Numerical prediction of recirculation flows with free convection encountered in gas-agitated reactors

T. Deb Roy

Department of Metallurgy and Materials Science, Imperial College of Science and Technology, Prince Consort Road, London SW7 2BP, UK

A. K. Majumdar and D. B. Spalding

Department of Mechanical Engineering, Imperial College of Science and Technology, Exhibition Road, London SW7 2BX, UK
(Received 6 February 1978)

Flows in a gas-agitated reactor have been predicted by a finite difference procedure. The free-convection phenomena in the gas–liquid mixtures have been accounted for by the calculation of a void fraction determined from the gas flow rate. Computations have been performed for two different situations: first, with the allowance of slip between gas and liquid phases, and second, without any slip. Reasonable agreement has been achieved between the measurements.

Introduction

In recent years, numerical methods[1,2] have been applied to predict flows in gas-agitated metallurgical reactors[3,4]. In the latter studies, the gas–liquid interaction was represented by prescribing the measured velocity distribution at an arbitrarily specified surface sufficiently distant from the two-phase region. Although significant success was achieved in the prediction of hydrodynamic variables in most of the reactor, such computations require prior knowledge of the measured velocity distribution at the said surface. This requirement is not easy to meet for practical high temperature reactors, e.g. those for converter steelmaking processes or for deoxidation of steel by argon injection.

In the present work, a method has been developed to represent the free-convection phenomena in gas–liquid mixtures. Two distinct situations have been envisaged: (a) No-slip: Gas and liquid move at the same speed without any slip between them. (b) With slip: The gas moves at a higher velocity than the liquid, allowing 'slip' between gas and liquid phases to take place. The difference in velocity between the gas and liquid equals the terminal-rise velocity of large gas bubbles in a stagnant liquid.

Predictions have been obtained for the physical situation shown in *Figure 1* by the finite difference procedure. The relevant data from the experimental situation[3] considered are presented in *Table 1*. The predicted flow field has been compared with the experimental results of Szekely *et al*[3]. Satisfactory agreement has been achieved by assuming slip between the phases.

Mathematical modelling

Governing equations

With reference to the coordinate system shown in *Figure 1*, the equations to be solved are:

Table 1 Data for experimental situation used by Szekely *et al.*[3]

Diameter of vessel	0.6 m
Height of water column in vessel	0.6 m
Velocity of air through orifice	1.62 m s
Orifice diameter	0.0127 m

0307-904X/78/0203-0146 $02.00

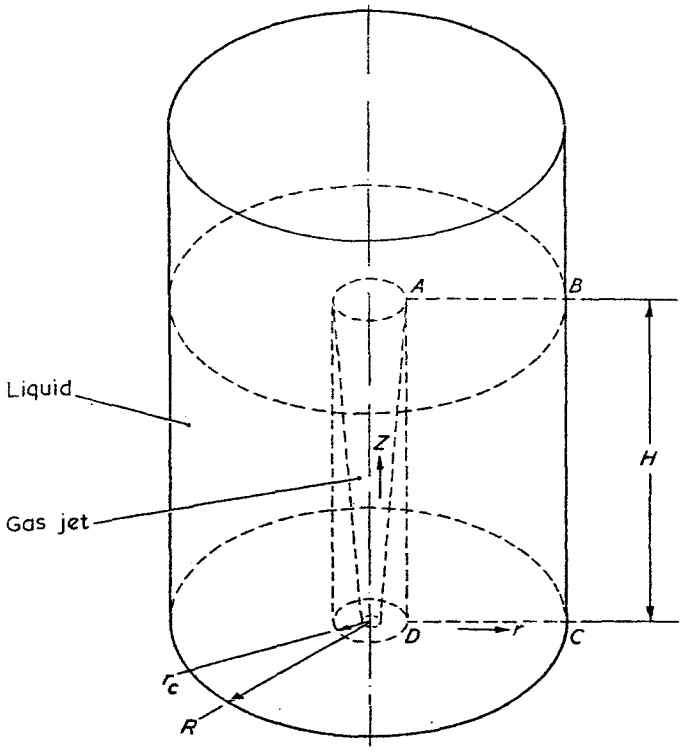

Figure 1 Experimental situation considered in present work

Continuity:

$$\frac{\partial}{\partial z}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(\rho r v) = 0 \tag{1}$$

