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PREDICTIVE MODELS FOR EROSION–CORROSION UNDER DISTURBED FLOW CONDITIONS

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Abstract—Recent advances in the development of predictive models for erosion–corrosion in disturbed turbulent flows are reviewed. The application of turbulence models permits the structure (velocity, pressure, turbulence fields) of the complex flow to be determined along with the calculation of local mass transfer rates of reactants and products. Particle/wall interaction statistics that are required for the application of erosion models are also determined.

NOMENCLATURE

D	diffusion coefficient, $m^2 s^{-1}$
K	mass transfer coefficient, $m s^{-1}$
k	kinetic energy of turbulence, $m^2 s^{-2}$
P	pressure, $N m^{-2}$
r	radial coordinate, m
Re	Reynolds number, $\mathrm{Re} = ud/\nu$
Sc	Schmidt number, $\mathrm{Sc} = \nu/D$
S	source term
$\overline{u_i}, \overline{u_j}$	components of the fluctuation velocity vector, $m s^{-1}$
U, V	components of mean velocity vector, $m s^{-1}$
x	axial coordinate, m
y^+	nondimensional distance from the wall
m	species mass fraction
Greek letters	
Γ	general diffusion coefficient
ε	dissipation of kinetic energy of turbulence, $m^2 s^{-3}$
ν	kinematic viscosity, $m^2 s^{-1}$
ρ	density, $kg m^{-3}$
σ_t	turbulent Prandtl–Schmidt number

INTRODUCTION

Computational fluid dynamics (CFD) has advanced to the stage where the modelling of transport processes in wall-bounded turbulent flows and the determination of particle/wall interactions have enabled the first steps to be taken in the development of predictive models for erosion–corrosion under conditions of disturbed flow.[1–8]

The most severe erosion–corrosion problems encountered in industry involve disturbed flow at sudden changes in the flow geometry, where there is often flow separation accompanied by recirculation and reattachment, and secondary flow. In the case of flow separation, for example at a sudden expansion in a pipe, turbulence is transported downstream from the point of separation. There is no simple relation between the bulk flow parameters and the local near-wall, hydrodynamic, mass transfer and erosion–corrosion conditions and the latter must be determined either experimentally[9–12] or by numerical simulation.[1–8,13] This paper discusses the advances in the application of turbulence models to the numerical simulation of erosion–corrosion during the past decade.

TURBULENCE MODELS

The task of turbulence models is to provide equations that will enable calculation of the Reynold stresses, $-\rho\overline{u_i u_j}$, and the turbulent diffusion fluxes, $-\rho\overline{m^s u_j}$, which arise when the time-averaged equations for turbulent flow and mass transport are obtained from the instantaneous equations.[14] The k–ε, turbulence models[15] which are presently[16] widely used for the computation of industrial flows are eddy viscosity models which are based on the concept proposed by Boussinesq in 1877 that assumes the effect of turbulence on the mean flow can be taken into account through viscosity. The turbulent viscosity, μ_t is determined from the kinetic energy of turbulence, k, and its rate of dissipation, ε;

$$\mu_t = C_\mu f_\mu \frac{\rho k^2}{\varepsilon}. \qquad (1)$$

The effective viscosity is given by

$$\underbrace{\mu_{\text{eff}}}_{\text{effective}} = \underbrace{\mu}_{\text{molecular}} + \underbrace{\mu_t}_{\text{turbulent}} \qquad (2)$$

and similarly the effective diffusivity is given by

$$\underbrace{D_{\text{eff}}}_{\text{effective}} = \underbrace{\frac{\mu}{\rho \text{Sc}}}_{\text{molecular}} + \underbrace{\frac{\mu_t}{\rho \sigma_t}}_{\text{turbulent}} \qquad (3)$$

where σ_t is the turbulent Schmidt number.[7,13]

The conservation equations for mass, momentum, kinetic energy of turbulence and its dissipation, and species, m, can be written in a general form. For axisymmetrical flow in 2D cylindrical coordinates:

$$\frac{\partial}{\partial x}(\rho U \Phi) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho V \Phi) = \frac{\partial}{\partial x}\left(\Gamma_\phi \frac{\partial \Phi}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\phi \frac{\partial \Phi}{\partial r}\right) + S_\Phi \qquad (4)$$

where $\Phi = U, V, k, \varepsilon, m, \ldots$

The values of Γ_ϕ, general diffusion coefficients and S_ϕ, the source terms, are given in Table 1.

