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Modelling thermal effects in agitated vessel and reactor design consideration

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Abstract:

The knowledge of the heat transfer coefficient on the inner side of a heated vessel wall is of utmost importance for the design of agitated vessels. The present contribution deals with heat transfer in an agitated vessel containing non-Newtonian liquid. The impellers used are six-blade Turbine (TPD) and a Propeller (TPI). The following aspects are discussed: description of the heat transfer process with the aid of dimensional analysis, heat transfer correlations for agitated liquid and influence of impeller speed on heat transfer.

Keywords: Mixing, Heat Transfer Coefficients, Viscous liquid.

1. Introduction

In the last few years, the important evolution of technology and Human needs have encouraged the development of many chemical processes without a basic knowledge of the potential risk involved, thus leading to a large number of accidents.

Accidents in the chemical processes are often due to the unexpected or undesired reactions, resulting from an over-heating of the reacting mixture and leading to a thermal-runaway. This happens when the heat generated by the reaction exceeds the heat removal capabilities of the equipment in which the process is carried out.

The standard equipment for this processes are:

Agitated vessels like stirred tanks, that involve mechanical mixing, they consist of a vessel, which can be heated or cooled by means of an external jacket or internal coils. The temperature evolution of the reactor contents depends on the heat transfer fluid temperature, agitated speed and apparent viscosity (Debab A., 2002). The heat transfer fluid can be temperature controlled for isothermal processes or may have a constant inlet temperature for isoperibolic ones (Yuce S., A. et al., 1999; Ziad Louleh et al. 1999).

Simulation and modeling for these equipment and processes are also on the increase due to the availability of high capacity computers (Kaminoyama et al., 1999; Ranade, 1997; Bakker et al., 1997 and Wei-Ming Lu et al., 1995).

From this study, it is possible to conclude that a thermal characterization and scale-up procedure are important aspects in the design of these installations. The present contribution deals especially with heat transfer between heated wall of a stirred vessel and a liquid exhibiting non-Newtonian time-independent flow behaviour. This work concentrate on Laboratory size stirred tank reactor and the later work will be on a pilot plant size reactor.

2. Apparatus and experimental method

An agitated vessel of 2.0 liters was made from stainless steel and surrounded by a jacket in which a heat-transfer fluid (e.g. water) circulates at a very high rate. It had an internal diameter D of 0.135m and an internal heat transfer surface A of 0.07307 m². Insulating the outside of the jacket by placing a 20 mm thick polypropylene lid on the reactor minimized heat exchange with the environment. A thermostat

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controls the jacket temperature and allows tracking a desired set point of the reactor temperature. The agitated vessel is equipped with a stirrer and PT-100 temperature sensors with a resolution of 1 mK.

A weighed amount of lubricating oil was placed inside the vessel and the agitator run at a constant speed. The viscosity was measured using a rotational viscometer (TA instruments). The rheological characterization was performed as a function of temperature in order to consider small variations due to energy dissipation during the mixing experiments. The dependence of the Newtonian viscosity with respect to temperature was expressed by an Arrhenius type equation given elsewhere (Debab, 2002). The density, heat capacity and thermal conductivity of this liquid at temperature in the range of (20- 80)°C were taken from (Strek et al., 1967).

A computer with an electronic devise is employed for data acquisition. The measured variables are the jacket inlet (T_{ji}) and outlet temperature (T_{jo}), the reactor temperature (T_a) and the stirrer speed (N_a) and sent to the computer. Water circulates through the heating/cooling loop by a centrifugal pump and the flow rate was measured by a flow meter.

Two impellers were employed: these were a turbine ($d= 78\text{mm}$) and a propeller ($d= 66\text{mm}$).

Further details on experimental equipment and procedure are given elsewhere (Debab, 2002).

The rate of heat evolution in the agitated vessel is related to the flow through the reactor wall. Hence, the temperature measurements have to be accurate and truly representative of the conditions existing in the various balance volumes. For example, it is necessary that the reactor and jacket zones are thermally homogeneous. In the jacket this is achieved by circulating the heat-transfer fluid at a very high flow rate. Consequently, the temperature difference between jacket inlet and outlet remains very small (typically 0.1K). Inside the reactor, a well-designed stirrer insures that the reactor zone is nearly homogeneous. Since it may be of interest to be able to follow fast thermal processes, the accumulation of heat within the wall has to be accounted for, and in addition, the thermally non-homogeneous wall needs to be modelled as a distributed system.

