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Technical Note

A CFD based correlation for mass transfer coefficient in elbows

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1. Introduction

Mass transfer has a very significant influence on corrosion rates. This is because the corrosion rate is proportional to the mass transfer coefficient raised to a power between 1 and 3, depending on solution chemistry and temperature [1]. Mass transfer and corrosion rates also depend on flow geometry and, in multiphase flows, on flow regime [2]. Due to the strong influence of local mass transfer coefficients on corrosion rate predictions, several investigators conducted experiments for single-phase flows to determine the maximum mass transfer coefficients in 90° elbows and 180° bends. For example, Poulson and Robinson [1] experimentally studied mass transfer in two 180° bends with r/D ratios of 1.25 and 2.72. An expression for the ratio of the maximum mass transfer coefficient for an elbow to the mass transfer coefficient for fully developed pipe flow (hereafter called the maximum elbow-to-pipe mass transfer coefficient ratio (MTCRE)) was also proposed by Poulson and Robinson based on the experimental data in the $r/D = 1.25$, 180° bend. The proposed expression contains only the Reynolds number and it was concluded that the MTCRE increases as the flow Reynolds number increases.

Coney [3] experimentally investigated the mass transfer in elbows and bends and developed an equation for the MTCRE

$$\frac{Sh_{\text{outside radius of bend}}}{Sh_{\text{fully developed pipe}}} = 1 + 2.2\left(\frac{R}{r}\right)^{1.2}\left(\frac{L}{D}\right)^{0.75}, \tag{1}$$

where $Sh = hD/D_{\mathrm{f}}$ is the Sherwood number, h the mass transfer coefficient, D_{f} the fluid diffusivity, D the inside pipe diameter, R the radius of the pipe ($R = D/2$), r the mean radius of the elbow, and L is the length along the center line of the curved section of the elbow. For a 90° elbow, $L = \pi r/2$, and Eq. (1) becomes

$$\frac{Sh_{\text{outside radius of 90°elbow}}}{Sh_{\text{fully developed pipe}}} = 1 + 1.343\left(\frac{r}{D}\right)^{-0.45}. \tag{2}$$

Eq. (2) is a function of the ratio of elbow radius to pipe diameter. This correlation suggests that the Reynolds number does not have an influence on the MTCRE. (It should be noted that the Reynolds number does influence the mass transfer coefficient in elbows.)

Sprague et al. [4] measured local mass transfer coefficients in a 45° bend and a 180° bend with an r/D of 2.72. Based on the experimental data, Sprague et al. concluded that the MTCRE in 45° and 180° bends decreases as the flow Reynolds number increases.

It is well known that the mass transfer coefficient in a straight pipe is a function of the flow Reynolds number ($Re = DU/\nu$, where U is the average flow velocity and ν is the kinematic viscosity of the fluid) and the Schmidt number ($Sc = \nu/D_{\mathrm{f}}$). The mass transfer coefficient in elbows also depends on the flow Reynolds number and the Schmidt number. Therefore, the MTCRE may be a weak function of the flow Reynolds number (Re) and the Schmidt number (Sc). It is also a function of the elbow radius to pipe diameter ratio (r/D). Since turbulent flow in a 90° elbow is not as well developed as compared with the flow in 180° bends, where most mass transfer experiments were performed, the conclusions for mass transfer in 180° bends may not be directly applicable to 90° elbows. Also, some of the conclusions from different sources of experimental observations [1,3–5] are not totally consistent.

This investigation was motivated by a need to predict mass transfer coefficients in short- and long-radius elbows for use in conjunction with a mechanistic model

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for calculating CO_2 corrosion rates [6] in oil and gas pipelines. In the present investigation, CFX [7], which is a commercially available three-dimensional computational fluid dynamics (CFD) code, is used to compute flow and mass transfer coefficients in elbows. Predicted mass transfer coefficients from the pipe wall to the fluid or from the fluid to the pipe wall are compared with available experimental data in the literature. Finally, based on the three-dimensional CFD modeling, an equation for estimating the maximum mass transfer coefficients for 90° elbows is developed.

