two consecutive exothermic chemical reactions of the first order, describe by Luyben (1996).
The heat of reaction is calculated by the equation:

$$Qr = Va\,(kl.Ca.\Delta H1 + k2.Cb.\Delta H2) \quad (9)$$

Qr: Reaction heat (W).
ΔH1, ΔH2: Enthalpies of the two consecutive reactions.

The equation of the global energy balance in the reactor becomes:

$$\rho_a VaCpa\frac{dTa}{dt} = -UiA\left[Ta(t) - Tj(t)\right] - Qp + P + Qr \quad (10)$$

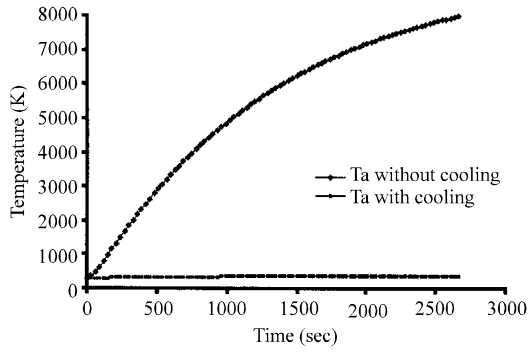

Fig. 9: Simulation of temperature profil Exothermic reaction

The simulation results is given by Fig. 9 (Baghli *et al*., 2005); representing the simulation profile of agitated liquid temperature with a turbine impeller with six flat blades (TPD) at speed of 650 rpm.

Model predictions imparts the average values of local and global transfer coefficients whatever the stirrer speed giving a number of Reynolds lower than 400, for the two mobiles studied.

According to the results gotten in this survey, we conclude that the proposed model can constitute a substantial tool for the simulation of this kind of process, in the domain of Reynolds defined higher.

This study with the example of simulation given reflects well the expected results, that is to say, the determination of the temperature profiles in the reactor, as well as, the determination of the different coefficients of transfer by simulation without making experience.

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