Momentum:

z direction

$$\frac{\partial}{\partial z}(\rho u^2) + \frac{1}{r}\frac{\partial}{\partial r}(\rho r v u) = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial z}\left(\mu_{\text{eff}}\frac{\partial u}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial u}{\partial r}\right) + S_u \tag{2}$$

where:

$$S_u = \frac{\partial}{\partial z}\left(\mu_{\text{eff}}\frac{\partial u}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\mu_{\text{eff}} r\frac{\partial v}{\partial r}\right) + \rho g\bar{\alpha}$$

with $\bar{\alpha} = 0$, $r > r_c$

r direction

$$\frac{\partial}{\partial z}(\rho u v) + \frac{1}{r}\frac{\partial}{\partial r}(\rho r v^2) = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial z}\left(\mu_{\text{eff}}\frac{\partial v}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial v}{\partial r}\right) + S_v \tag{3}$$

where:

$$S_v = \frac{\partial}{\partial z}\left(\mu_{\text{eff}}\frac{\partial u}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial v}{\partial r}\right) - \frac{2v\mu_{\text{eff}}}{r^2}$$

$$\rho = (1 - \bar{\alpha})\rho_l, \quad \text{for} \quad r < r_c \tag{4}$$

$$\rho = \rho_l \quad \text{for} \quad r > r_c \tag{5}$$

Boundary conditions

At the axis:

$$\frac{\partial u}{\partial r} = 0, \quad v = 0 \tag{6}$$

At walls,

$$u = v = 0 \tag{7}$$

At the free surface,

$$\frac{\partial v}{\partial z} = 0, \quad u = 0 \tag{8}$$

Calculation of $\bar{\alpha}$

The term involving the void fraction $\bar{\alpha}$, in the *z*-direction momentum equation, represents the body force (buoyancy) due to free convection in gas–liquid mixtures. It is important to recognize that this term plays a key role in determining the overall flow pattern in gas-agitated systems.

The present calculation scheme uses a simple, but approximate method for calculating $\bar{\alpha}$. The following assumptions are made: (1) An estimate for the radial width of the gas–liquid mixture (r_c) is made. In the present case the assumption for $r_{c/R}$ was 0.24. (2) The cross-sectional average value of void fraction ($\bar{\alpha}$) is the only relevant void fraction; $\bar{\alpha}$ is a function of *z* only.

Assuming that there is no slip between the gas and the liquid phase, the void fraction $\bar{\alpha}$ has been calculated from the following expression:

$$\bar{\alpha} = \frac{1}{2\pi}\frac{V_{\text{gas}}}{\int_0^{r_c} ru\,dr} \tag{9}$$

where V_{gas} is the volumetric flow rate of gas.

In another set of calculations, it has been assumed that the gases move with their 'terminal velocity', U_{slip} relative to the liquid. The expression for $\bar{\alpha}$ for this (slip) condition assumes the form:

$$\bar{\alpha} = \frac{1}{2\pi}\frac{V_{\text{gas}}}{\int_0^{r_c} r(u + U_{\text{slip}})\,dr} \tag{10}$$

U_{slip} is taken to be 40 cm/sec. (Davenport *et al.*[5])

Turbulence modelling

The effective viscosity μ_{eff} in equations (2) and (3) has been calculated by an *ad hoc* viscosity hypothesis proposed by Pun and Spalding[1]. It has been demonstrated (equation 4) that, in the systems such as the present one, the *ad hoc* viscosity model provided a reasonable prediction of the velocity field with very little computational costs. The following expression has been used:

$$\mu_{\text{eff}} = K(2R)^{2/3}(H)^{-1/3}\rho_l^{2/3}(m_j u_j^2)^{1/3} \tag{11}$$

According to Pun and Spalding[1], $K = 0.012$. In the experimental situation[3] considered in the present work,

μ_{eff} has been found to be 9×10^{-4} kg/cm s. No special treatments in turbulence modelling were made in the near-wall regions (e.g., use of wall functions).