2. Model description and verification

In CO_2 corrosion of oil and gas pipelines, concentrations of chemical reacting species can be dilute. Thus, their reactions with the pipe wall may not significantly change the fluid or flow behavior. Therefore, it is assumed the flow field results will not be affected by chemical reactions. This de-couples the governing flow equations from the governing equations for mass transfer. Based on this assumption, the CFD code was used to simulate flow and mass transfer in elbows. Flow in an elbow is assumed to be turbulent and turbulent flow models are needed to calculate the turbulent viscosity that is needed in the Reynolds (time-averaged Navier–Stokes) equations. There are several turbulence models available in the CFD code. Among them, the standard k–ε model and a low-Reynolds-number version of the k–ε model were used to predict turbulent flow and mass transfer in elbows. It is also noticed (see [7–9]) that mass transfer model, if used in conjunction with the standard k–ε model, is limited to calculation of mass transfer for low Schmidt number species ($Sc < 25$). In an actual CO_2 corrosion process, the Schmidt number for some species, such as Fe^{++}, is much higher than this limit. Therefore, the low-Reynolds-number version of the k–ε turbulence model was used in conjunction with Fick's law to investigate the effects of the Schmidt number on the MTCRE.

A description of the governing equations that are used to solve the flow field and mass transfer coefficient is given in [7–9].

The experimental data of Enayet et al. [10] for turbulent flow in a 90° elbow were used to evaluate the turbulence models used in this study. Mass transfer results were compared with experimental data of Achenbach [5] to verify the models.

2.1. Flow model verification in a 90° elbow

The experimental data provided by Enayet et al. [10] with a Reynolds number of 43 000 were simulated with the CFD code. The turbulence models used to simulate the flow were the standard k–ε model and the low-Reynolds-number version of the k–ε model [7–9]. The simulation started at a plane 5 diameters upstream of the elbow inlet (i.e., $x/D = -5$) assuming a uniform inlet velocity profile (Enayet et al. data did not give details of flow upstream of the elbow). For the standard k–ε model, the grid was generated in a way that the y^+ value for the first grid point away from the wall was in the range of 50–100. For the standard model, the total number of grid points used was 29 520 with 80 in the streamwise direction. The total number of grid points in the normal (cross-section) plane is 369 with 36 grid points in the circumferential direction. A grid refinement study was performed using the standard version of the k–ε model by doubling the number of grid points in the radial direction. The solutions for the velocity profiles and the mass transfer coefficient ratios (discussed below) that were obtained by the finer radial grids were compared to the solutions presented below. The differences between the solutions for the finer grid and the results presented in this section were generally less than one or two percent.

When the low-Reynolds-number version of the k–ε model was used, the grid generated resulted in a y^+ value ranging from 0.4 to 1.0. For this case, the total number of grid points was 67 560 with 80 in the streamwise direction. The total number of grid points in the normal plane is 832 with 32 grid points in the circumferential direction. Only sample results are presented in this paper; further results and details are discussed by Wang [8] and Wang et al. [9].

The predicted velocity profiles at the 30° station of the elbow are compared with the experimental data [10] and are shown in Fig. 1. It can be seen that at the 30° station, both the standard and the low-Reynolds-number k–ε turbulence models overpredict the streamwise velocity near the inner wall of the elbow. But, in the

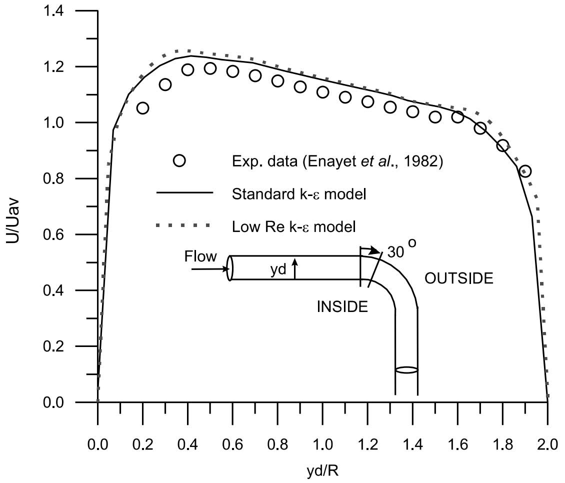

Fig. 1. Predicted velocity profiles and experimental data [10] at the 30° station.