3. Reactor modeling

The differential heat balance (Equation 1) included the thermal capacities of the agitated liquid and the tank itself and also the energy dissipation of the impeller, reads:

$$(m_i C_{p_i} + m_a \cdot C_{p_a}) \frac{dT_a}{dt} = q_1 + q_2 \quad (1)$$

Where, q_1 and q_2 are the power terms associated with the energy transfer from the heating/cooling medium and the secondary heat effects (stirrer energy, heat transfer from the surroundings), respectively. The first term on the right-hand-side of the equation is often referred to as q_R , the total rate of heat evolution in the mixing fluid.

The heat flow q_1 , which is defined by the Equation (2) below, requires for its computation the knowledge of T_{wi} , the wall temperature in contact with the reactor contents :

$$q_1 = - h_i A_i (T_a - T_{wi}) \quad (2)$$

Since the wall is thermally non-homogeneous in the direction of the heat transfer, its temperature T_w is described by the following heat conduction equations and T_{wj} being the wall temperature in contact with the heating/cooling medium.

$$\frac{\partial T_w}{\partial t} = \frac{\lambda_w}{\rho_w C_{p_w}} \frac{\partial^2 T_w}{\partial l^2} \quad (3)$$

with the boundary conditions:

$$\lambda_w \frac{\partial T_w}{\partial l} \Big|_{l=0} = h_i (T_{wi} - T_a) \quad (4)$$

$$\lambda_w \frac{\partial T_w}{\partial l} \Big|_{l=x} = h_j (T_j - T_{wj}) \quad (5)$$

The partial differential Equation (3) can be put in discrete form within the space with respect to its thickness by applying the method of orthogonal collocation (Villadsen, 1978), using N interior collocation points (N being a design parameter at this stage of the development).

The secondary heat effects comprise the power input due to the stirrer (modelled as a linear function of the stirrer speed) and the heat loss through the insulated parts of the vessel (the heat-loss coefficient is treated as a linear function of the reactor temperature).

4. Determination of the heat transfer coefficients

4.1 Internal partial heat transfer coefficient h_i

From dimensional analysis, using the Nusselt Equation (6), it is possible to correlate empirically the internal partial heat transfer coefficient as a function of operating conditions and mixture properties by means of equation (7).

$$Nu = C_1 Re^\alpha Pr^{0.33} Vi^{0.14} \quad (6)$$

$$h_i = C_0 \cdot N_a^\alpha \quad (7)$$

The constants C_1 and α are depending on the type of impeller and system geometry, they are reported by (Bourne et al., 1981 and Fletcher, 1987).

According to Equation (7), only the stirrer speed can modify the value of internal partial heat transfer coefficient for a given reactor, with the same mixture and temperature conditions inside it. The value of C_0 is described by dimensionless analysis (Nusselt equation) in Equation (8):

$$C_0 = C_1 \cdot \frac{\lambda_{av}}{D_0} \cdot Pr^{0.33} \cdot Vi^{0.14} \cdot \left[\frac{d^2 \cdot \rho_{av}}{\mu_{ap}} \right]^\alpha \quad (8)$$

Assuming that C_1 has a constant value under the conditions previously mentioned, it is possible to determine experimentally the value of h_i , using the Modified Wilson plots (Chapman et al., 1965). For every vessel, the values of h_i and C_1 must be experimentally determined in order to derive the characteristic values for a specific system. The correct values of h_i and C_0 can be simply obtained using Equation (9).

$$\frac{1}{U_i} = \frac{1}{h_i} + \frac{A_i x}{A_{av} \lambda_w} + \frac{Di}{Do \cdot h_j} \quad (9)$$

It should be noticed that every liquid could produce or deposit a layer of extraneous materials on the heat transfer surface, which will provoke a time modification of both partial heat transfer coefficients. In these cases, the heat transfer resistance increases considerably due to the fact that this type of materials normally has a lower thermal conductivity. This effect is referred to as the fouling or dirt factor, and should be avoided or, if this is not possible, which should be taken into account as a further resistance to the heat transfer.