Solution procedure

The finite difference equations derived from equations (1) to (3) have been solved by a version[6] of the finite difference procedure of Patankar and Spalding[2] embodied in the computer code 2/E/FIX (Two-dimensional, elliptic, and fixed grid). The details of the method can be found elsewhere[6]. However, in the present context the calculation procedure assumes the following form:

(1) The calculation starts from the known velocity distribution at $z = 0$.
(2) The pressure distribution $p(r, z)$ and $\bar{\alpha}(z)$ are guessed.
(3) The momentum equations in r and z-directions are solved at the next higher z station to get a first approximation to the velocity distribution.
(4) Since the velocities do not satisfy the continuity equation, a pressure-correction equation is derived from the continuity and linearized momentum equations.
(5) The pressure–correction equation is then solved for corrections to the pressure field.
(6) The velocities are corrected accordingly.
(7) $\bar{\alpha}$ is then calculated either from equation (9) or equation (10) depending upon the presumption of the 'no slip' or 'slip' condition respectively.
(8) A new z station is chosen, and steps 2 to 7 are repeated.
(9) Integration proceeds until the end of the flow domain ($z = H$) is reached. This completes one iteration cycle.

In the present computations, it has been found useful to reverse the sweeping direction in each iteration, i.e. the calculation starts from $z = 0$ and $z = H$ in every odd and even number of iteration respectively.

Computational details

The finite difference grid possessed 12 intervals in the z direction and 15 in the r direction distributed as in *Table 2*. The convergence of the numerical scheme was

Table 2 Details of finite difference grid distribution

z/H	r/R
0	0
0.017	0.033
0.100	0.087
0.192	0.140
0.395	0.180
0.560	0.210
0.680	0.280
0.810	0.347
0.920	0.440
0.958	0.560
0.978	0.700
1.000	0.820
	0.900
	0.960
	1.000