Flow separation with recirculation and reattachment for example is observed at a sudden expansion and knowledge of the concentration field enables the rate of wall mass transfer to be calculated[6,13] throughout the expansion. The calculation of the concentration field close to the wall requires the use of a low Reynolds number (LRN) k–ε model since the mass transfer boundary layer is deeply embedded within the viscous sublayer. The concentration is required at $y^+ \sim 0.1$, deep within the viscous sub-layer where the mass transport is diffusion controlled, in order to

TABLE 1. CONSERVATION EQUATIONS

Conservation of:	Φ	Γ_Φ	S_Φ
Mass	l	0	0
Axial momentum	U	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{\text{eff}}\frac{\partial U}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial V}{\partial x}\right)-\frac{\partial P}{\partial x}$
Radial momentum	V	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{\text{eff}}\frac{\partial U}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial V}{\partial r}\right)-2\mu_{\text{eff}}\frac{V}{r^2}-\frac{\partial P}{\partial r}$
Turbulent kinetic energy	k	$\frac{\mu_{\text{eff}}}{\sigma_{\text{k}}}$	$P_k-\rho\varepsilon$
Turbulent dissipation rate	ε	$\frac{\mu_{\text{eff}}}{\sigma_\varepsilon}$	$\frac{\varepsilon}{k}(C_{\varepsilon 1}f_1P_k-C_{\varepsilon 2}f_2\rho\varepsilon)$
Species	m	ρD_{eff}	0

$$P_k=\mu_{\text{eff}}\left\{2\left[\left(\frac{\partial U}{\partial x}\right)^2+\left(\frac{\partial V}{\partial r}\right)^2+\left(\frac{V}{r}\right)^2\right]+\left(\frac{\partial U}{\partial r}+\frac{\partial U}{\partial x}\right)^2\right\}$$

calculate the wall mass transfer rate. The latter requirement is a consequence of the small amount of turbulence in the viscous sublayer having a major effect on mass transfer at the high Schmidt numbers Sc $\sim$ 1000 often encountered in aqueous mass transfer. LRN models utilize turbulence damping functions[13,16] as the most effective way of modelling wall-bounded flow with heat/mass transfer under separated flow conditions.[17] The alternative wall function (WF) closure places the first computation node in the logarithmic law region ($30 < y^+ < 150$) and bridges over the important viscous sub-layer.

The motion of a dispersed particulate phase within a turbulent flow field can be modelled by either a Lagrangian or Eulerian approach.[18] In Lagrangian models a large number of individual particle trajectories are calculated in the flow domain whereas in the Eulerian approach the particles are treated as a second fluid. From an erosion modelling standpoint the direct calculation of particle/wall interaction statistics, impact frequency, angle and velocity with the Lagrangian approach is an advantage; at least in dilute particulate suspensions. As pointed out by Nešić,[7] the Eulerian approach would be more appropriate in concentrated suspensions.

EROSION—CORROSION SIMULATIONS

Modelling of phenomena such as erosion–corrosion and flow-induced corrosion in general is done with the immediate objective of gaining a greater understanding of the mechanisms involved. With this objective in mind the models should be based on fundamental equations and involve as few empirical relationships as possible. The ultimate objective of modelling is to develop predictive models that can be used for design purposes, and the more fundamentally based the greater the generality and utility of the model.

The k–ε turbulence model meets these criteria. There are more fundamental models such as the Reynolds stress transport model (RSTM) which solves the transport equations for the turbulent stress directly. However, the improvements in mimicking the behaviour of the turbulent flow are offset by the complex problem of the prescription of boundary conditions for all stresses along the various boundaries.

The major problems that arise relate to the modelling of the actual erosion–corrosion processes at the wall.

Single phase studies

An LRN, k–ε model has recently been successfully applied to the calculation of pipe-wall mass transfer rates at a sudden expansion,[7,13] a sudden constriction[19] and flow over a groove.[6,19] In addition[19] mass transfer rates have been calculated to the pipe wall at a sudden expansion where small patches of a protective 'rust' film were assumed to have been removed. The above results indicate that the mass transfer aspects of erosion–corrosion processes in disturbed flow conditions can be satisfactorily dealt with by the application of turbulence models.

