Proceedings of the 18th UK Heat Transfer Conference

9-11 September 2024, Birmingham

UKHTC2024-123

EXTENDED HEAT TRANSFER MODEL OF A JACKETED BATCH STIRRED TANK REACTOR

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1. ABSTRACT

An extended thermal model for jacketed batch stirred tank reactors (STRs) has been expanded for applications to both non-reactive and reactive systems. It is not only able to replicate the predicted process temperature profile by the reduced thermal model, but also provides information about how the jacket outlet temperature and the heat flows vary with time. It is revealed that values of the overall heat transfer coefficient obtained from experimental data and the reduced thermal model inherently include several thermal effects not covered in the model equations and thus should not be used to predict other experimental equipment, process and ambient conditions.

2. INTRODUCTION

Jacketed stirred tank reactors (STRs) are widely used in academic laboratory teaching and research, in industrial pilot plants and in full scale processes. It is imperative that the transient temperature response of the contents of the reactors are predicted as accurately as possible, so that exothermic reactions can be controlled to avoid the dangers of thermal runaways in any of the previous mentioned situations. The most simplistic and commonly used mathematical predictor of process temperature is the adiabatic reduced thermal model, but this requires experiments to generate transient temperature profiles and then to use measurement data in the model to back calculate an overall heat transfer coefficient (OHTC). The values of these OHTCs are extremely limited in their use for predicting process temperature profiles other than for exactly the identical sized equipment, processing fluids and ambient conditions.

Snee and Hare [1] reported results from an investigation of the control and stability of exothermic reactions in a pilot scale STR, fitted with a retreat curve impeller and an outer plain jacket. This STR had been chosen in order to reproduce conditions similar to those in industry. The heat transfer characteristics of the 250 L glass-lined reactor (DIN Standard 28136) were investigated by four experiments performed with two agitation rates and two flow rates of cooling water circulating through the reactor jacket at a fixed inlet of around 12 °C. The 200 L of water in the vessel was raised to around 50 °C by an electrical immersion heater and then cooled by the water in the jacket.

No cooling temperature profiles of the vessel contents nor temperatures at the inlet and outlet of the jacket were reported in the paper [1], but they must have been recorded as the four Newtonian cooling times of the experiments were reported. These revealed that shorter cooling times occurred with a greater stirring rate and a larger flow through the jacket. However, the so called reduced thermal model, Equations (1) and (2), is used for the prediction of the transient temperature response (T_p^*) of the well mixed contents of a vessel and depends

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upon the heat capacity of the water in the vessel, an OHTC, a transfer area and ignores any coolant effect of the water flow through the jacket.

The Newtonian Cooling Time (NCT), $\left(Mc_p\right)_p/(U^*A)_p$, is the gradient of the analytical solution, Equation (3), of the reduced thermal model and a semi-log plot of experimental data of t against $\ln\left\{(T_p^* - T_{j1})/(T_{pi} - T_{j1})\right\}$ would have provided these values of the gradient. Four different values of $(U^*A)_p$ are obtained from these gradients, see Table 1. Each of these values of $(U^*A)_p$ in equations (1) and (2) will provide reasonable cooling temperature profiles for the experiments.

$$\left(Mc_p\right)_p \frac{\mathrm{d}T_p^*}{\mathrm{d}t} = (U^*A)_p \left(T_{j1} - T_p^*\right) \tag{1}$$

$$\text{Initial conditions: } t \le 0, T_p^* = T_{pi} \text{ and } t > 0, T_{j1} \text{ remains fixed.} \tag{2}$$

$$t = \left(Mc_p\right)_p \times \ln\left\{(T_p^* - T_{j1})/(T_{pi} - T_{j1})\right\}/(U^*A)_p \tag{3}$$

Recently, a more detailed thermal model has been reported [2], which reduces the experimental requirements for determining the OHTC in the reduced thermal model. Equation (4), along with the initial conditions in Equation (2), permit the process temperature profile $\left(T_p\right)$ to be predicted. There are now three OHTCs $\left(U_p, U_{jloss} \text{ and } U_{ploss}\right)$ and associated transfer surface areas $\left(A_p, A_{jloss} \text{ and } A_{ploss}\right)$ required as well as a full complement of added thermal inertia terms $\left(Mc_p\right)_n$ and the ambient temperature (T_{amb}). Note that the asterisk $(*)$ used for U_p and T_p do not apply for this extended model. Hopefully, with knowledge of the type of agitator, the agitation rate, the vessel and jacket dimensions and materials, correlations to predict the film heat transfer coefficients for the vessel and jacket, then the various thermal resistances for the OHTCs can be evaluated without the need for experimentation.

$$\begin{aligned}\sum_{n=1}^{N}\left(Mc_p\right)_n \frac{\mathrm{d}T_p}{\mathrm{d}t} &= \frac{\left(\dot{M}c_p\right)_j}{1+\dfrac{(UA)_{jloss}}{(UA)_p}}\left[\frac{\left(T_{j1}-T_p\right)+\left(T_{j1}-T_{amb}\right)\dfrac{(UA)_{jloss}}{(UA)_p}}{1+\dfrac{(UA)_{jloss}}{(UA)_p}}\right] \\ &\times\left[1-\exp\left(-\frac{(UA)_p+(UA)_{jloss}}{\left(\dot{M}c_p\right)_j}\right)\right]+\frac{(UA)_{jloss}\left(T_{amb}-T_p\right)}{1+\dfrac{(UA)_{jloss}}{(UA)_p}} \\ &+(UA)_{ploss}\left(T_{amb}-T_p\right)\end{aligned} \tag{4}$$