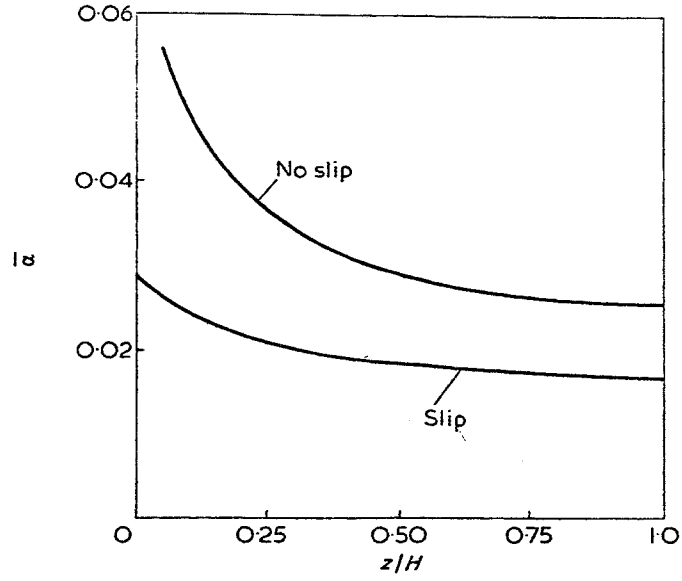

Figure 2 Variation of $\bar{\alpha}$ with z/H. $r_c/R = 0.24$

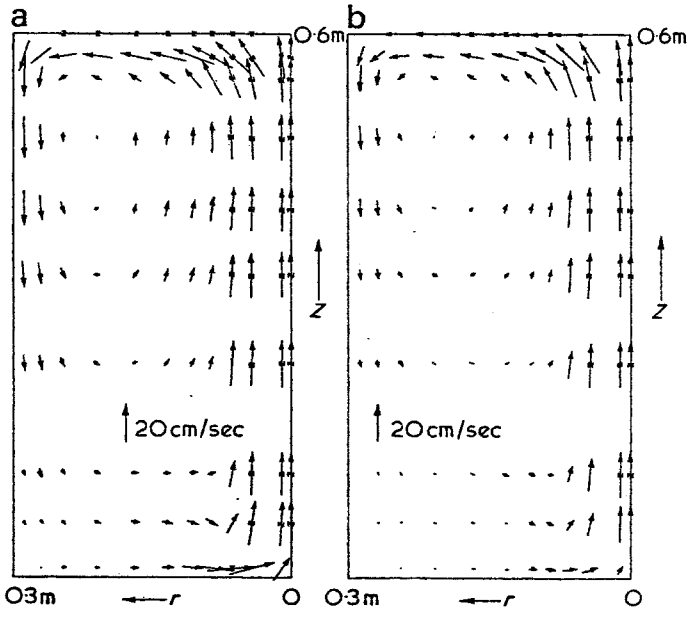

Figure 3 Predicted velocity fields for (a) slip and (b) no slip conditions. $r_c/R = 0.24$. (→) velocity <20 cm/sec

checked by examining the magnitude of the mass and momentum imbalance, normalized with respect to suitably-chosen reference values. In the present computations, the reference values chosen for normalizing the mass continuity and momentum imbalance are 0.5 kg/s and 0.03 kg m/s^2 respectively. These values are derived from the knowledge of a representative velocity in the flow domain, the cross-sectional area of the flow domain and the density of the liquid (see *Table 1*). The maximum permissible value of these non-dimensional measures of mass and momentum imbalance was set at 0.001. About 550 iterations were necessary to satisfy the present convergence criteria for the no-slip condition. The computations required 52 seconds in a CDC 6600 computer. The corresponding figures for the computations for the slip condition were 295 iterations and 28 seconds.

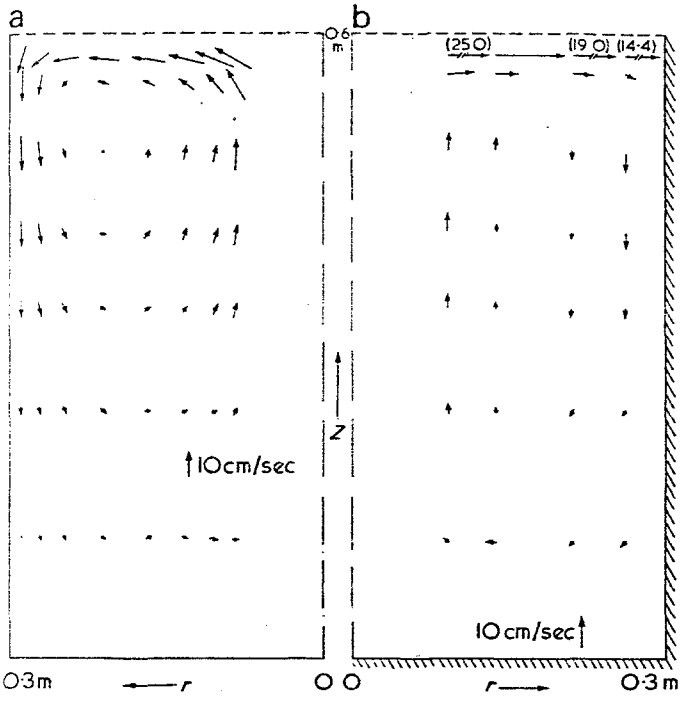

Figure 4 (a), predicted velocity fields. (b), experimental velocity fields. $r_c/R = 0.24$

Results and discussion

The predicted variations of the void fraction $\bar{\alpha}$ for two different models appear in *Figure 2*. Evidently, the predicted $\bar{\alpha}$ with the no-slip model is higher than that of the model employing full slip.