outer wall region the predicted velocity profiles from both models agree with the experimental data. The overprediction of the velocity profile in the inner wall influences the prediction of mass transfer coefficients in this region. Fortunately, as it is shown later, the maximum corrosion rate or the mass transfer coefficient occurs at the outer wall region and at $x/D \approx 1$, where velocity predictions agree well with the data. The flow model predictions downstream of the elbow were also carefully studied. This is because the maximum mass transfer occurs downstream of the exit of the elbows. Fig. 2 shows the comparison of the predictions with the experimental data downstream of the elbow at $x/D = 1$ station. From Fig. 2, it can be seen that in the downstream region, the standard k–ε model and the low-Reynolds-number k–ε model predictions are in better agreement with the experimental data at the outer wall than the inner wall region. Since the maximum mass transfer occurs at the outer surface of the elbow and downstream (about one to one half diameter-downstream) of the elbow exit, where the predicted velocity profiles agree with the data, it was decided that the available flow model can be used to predict the mass transfer coefficient in the outer wall of the elbow. The standard k–ε turbulence model was used to predict turbulent flow and mass transfer coefficients in the elbows because of its computational efficiency. Since, as shown in Fig. 2, the low-Reynolds-number k–ε model gives only slightly better predictions for the streamwise velocity profile in the outer wall region of the elbow than the standard k–ε model predictions, the low-Reynolds-number k–ε model was used only for high Sc number where the standard k–ε model cannot be used to resolve the viscous sublayer region where the mass transfer takes place (see [7–9]). Further details of flow model verification and the effects of the grid refinement studies on the results are provided by Wang [8] and Edwards et al. [11].

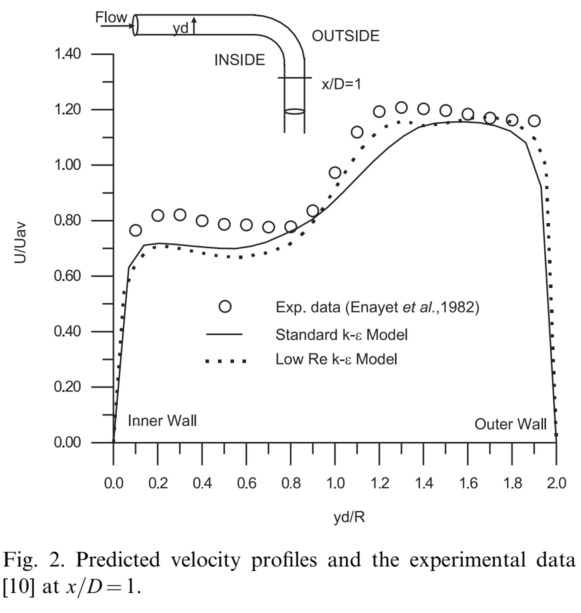

Fig. 2. Predicted velocity profiles and the experimental data [10] at $x/D = 1$.

2.2. Mass transfer model verification

Mass transfer coefficient predictions using the CFD code were compared with the experimental data of Achenbach [5] for a naphthalene–air system. Achenbach measured mass transfer between an elbow wall and air in a 90° elbow ($r/D = 1.5$, a Schmidt number ($Sc = \nu/D_f$) of 2.53). To simulate this experiment, the following boundary conditions were applied. At the inlet, it was assumed that there is no naphthalene concentration and the velocity profile is uniform. At the pipe wall, the mass concentration of naphthalene is one and no-slip velocity boundary condition was applied. The predicted results of the ratio of the local mass transfer coefficient (or the Sherwood number) in an elbow to the mass transfer coefficient of fully developed flow in a pipe (MTCRE) are shown in Figs. 3 and 4. Figs. 3 and 4 show the comparison of predicted values (using the standard k–ε turbulence model) with the experimental data of Achenbach [5] for the outer wall of the elbow at a Reynolds number of 9×10^4 and 3.9×10^5, respectively. For both cases considered here, it was observed that the trend of the predictions agrees with the data. Further details of flow model and mass transfer evaluations are described by Wang [8].

The predictions from the CFD code using the low-Reynolds-number k–ε turbulence model were also compared with the elbow mass transfer data of Achenbach [5]. As compared with the data, the mass transfer profiles in the elbow predicted by this turbulence model gave the right location and magnitude of the maximum mass transfer rate in the elbow. Therefore, the low-Reynolds-number k–ε model was used only to determine the effects of Schmidt number on the predicted mass transfer coefficients.

3. Mass transfer coefficients in elbows

The mass transfer coefficient in an elbow varies with the flow Reynolds number (Re), the Schmidt number of the system (Sc) and the elbow radius to pipe diameter ratio (r/D). By performing many CFD simulations based on different Reynolds numbers, Schmidt numbers and elbow r/D, a curve fit relation which defines the maximum mass transfer coefficients in elbows was obtained. The relation depends on Reynolds number, Schmidt number and elbow r/D and is given in Eq. (3).

$$\mathrm{MTCRE} = 0.68 + (1.2 - 0.044\ln(Re))\mathrm{e}^{-0.065r/D} + \frac{0.58}{\ln(Sc + 2.5)}, \quad (3)$$