3. RESULTS

The NCT values and other calculated values for all four experiments are listed in Table 1. The $(U^*A)_p$ value for experimental run 1 was used in the reduced model to generate the predicted T_p^* profile in Figure 1a. U_{ploss} and U_{jloss} were calculated from a combination of literature correlations and then implemented into the extended thermal model. Parameter estimation was applied to profiles from the extended thermal model to generate a value of $(UA)_{p,f}$, that fitted the T_p^* profile in Figure 1a. A NTC value was obtained from the final extended temperature profile and used to calculate $\left(U_f^*A\right)_p$. There is <0.2% difference between $\left(U_f^*A\right)_p$ and $(U^*A)_p$, which indicates that any values of U_p^* generated from the reduced thermal model inherently include thermal contributions from physical values of terms such as the likes of $\sum_{n=1}^{N}\left(Mc_p\right)_n$, $(UA)_p$, $(UA)_{ploss}$, $(UA)_{jloss}$ and T_{amb}, which are accounted for in the extended thermal model. Figure 1b shows how the predicted heat transfer rate between the jacket and the process (Q_{jp}) and rate of heat losses from the process (Q_{ploss}) and the jacket (Q_{jloss}) changed over time for experimental run 1.

Table 1: Comparison between $(U^*A)_p$(calculated NCT data), $(UA)_{p,f}$ (fitted using the extended thermal model) and $\left(U_f^*A\right)_p$(calculated from the extended thermal model using the NCT method).

Run	Flow (L min^{-1})	Agitation (RPM)	NCT (s)	NCT $(U^*A)_p$ (WK^{-1})	Extended $(UA)_{p,f}$ (WK^{-1})	$\left(U_f^*A\right)_p$ (WK^{-1})	$\left(U_f^*A\right)_p/(U^*A)_p$ Difference (%)
1	10	69	5630	145.96	188.4	145.97	0.005
2	10	139	5430	151.33	197.1	151.36	0.015
3	20	69	4606	178.41	222.2	178.69	0.158
4	20	139	4465	184.04	230.2	184.23	0.105

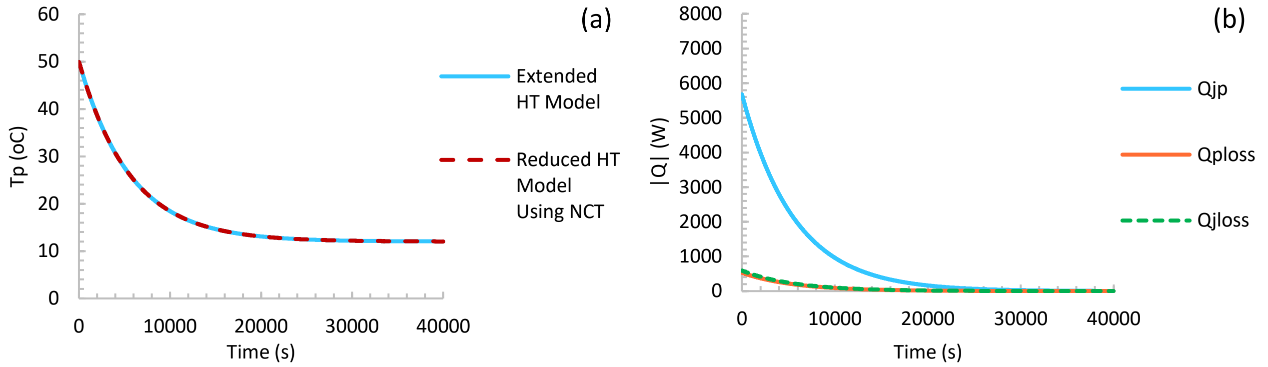

Figure 1: The process temperature (a) and heat flow rates (b) predicted by the reduced and extended thermal models.

The fitted U_pA_p can then be used to calculate the jacket side film heat transfer coefficient (161.0 Wm^{-2}K^{-1} for experimental run 1) by using a literature correlation for the process side. This would enable the extended thermal model to be applied to a reactive system in future work, with only the jacket side coefficient needing to be determined from experimental data of a non-reactive system.

5. CONCLUSIONS

The extended thermal model replicates the predicted T_p^* profile by the reduced thermal model and provides information regarding the heat losses and the jacket outlet temperature. Additionally, values of U_p^* inherently include thermal contributions of terms $\sum_{n=1}^{N}\left(Mc_p\right)_n$, $(UA)_p$, $(UA)_{ploss}$, $(UA)_{jloss}$ and T_{amb}.

ACKNOWLEDGMENT

The first author acknowledges the UK Engineering and Physical Sciences Research Council (EPSRC) for funding through the Doctoral Training Partnership award.

REFERENCES

[1] T. J. Snee and J. A. Hare, “Development and application of a pilot scale facility for studying runaway exothermic reactions,” J. Loss Prev. Process Ind., vol. 5, no. 1, pp. 46–54, 1992.

[2] M. Johnson, K. H. Al-Dirawi, E. Bentham, T. Mahmud, and P. J. Heggs, “A non-adiabatic model for jacketed agitated batch reactors experiencing thermal losses,” Ind. Eng. Chem. Res., vol. 60, no. 3, pp. 1316–1325, 2021.