Figure 3 represents the computed velocity field for the two different cases as mentioned above. It may be noted that two different methods predict similar flow fields which are in reasonable agreement with the expectation. However, the no-slip model predicts relatively higher velocities in an otherwise identical situation. This observation can be explained with reference to *Figure 2* which demonstrates a higher $\bar{\alpha}$ in the no-slip model and hence a higher buoyancy (equation 2).

In *Figure 4*, a comparison has been made between the predictions of velocity field with the no-slip model along with the experimental measurements of Szekely *et al.*[3] Reasonable agreement between the measurements and the predicted values are evident.

In the present work, r_c has been chosen arbitrarily. It was therefore necessary to examine the sensitivity of the variation of r_c on the predicted flow field. The predicted void fraction for different values of (r_c/R) appear in *Table 3*. The cross-sectional average of the void fraction, determined from the following expression also appears in the table:

$$\alpha_{AV} = \bar{\alpha} r_c^2 / R^2 \qquad (12)$$

It may be noted that the predicted value of α_{AV} is not significantly influenced by the variation of r_c/R. *Figure 5* shows the predicted values of u velocity distribution for three different values of r_c/R, assuming slip between gas and liquid phases. Considerable variation of the predicted flow field is observed with the variation of r_c/R in the regions close to the axis of the vessel $(r/R < 0.3)$. However, in most parts of the flow domain away from the axis $(r/R > 0.3)$, the variation of the predicted velocity field with the variation of r_c/R was insignificant.

Table 3 Tabulated values of predicted α and $\bar{\alpha}$ for different r_c/R. $\alpha_{AV} = [r_c/R]^2 \bar{\alpha}$

		z/H			
r_c/R		0.02	0.19	0.56	0.81
0.16	$\bar{\alpha}$	0.063	0.043	0.035	0.033
	α_{AV}	1.61×10^{-3}	1.11×10^{-3}	0.90×10^{-3}	0.84×10^{-3}
0.19	$\bar{\alpha}$	0.043	0.031	0.026	0.024
	α_{AV}	1.65×10^{-3}	1.20×10^{-3}	0.99×10^{-3}	0.92×10^{-3}
0.24	$\bar{\alpha}$	0.029	0.022	0.018	0.017
	α_{AV}	1.72×10^{-3}	1.31×10^{-3}	1.09×10^{-3}	1.02×10^{-3}