A more intractable problem is the ability to predict protective film removal under single phase aqueous flow conditions. The partial removal of a protective surface film is often the precursor to rapid corrosion and component failure. For example failures in copper piping in apartment buildings often relate to rapid corrosion at a sudden change in the geometry where the normally protective film has been damaged by the enhanced turbulence. Recent observations have shown that although much of this type of corrosion occurs near the outlet of 90° bends that the film breakdown and subsequent failure started at the sudden step where the downstream pipe was soldered into the elbow. The concept of a critical shear stress[20] for the removal of protective layers has been questioned[21] on the basis that the small stresses involved would not be adequate to mechanically remove a surface oxide film. As pointed out by Launder,[17] pressure fluctuations unlike velocity fluctuations do not vanish at the wall. Heitz[22] has suggested that pressure fluctuations at the wall, in disturbed flow, add to the overall shear stress and may produce mechanical damage. Following a study of the relationship between the structure of the flow and corrosion in disturbed flow, Nešić and Postlethwaite[3] concluded that the local near-wall turbulence is the governing factor rather than the wall shear stress in the disruption of the protective corrosion layer; pointing out that in simple undisturbed flows the patterns of wall shear stress are the same as the patterns of near-wall turbulent intensity. The mechanical properties of *in situ* and developing corrosion product films are not well documented. Further work is required in this area to clarify the stability of corrosion product films under conditions of disturbed flow which are amenable to both experimental observation and numerical simulation. Such a study involving copper is presently being conducted by Wang at the University of Saskatchewan.

Liquid/solid flow

The presence of solid particles enhances the destruction of protective films giving rise to increased corrosion rates and may add to the overall metal loss by the mechanical erosion of the underlying metal. As with single phase flow these destructive effects are more pronounced under disturbed flow conditions.

Nešić and Postlethwaite[5–7] have developed a predictive model for localized erosion–corrosion under disturbed flow conditions based on the application of a two phase flow version of an LRN, k–ε model of turbulence. The motion of the particles was predicted by means of a Lagrangian Stochastic–Deterministic (LSD) model proposed by Milojevic.[23] The model which was applied to various pipe geometries including a sudden expansion, constriction and a groove (Fig. 1) was based on an oxygen-mass-transfer controlled corrosion model with the assumption that the

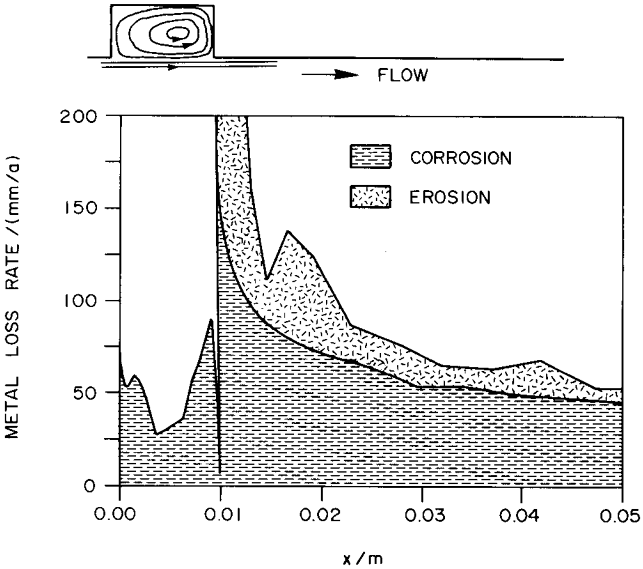

FIG. 1. Simulation of erosion–corrosion at a 10 mm groove in a 100 mm diameter pipe: U = 15 m s^{-1}; 2 vol% sand in water (after Nešić and Postlethwaite[6]). © 1991 NACE. Reprinted with permission.

particles removed the protective rust film, and an erosion model based on the Finnie[24] cutting wear erosion equations as modified by Bergevin.[25] The model successfully simulated the erosion results for a sudden expansion in a stainless steel pipe determined by Lotz and Postlethwaite[26] (Fig. 2) and the erosion–corrosion of a carbon-steel sudden expansion.[5,6]

Zeisel and Durst[2] have successfully applied a two phase k–ε model to the numerical simulation of uniform CO_2 erosion–corrosion under separated flow conditions at a sudden expansion. The particles were modelled by an Eulerian approach. The corrosion model was based on the DeWaard–Milliams equation[27] for bare surfaces and Fick's law of diffusion when a film was present. The erosion model was a mixed model based on Finnie's equations for low angle cutting erosion and the Sundararajan and Shewmon[28] equation for high angle impacts. The erosion simulation was used to predict corrosion layer destruction as well as erosion of the wall material. Details of the implementation of the model such as boundary conditions were not presented. An important aspect of the Zeisel and Durst model was that it was an unsteady state model taking into account the changing erosion–corrosion rate as the corrosion product film developed.

