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Numerical investigation on mass transfer enhancement downstream of an orifice

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ABSTRACT

Mass transfer enhancement is an indispensible element in flow accelerated corrosion (FAC). In order to investigate mass transfer enhancement downstream of an orifice, the two-dimensional computational fluid dynamics (CFD) calculation is conducted. First, validation of turbulence model, the ζ–f model, is conducted in the fully developed pipe flow, the flow through an orifice and the flow downstream of a sudden expansion. The validation shows that the model is adequate to predict mass transfer enhancement in all the tested flows. Effects of Reynolds number, orifice thickness and diameter ratio on mass transfer enhancement downstream of an orifice are then investigated based on the numerical calculation. The investigation shows that the mass transfer enhancement ratio decreases with the increasing Reynolds number. However, the locations of reattachment point and the peak transfer rate point are not affected by the Reynolds number. Parametric study on the orifice thickness shows that a thin orifice helps mass transfer enhancement in its downstream. This is attributed to more intense turbulence generation downstream of a thin orifice. Moreover, the peak transfer point appear about $0.4L_r$ (reattachment length) downstream of the orifice. The results of the parametric study are synthesized as a correlation,

$$\frac{St_{max}}{St_{fd}} = 4.78Re^{-0.12}\left(\frac{d}{D}\right)^{-1.16}\frac{1+0.82(L_1/d)^3}{1+(L_1/d)^3}$$

which is expected to be valid in the range of $4.2\times10^4 \leqslant Re \leqslant 1.3\times10^5$, $0.4 \leqslant d/D \leqslant 0.75$, $0.13 \leqslant L_1/d \leqslant 2.61$.

1. Introduction

Mass transfer enhancement is regarded as one of the elements leading to flow-accelerated corrosion (FAC) in the piping system of nuclear and fossil power plants. The flow in the piping system of plants can hardly reach its fully developed condition because it keeps receiving disturbance from the components installed in the system, such as orifices. These components can change flow direction and consequently leads to flow impingement or reattachment on the pipe wall in their downstream. Peak local mass transfer rates usually appear in the neighborhood of impinged and reattaching point. These regions are identified as the FAC high-risk zone and demand careful examination. In order to assist the FAC analysis, this paper is dedicated to investigate the mass transfer enhancement downstream of an orifice based on the computational fluid dynamics calculation.

It is a well-known challenging task to model the turbulence near impinged or reattaching points with the eddy viscosity models because at these locations the wall shear stress, τ_w, and the friction velocity, $u_\tau = \sqrt{\tau_w/\rho}$, approaches to zero and, consequently, ν/u_τ is not a valid wall characteristic length any more. The restriction eliminates application of the low-Reynolds number model which fits the wall behaviors based on y^+. Partially motivated by the above mentioned challenge, models utilizing other dimensionless wall distances were developed, such as $R_y = \sqrt{k}y/\nu$ in the Lam–Bremhorst model [1] and $R_\varepsilon = y/(\nu^3/\varepsilon)^{1/4}$ in the Abe–Kondoh–Nagano model [2].

Another point worth noting is that the Schmidt number, Sc, is on the order of 10^3 in the ordinary mass transfer cases. Based on the relation between concentration and momentum boundary layer thickness, $\delta_c = Sc^{-0.3}\delta_u$, given by Shaw and Hanratty [3], the concentration boundary layer can be at least one order thinner than the momentum one. It can be expected that modeling of turbulent mass transfer is very sensitive to local model performance in the wall vicinity, if the model is designed to resolve the wall region. Most of the models based on the dimensionless wall distances were developed via fitting the direct numerical simulation (DNS) data in the fully developed flow. Hence, these models should be carefully applied in the impinging and reattaching flows,

