Fixed Bed Heat Transfer Parameter Estimation – A New Look at an Old Problem

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Highlights

- Particle-resolved computational fluid dynamics (PRCFD) simulates heat transfer experiment.
- Wall coefficient (h_w) and radial thermal conductivity (k_e) estimated by two methods.
- Values of h_w are very sensitive (biased low) to experimental mixing cup heat losses.
- k_r, h_w from radial temperature profiles give correct Q (total bed heat transfer).

1. Introduction

The pseudo homogeneous 2D $k_r - h_w$ fixed bed heat transfer model is still frequently used for fixed bed reactor simulation and design because of its simplicity, despite having been criticized as being either inadequate or non-physical [1]. The two parameters are usually estimated from non-reacting heat transfer experiments, by one of two main approaches, designated Method 2 and Method 4 [2]. In Method 2 the bed centerline temperature is measured either by embedded thermocouples or a thermowell, as well as either the exit mixing-cup temperature or the tube exit temperature profile [3]. This method is intrusive in the bed, and uses very little data to separate the two radial parameters, whose estimates may be statistically biased and/or have large variance. Method 4 uses radial temperature profile measurements at the exits of a series of progressively longer beds, then fits the profiles using nonlinear least squares parameter estimation, which allows statistical analysis such as estimation of confidence intervals [4]. Method 4 has been criticized for using measurements outside the bed itself and for observed bed length effects on the parameters. It has been shown for method 4 that the parameter estimates can depend on the radial thermocouple locations, especially for h_w [5].

It is difficult to obtain experimental data from the same tube to make a fair comparison between the methods. This is possible, however, using particle-resolved computational fluid dynamics (PRCFD) in which heat transfer in computer-generated beds of particles can be simulated. PRCFD simulations give temperatures at all locations within the bed, without disturbing the packing. This work simulates an experiment carried out by Yagi and Wakao [3] of a bed of spheres with tube-to-particle diameter ratio $N = 6$ to answer the question of whether the two methods give the same parameter values, and whether models that use the estimated parameters give the correct total heat transfer to or from the fixed bed.

2. Methods

PRCFD simulations were carried out in a computer-generated randomly packed bed of 1014 6 mm glass spheres. An adapted "soft-sphere" Monte Carlo collective rearrangement algorithm [6] was used to generate the packing. The bed length was 0.2 m which was meshed with tetrahedra. A range of mesh sizes was used to show mesh independence, with the final chosen mesh at 43.45×10^6 cells. Small bridges of effective thermal conductivity between that of glass and air (the fluid) were placed at particle-wall contact points. Comparison to the experimental data of the original study [3] for values of Re = 234, 382 and 691 validated the model simulations, which were run under ANSYS Fluent 2023 R1.

Centerline temperature profiles as well as bed exit mixing-cup temperatures were output and used in method 2, in which the slope of the straight-line part of a plot of ln $(T_w - T_c)$ vs. z gave k_r and the characteristic equation of the PDE and an equation relating the mixing cup temperature to the first eigenvalue of the model gave h_w. Radial temperature profiles were output at 16 positions and 8 axial positions. Selected profiles were fitted by method 4 which used the nonlinear least squares Marquardt-Levenberg method. The total heat transfer Q from the tube wall to the bed was also evaluated.

3. Results and discussion

The computer-generated fixed bed model and a sample fit to the centerline temperature profile for method 2 are shown (Fig. 1). A preliminary sensitivity analysis for method 2 showed that a measurement of the mixing cup temperature 1K low would give a low value of h_w by 18%. PRCFD can avoid this.

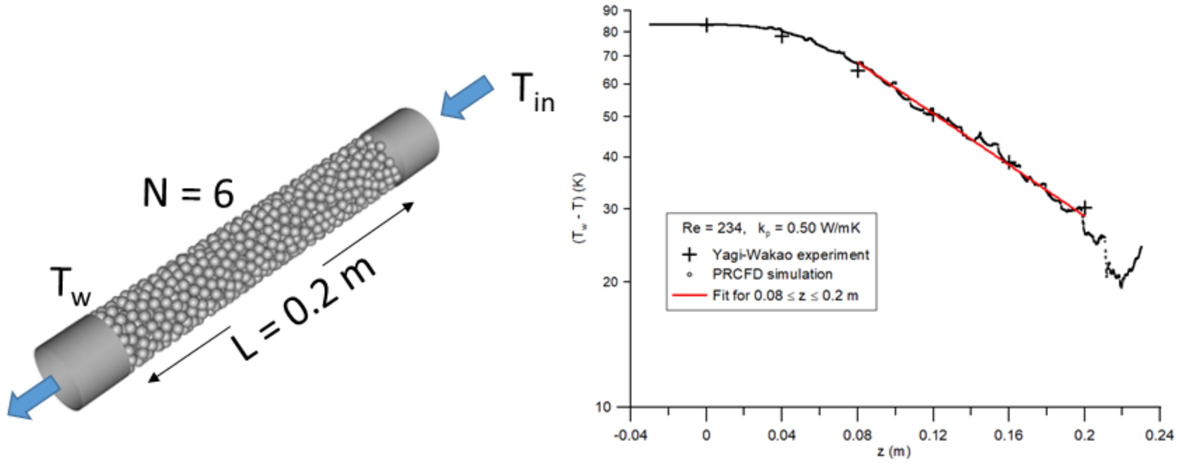

Figure 1. Isometric view of simulated fixed bed (left); fit of straight line to PRCFD axial temperatures (right).

Length effects on the parameters in method 4 were observed for $z < 0.04$ and were avoided by fitting to radial temperature profiles from bed depths between 0.08 and 0.2 m, corresponding to the straight-line portion of the centerline profile used by method 2 (Fig. 1). Comparisons of the parameter values estimated by both methods, as well as the predicted total wall heat flow Q, are given in Table 1.

	k_r/k_f		Nu_w		Q (W)		
Re	Method 2	Method 4	Method 2	Method 4	PRCFD	Method 2	Method 4
234	15.90	17.19	28.21	28.94	53.76	52.17	53.26
382	22.33	24.69	32.10	35.34	80.90	76.52	80.01
619	28.56	39.47	48.44	44.88	129.33	121.60	128.84

Table 1. Comparison of estimated parameter values and predicted total heat transfer using both methods.

4. Conclusions

Sensitivity analysis of method 2 showed that h_w was strongly affected by mixing cup temperature, which would be likely measured low in an experiment due to heat loss, giving underestimated values of h_w. In method 4 length effects on the parameters were found at small z, and attributed to developing radial profiles. These could be eliminated by fitting model 4 to the same range of z as used to fit the straight line of method 2. Values of $Nu_w = h_w d_p / k_f$ were in good agreement for the two methods, contrary to previous literature, while values of k_r/k_f were slightly higher from method 4. Use of the parameters in a 2D pseudo homogeneous fixed bed heat transfer model showed the parameters from method 4 reproduced the total bed heat transfer accurately, the parameters from method 2 under predicted Q, especially at higher Re. These findings have implications for the prediction of hot-spots in fixed bed reactors and for the evaluation of the thermal performance of novel catalyst particle shapes.

References

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Keywords

Particle Resolved CFD; Fixed Bed; Heat Transfer; Parameter Estimation.