Another important time dependent factor pointed out by Lotz and Heitz[29] is the interrelation between the wall geometry, erosion–corrosion and flow structure. As erosion–corrosion proceeds the computational grid which may start out as a simple cartesian grid will not be satisfactory, as for example sharp edges are rounded requiring the introduction of curvilinear coordinates at a sudden constriction. Bends which may be initially modelled using analytically produced curvilinear coordinates will require numerically generated grids as the asymmetrical erosion progresses.

Fluid flow is much more reproducible than the kinetics of corrosion reactions and the ultimate barrier to the predictive modelling of erosion–corrosion will not be the

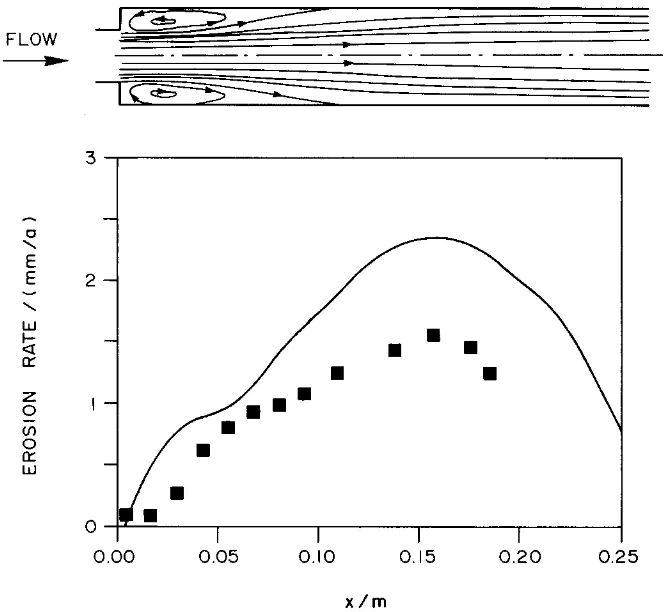

Fig. 2. Flow structure and simulation and experimental erosion rates for stainless steel pipe expansion: $d_{in} = 21.1$ mm, $d_{out} = 42.5$ mm; $U_{in} = 13.2$ m s^{-1}; 2 vol% sand in water; ■ measurements,[10] ——— model predictions (after Nešić and Postlethwaite[6]). © 1991 NACE. Reprinted with permission.

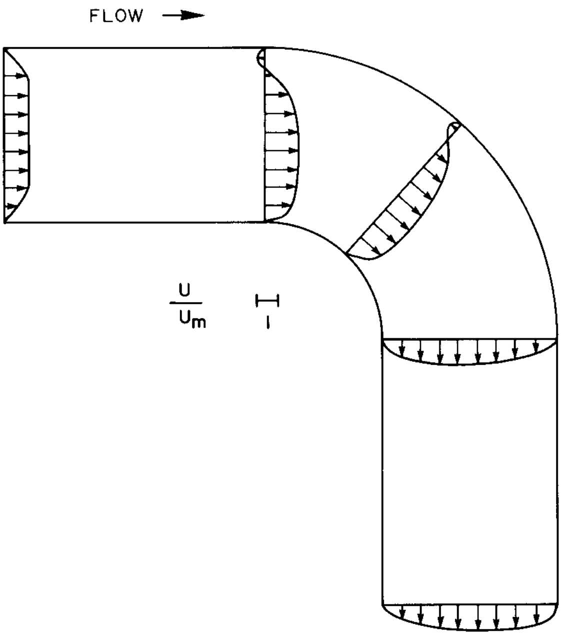

Fig. 3. Modelling the flow structure for water, Re = 10^5, at a 90° 2D bend illustrating flow separation and recirculation.

inability to predict the complex interaction between fluid and suspended solids with the corroding wall but the inability to calculate totally or partially activation-controlled corrosion rates, with a degree of confidence. This of course does not preclude the use of such modelling for mechanistic and parameter sensitivity studies.

FUTURE DEVELOPMENTS

Several corrosion groups in Europe, North America and Australia are presently engaged in the numerical simulation of erosion–corrosion processes under disturbed flow conditions and substantial progress should be made in the next decade. The corrosion group at the University of Saskatchewan is developing codes for the simulation of erosion–corrosion at bends, where many problems occur in mineral processing. The flow structure at a curved 2D duct has been simulated (Fig. 3) and the simulation of the erosion–corrosion is now underway.

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