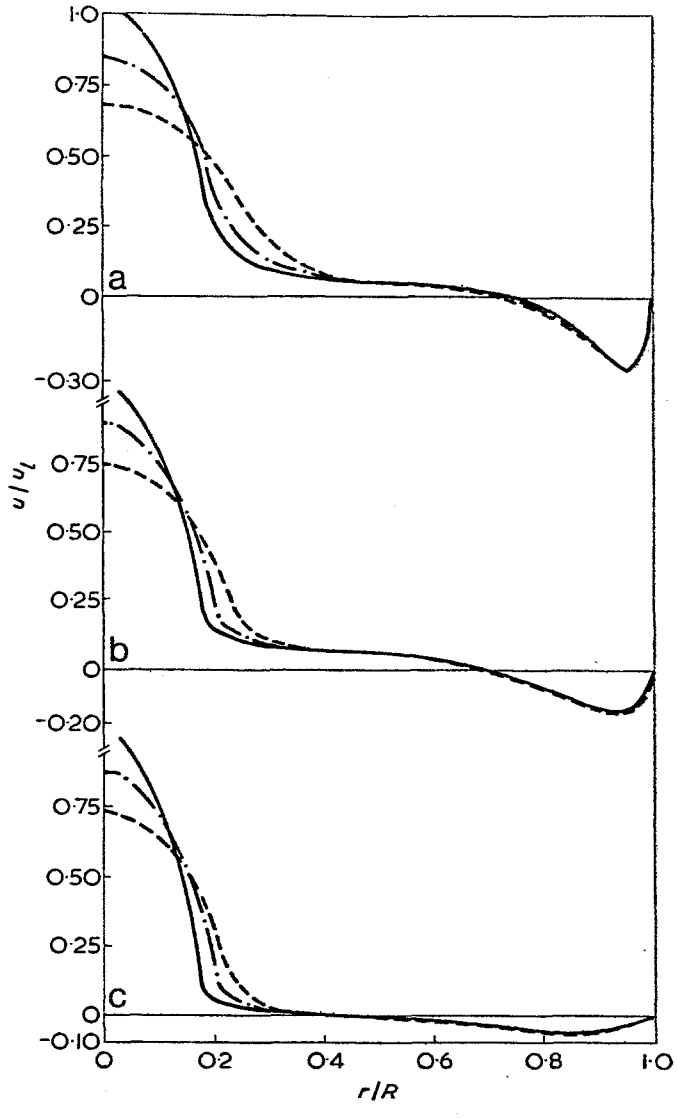

Figure 5 Quantitative comparison of predicted u velocity distribution at different values of z/H. (a), $z/H = 0.86$; $u_l = 0.564$ m/s. (b), $z/H = 0.62$; $u_l = 0.542$ m/s. (c), $z/H = 0.29$; $u_l = 0.438$ m/s. (—) $r_c/R = 0.16$; (—·—), $r_c/R = 0.19$; (– – –), $r_c/R = 0.24$

Conclusions

Predictions of the flows in a gas-agitated cylindrical reactor have been obtained by a finite difference method. The present method accounts for the free convection in a gas–liquid mixture and therefore does

not require any measured velocity distribution as input. The flow field could be predicted with reasonable accuracy by supplying only the gas flow rate.

Acknowledgements

One of the authors (TDR) acknowledges financial support received from the Wolfson Foundation. Thanks are also due to Christine MacKenzie for preparing the typescript.

References

1 Gosman, A. D. *et al.* 'Heat and Mass Transfer in Recirculating Flows'. Academic Press, London and New York, 1969
2 Pantakar, S. V. and Spalding, D. B. *Int. J. Heat Mass Transfer*, 1972, **15**, 1787
3 Szekely, J. *et al. Met. Trans.*, 1976, **78**, 287
4 Deb Roy, T. and Majumdar, A. K. 'Turbulent recirculating flows in a cylindrical reactor agitated by gases'. (*Unpubl. Rep.*) Imperial College, London, 1977
5 Davenport, W. G. *et al. J. Iron Steel Inst.*, 1967, **205**, 1034
6 Pun, W. M. and Spalding. D. B. *Rep. HTS 76/2* Heat Transfer Section, Imperial College. London, 1976

Nomenclature

H Height of liquid column in vessel, m
K Constant, defined after equation (8)
m_j Mass-flow rate of gas, kg/s
p reduced pressure, $P - \rho gz$, kg/m-s^2
P pressure, kg/m-s^2
R Radius of vessel, m
r Radial distance from axis of symmetry, m
r_c Radius of core (*Figure 1*)
u Velocity in axial direction, m/s
u_j Inlet gas velocity, m/s
v Velocity in radial direction, m/s
V_{gas} Volumetric flow rate of gas, m^3/s
z Axial distance from bottom of vessel, m
μ_{eff} Effective viscosity, kg/m-s
ρ_ℓ Density of water, kg/m^3
ρ Density of gas–liquid mixture, kg/m^3
$\bar{\alpha}$ Void fraction defined by equation (9) or (10)