With the same operating conditions in the jacket, R_w and h_j will not change, and h_i can be modified varying only the stirrer speed. A straight line can be plotted in a graph using Equation (10).

$$\frac{1}{U_i} = \left[R_w + \frac{D_0}{D_1 \cdot h_j} \right] + \frac{1}{C_0} N_a^{-\alpha} \quad (10)$$

4.2 External partial heat transfer coefficient h_j

Determination of the external partial heat transfer coefficient for a given vessel can be done following the dimensional analysis mentioned previously for the calculation of the internal one. Again, the Nusselt Equation (6) can be used to correlate empirically the influence of the flow of the circulating heat transfer fluid through the jacket.

Many different authors (Fletcher, 1987, Werner, et al 1986 ; Strek et al., 1967) have reported studies on Nusselt's dimensionless equation for different systems through a large range of Reynolds numbers (Re). The heat transfer coefficient h_j is determined according to following correlation (12) given in (Werner A., et al 1986):

$$Nuj = \left[3.65^3 + 1.61^3 Re_j Pr \left(\frac{D_1}{H} \right) + 0.664^3 Re_j^{1.5} Pr \left(\frac{D_1}{H} \right)^{1.5} \right]^{0.33} \left(\frac{\mu(T_j)}{\mu(T_p)} \right)^{0.14} \quad (12)$$

4.3 Overall heat transfer coefficient U_i

In some cases it may be useful to know the variation of the overall heat transfer coefficient during a chemical process. It might happen during a chemical reaction that the physical properties of the mixture change drastically and, with them, its heat transport characteristics. Under such conditions, the internal heat transfer coefficient might decrease due to the variation of the reaction mixture properties, and a large quantity of heat than expected can be accumulated in the reactor, increasing the temperature of the mixture. In such cases, undesired reactions may take place and, in the worse case, reaction can lead to a thermal runaway.

There are two different methods to measure the overall heat transfer coefficient using calorimetric principles. The first one uses a control system to keep the reactor temperature constant while a known power is given to the mixture, which causes a decrease of jacket temperature. The second one is in isoperibolic mode, where a known power (q_i) is given to the mixture and the reactor temperature is followed to reach a steady state. In both cases the measure of the ΔT generated will be used to determine the value of U_i .

The overall heat transfer coefficient can then be calculated using Equation (13).

$$U_i \cdot A_i = \frac{q_i}{\Delta T_{ln1} - \Delta T_{ln0}} \quad (13)$$

Where: ΔT_{ln0} and ΔT_{ln1} are the temperature difference between the mixture and the jacket before and during the power input (when reactor temperature steady state is reached) respectively.

5. Results and discussion

A computer programme was used to analyse the data taken in this heat transfer study.

The first step deals with the temperature-time data, the second with the calculation of the Overall heat transfer coefficients U_i and the third step with the estimation of the partial heat transfer coefficient h_i .

Step 1:

The temperature of the liquid inside the vessel, as function of time, has been fitted with polynomial and exponential equations and the last one has been found to accurately represent these heat transfer data, it is given by equation of the form:

$$\frac{T_t - T_\infty}{T_0 - T_\infty} = \exp(\xi t) \quad (14)$$

ξ is a number whose value depends on the shape of the heating curve. The computer uses regression analysis to find values of ξ and T_∞ that best fit the experimental data.

Table 1 gives a comparison of the observed temperature data for a typical run with that calculated by the computer using Equation (14). The percent differences between the observed and calculated values are seen to be small.

Table 1. Theoretical and experimental temperature-time data for TPD. System: lubricate oil, impeller speed: 250rpm

Observed temperature (°K)	Calculated temperature (°K)	Obs. – Calc. (°K)	Percent difference	Time (mn)
301.018	300.57	0.443	0.147	1
305.15	306.553	-1.383	-0.453	2
309.395	311.220	-1.825	-0.589	3
312.602	314.907	-2.305	-0.737	4
315.552	317.807	-2.225	-0.714	5
318.057	320.089	-2.032	-0.639	6
320.193	322.910	-2.717	-0.848	7
321.915	324.103	-2.188	-0.679	8
323.33	325.041	-1.71	-0.529	9
324.4	325.779	-1.379	-0.45	10
325.34	326.35	-1.011	-0.311	11
326.037	326.81	-0.77	-0.23	12

Typical plots of time-temperature have been presented in Figure 1 for TPD. From these plots it could be clearly seen that the agreement between the experimental data and the theoretical values is satisfactory. Similar plots prepared for the TPI also indicated satisfactory agreement.