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Nomenclature

C	concentration, mol/L
C_f	skin friction coefficient, $2\tau_w/(\rho U_b^2)$
c'	concentration fluctuation, mol/L
d	orifice inner diameter, m
D	tube inner diameter, m
h_m	mass transfer coefficient, $q_m/(C_b - C_w)$, m/s
k	turbulent kinetic energy, m^2/s^2
L_r	reattachment length, m
p	mean pressure, Pa
P_k	production rate of turbulent kinetic energy, m^2/s^3
q_m	wall mass flux, mol/(m^2 s)
Re	Reynolds number, $\rho UD/\mu$
Sc	Schmidt number, ν/D
St	Stanton number, h_m/U_b
U	mean streamwise velocity, m/s
U_i	mean velocity in the ith direction, m/s
u'_i	velocity fluctuation in the ith direction, m/s
u_τ	wall friction velocity, $\sqrt{\tau_w/\rho}$, m/s
v	velocity fluctuation in wall normal direction, m/s
x_i	coordinates in the ith direction, m
y	wall distance, m
y^+	dimensionless wall distance, yu_τ/ν
z	streamwise coordinate, m
Greek letters	
δ_c	thickness of concentration boundary layer, m
δ_u	thickness of momentum boundary layer, m
ε	dissipation rate of turbulent kinetic energy, m^2/s^3
Γ	mass diffusivity, m^2/s
ν	molecular viscosity, m^2/s
ν_t	eddy viscosity, m^2/s
ρ	density, kg/m^3
σ_t	turbulent Prandtl number
τ_w	wall shear stress, kg/(m s^2)
ζ	normalized wall normal Reynolds stress, v^2/k
Subscripts	
b	bulk
fd	fully developed
m	mass
max	maximum
w	wall

especially when we are interested in mass transfer. One of the authors has evaluated the performance of five models utilizing the dimensionless wall distances other than y^+ and found that none of these models can fairly predict mass transfer, especially in the case of high Reynolds number [4].

The k–ε–v^2–f model proposed by Durbin [5] introduces an elliptic equation to consider the wall blocking effect and avoids utilizing wall damping function for which the proper wall characteristic length is still an open question. This feature makes the k–ε–v^2–f model more promising for solving mass transfer problem in the impinging and reattaching flows. A modified version of k–ε–v^2–f model, i.e. the ζ–f model, was proposed by Hanjalic et al. [6], appealed with the improved numerical robustness. In the present paper the ζ–f model is applied to model turbulent mass transfer in the downstream of an orifice. Since the ζ–f model has been implemented by the authors into the open-source code, OpenFOAM [7], a fully developed pipe flow is calculated first to justify the implementation. Then the model is examined with Sydberger and Lotz's [8] and Tagg et al.'s [9] mass transfer experiments to show its performance in predicting mass transfer enhancement downstream of an orifice or sudden expansion. Based the justified model performance the model is further applied to investigate the influence of flow and geometry parameters on mass transfer enhancement downstream of an orifice.

2. Turbulence model

2.1. Reynolds averaged Navier–Stokes model

The incompressible Reynolds-averaged continuity equation

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{1}$$

the incompressible Reynolds-averaged Navier–Stokes equation

$$\frac{\partial U_i}{\partial t} + \frac{\partial U_i U_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left\{\nu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \overline{u'_i u'_j}\right\} \tag{2}$$

and the Reynolds averaged concentration equation

$$\frac{\partial C}{\partial t} + \frac{\partial U_j C}{\partial x_j} = \frac{\partial}{\partial x_j}\left\{\Gamma\frac{\partial C}{\partial x_j} - \overline{c' u'_j}\right\} \tag{3}$$

are solved in the calculation. The fluid properties are assumed to be constant. The Reynolds-stress tensor in Eq. (2) is modeled with the eddy viscosity model

$$-\overline{u'_i u'_j} = \nu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{2}{3}k\delta_{ij} \tag{4}$$

The turbulent mass flux in Eq. (3) is obtained using a gradient diffusion model

$$-\overline{c' u'_j} = \alpha_m \frac{\partial C}{\partial x_j} \tag{5}$$

2.2. ζ–f Model

In the ζ–f model [6] the eddy viscosity is defined as

$$\nu_t = C_\mu^\zeta \zeta k \tau \tag{6}$$

The mass eddy diffusivity is calculated with

$$\alpha_m = \frac{\nu_t}{\sigma_t} \tag{7}$$

where the turbulent Prandtl number, σ_t, is set as 0.9.

Four basic equations are included in the ζ–f model.

$$\frac{Dk}{Dt} = P_k - \varepsilon + \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] \tag{8}$$

$$\frac{D\varepsilon}{Dt} = \frac{(C_{\varepsilon1}P_k - C_{\varepsilon2}\varepsilon)}{\tau} + \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] \tag{9}$$

$$\frac{D\zeta}{Dt} = f - \frac{\zeta}{k}P_k + \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\zeta}\right)\frac{\partial \zeta}{\partial x_j}\right] \tag{10}$$

$$L^2\nabla^2 f - f = \frac{1}{\tau}\left(c_1 + C'_2\frac{P_k}{\varepsilon}\right)\left(\zeta - \frac{2}{3}\right) \tag{11}$$