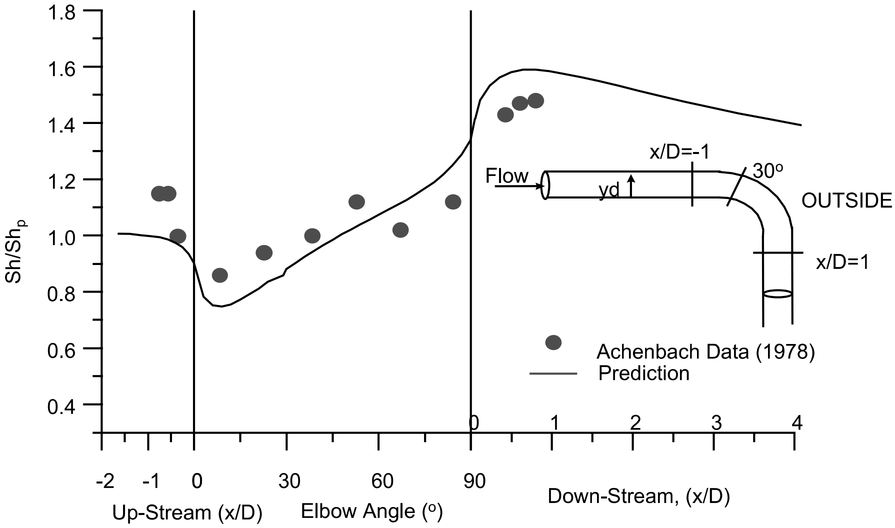

Fig. 3. Predicted mass transfer coefficients in a 90° elbow vs. data of Achenbach [5] ($Re = 9 \times 10^4$, $Sc = 2.53$).

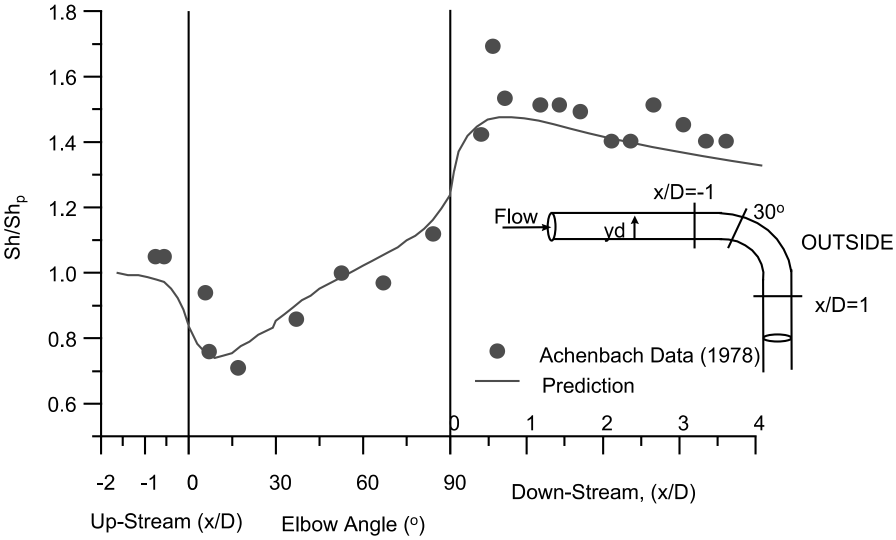

Fig. 4. Predicted mass transfer coefficients in a 90° elbow vs. data of Achenbach [5] ($Re = 3.9 \times 10^5$, $Sc = 2.53$).

where MTCRE is the ratio of the maximum mass transfer coefficient in an elbow to the mass transfer coefficient in a fully developed turbulent flow in a straight pipe upstream of the elbow as calculated by the CFD code. Note that this equation is expected to represent only the regions for which calculations were performed (see Figs. 5–7). Therefore, if the mass transfer coefficient is known in a pipe, then Eq. (3) can be used to estimate the maximum mass transfer coefficient in an elbow of the same diameter as the pipe.

The simulated results for mass transfer as a function of the Reynolds number in a 90° elbow with $r/D = 1.5$ and $Sc = 2.53$ are shown in Fig. 5. It can be observed that Eq. (3) agrees well with the CFD code simulation results and is in good agreement with the magnitude of the experimental data. The accuracy of the data is not known. But, other data for elbows [4] indicate that MTCRE decreases as the flow Reynolds number increases as indicated by Eq. (3) and the CFD code simulations.