Step 2:

The asymptotic heating curve parameters from step 1 are used to calculate values of the Overall heat transfer coefficients U_i . Equation (1) can be rewritten as:

$$(m_i C_{p_i} + m_a C_{p_a}) \frac{dT_a}{dt} = U_i A_i (T_{js} - T_a) \quad (15)$$

which can be written in the form:

$$U_i = \frac{(m_i C_{p_i} + m_a C_{p_a})(T_{af} - T_{ai})}{A_i (T_{js} - T_a) \Delta t} \quad (16)$$

the term C_{p_a} is a function of temperature. Equation (16) enables values of U_i , the overall heat transfer coefficient, to be calculated. U_i is related to the film heat transfer coefficient, h_i , of the liquid inside the vessel. In addition the computer also calculates the Reynolds numbers at these temperatures. The values calculated from Equation (16) are presented in Table 2.

Table 2. Values of U_i , Na and Re

TPD			TPI	
Na (rpm)	Re	U_i (W.m ⁻² .°C)	Re	U_i (W.m ⁻² .°C)
250	142.80	129.30	140.78	83.95
450	241.95	188.68	265.07	116.22
650	353.75	240.82	373.49	146.68
850	430.91	276.19	573.08	189.721

From the above table it can be seen that the heat transfer coefficient is calculated in the Transition regime.

Step 3:

The partial heat transfer coefficient h_i is calculated by Equation (10), which can be rewritten as:

$$\frac{1}{U_i} = \Phi + \frac{1}{h_i} \quad (17)$$

where $\Phi = R_w + \frac{D_0}{D_1 \cdot h_j}$ which is a constant for any one tank.

The calculated values of the local heat transfer coefficient h_i has been plotted against the speed of the impeller for each of the impellers. From this plots it has been deducted the correlations given in Table 3.

Table 3. Correlations of the local heat transfer coefficient “ h_i ” with the speed N

TPD	TPI
$h_i = 3.697 N^{2/3}$	$h_i = 2.158 N^{2/3}$

6. Conclusion

The heat transfer behavior at unsteady states in the stirred vessel with two types of impellers for viscous liquid is analyzed. The method of estimating the local heat transfer coefficient on the vessel side wall is presented based on theoretical and experimental results.

Notation

A_i :	heat transfer surface area (m^2)
c :	parameters for correlations
C_p :	specific heat capacity ($J.Kg^{-1}.K^{-1}$)
d :	impeller diameter (m)
D_0 :	tank internal diameter (m)
D_1 :	jacket internal diameter (m)
g :	gravitational acceleration ($m.s^{-2}$)
h_i :	partial internal heat transfer coefficient ($W.m^{-2}.K^{-1}$)
h_j :	partial internal heat transfer coefficient ($W.m^{-2}.K^{-1}$)
m :	mass (Kg)
N_a :	stirrer speed (s^{-1})
Q :	volumetric flow ($m^3.s^{-1}$)
q :	thermal flow (W)
P :	power (W)
T_{ji} :	inlet jacket temperature (K or $^{\circ}C$)
T_{jo} :	outlet jacket temperature (K or $^{\circ}C$)
t :	time (s)
U_i :	overall heat transfer coefficient ($W.m^{-2}.K^{-1}$)

Greek symbols

λ :	Thermal conductivity ($W.m^{-1}.K^{-1}$)
μ :	Dynamic viscosity ($kg.m^{-1}.s^{-1}$)
μ_{ap} :	apparent viscosity ($kg.m^{-1}.s^{-1}$)
ρ :	Density ($kg.m^{-3}$)

Dimensionless groups

$N_p = P. \rho^{-1}. N^{-3}. d^{-5}$	Power number
$Nu = h.D.\lambda^{-1}$	Nusselt number
$Pr = \mu.C_p. \lambda^{-1}$	Prandtl number
$Re = \rho_m.N_a.d^2.\mu^{-1}$	Reynolds number
$Vi = \mu_{bulk}/\mu_{atwall}$	Viscosité ratio

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