The predictions from Eq. (3) are also compared with the CFD code simulations, the experimental data of Achenbach [5], and Coney's correlation for different elbow r/D values. The results are shown in Fig. 6. The

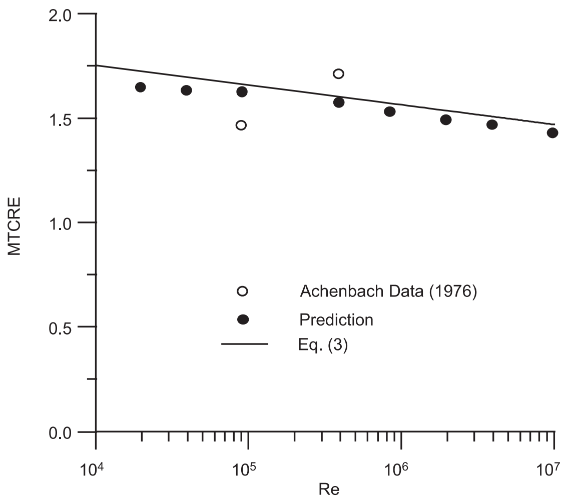

Fig. 5. Variation of MTCRE with the Reynolds number ($Sc = 2.53$).

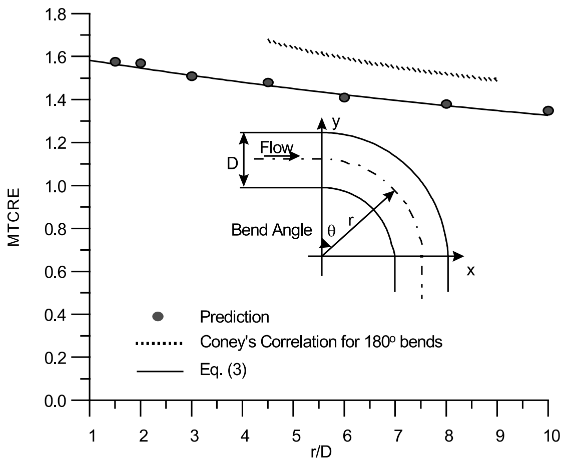

Fig. 6. Variation of MTCRE with r/D ($Re = 390\,000$, $Sc = 2.53$).

agreement between the predictions using Eq. (3) and the CFD simulation results is very close. The Coney correlation (Eq. (2)) is valid in a smaller range of r/D values and it was developed for predicting mass transfer in 180° bends where the mass transfer coefficient ratio of an elbow to a pipe is higher than in 90° elbows because the flow is not well developed in 90° elbows as compared to the 180° bends.

The predicted mass transfer coefficient ratio of an elbow (MTCRE), at a r/D of 1.5 with $Re = 390\,000$, as a function of the Schmidt number is shown in Fig. 7. For high Sc numbers, the predictions indicate that the Schmidt number does not have a significant influence on the MTCRE. Note that the mass transfer model based

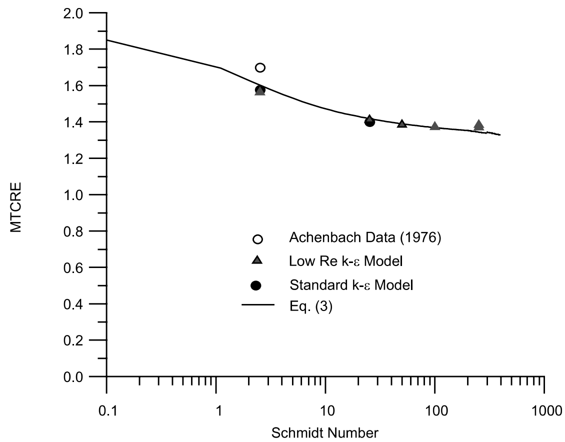

Fig. 7. Variation of MTCRE with Sc ($Re = 390\,000$).

on the low-Reynolds-number k–ε turbulence model was used to predict mass transfer coefficients in elbows due to the fact that the mass transfer model based on the standard k–ε model is not applicable (or valid) for high Schmidt numbers. From this figure, it can be seen that the mass transfer model based on the low-Reynolds-number k–ε turbulence model gives the same prediction as the mass transfer model based on the standard k–ε turbulence model for the maximum mass transfer coefficient in an elbow.

4. Conclusions

A correlation for predicting the maximum mass transfer coefficient in elbows based on three-dimensional computational flow modeling and mass transfer predictions was developed. The correlation is a function of the flow Reynolds number, the Schmidt number and the elbow radius to diameter (r/D) ratio. The correlation for the maximum mass transfer coefficient in an elbow to the mass transfer coefficient in a fully developed pipe flow (MTCRE) is in good agreement with the CFD code results that are verified with the available experimental data for flow and mass transfer in elbows. The correlation for the MTCRE is found to decrease slightly with the flow Reynolds number, with Schmidt number, and with r/D for moderate r/D values.

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