A STRUCTURED STOCHASTIC FLOW MODEL FOR INTERPRETING FLOW-FOLLOWER DATA FROM A STIRRED VESSEL

By R. MANN (GRADUATE), P. P. MAVROS and J. C. MIDDLETON (MEMBER)
Department of Chemical Engineering, UMIST, Manchester

A new flow model has been developed for a stirred vessel which makes use of an overall circulation structure of velocities to represent the average flow of fluid, but which incorporates stochastic switching between adjacent flow streams. The model thus provides the general time-averaged properties of the flow determined by the size, location and rotation speed of the impeller, but in addition is capable of incorporating randomness into the pathways traced by circulating particles of fluid moving around the vessel under the influence of the impeller. The model therefore gives directly times between passages through the impeller region and for a sufficient number of simulations gives the passage time distribution. It can thus be used to interpret data obtained with the radio-pill neutrally buoyant flow-follower technique. Moreover, the model automatically provides the frequency of appearance of the flow follower at any location within the vessel. Thus measurements remote from the impeller region with a loop aerial can provide further insights into correct model parameter selection. Predictions of the model closely match experimental results from a stirred vessel. The theory shows that flow maldistribution of liquid due to the passage of a gas in a stirred gas-liquid mixing vessel results in a significant distortion of the passage time distribution function. Such flow maldistributions, which have an impact upon yield in gas–liquid reactors, should be detectable and quantifiable by the radio-pill flow-follower technique.

INTRODUCTION

The design of industrial-scale reactors is usually based on data obtained on laboratory or pilot-plant equipment. In the case of gas–liquid stirred tank reactors, lack of detailed knowledge of the physical and chemical processes occurring within the vessel leads to imprecise or arbitrary scale-up criteria such as the equal tip speed or equal power per unit volume rules. These criteria, not being connected with the chemical reaction processes taking place in the reactor, can possibly lead to a chemically inefficient design. A clear example of this has been given by Mann et al., where for a complex gas–liquid reaction, changes in the gas–liquid internal flow structure using a constant tip speed scale-up criterion gave rise to increasing yield losses with increasing scale of the reactors. This theoretical investigation based upon a “multi-zones in loops” flow model depicted in Figure 1 (itself based upon a development of Van de Vusse’s model2), highlighted two new factors relevant to the rigorous design of large-scale reactors. Firstly, that the time scales of the mixing, recirculation rate and chemical reaction speed within an impeller-agitated stirred vessel do not inevitably lead to even a reasonable approach to perfect backmixing. Thus reactor designs which commence with the assumption of perfect backmixing must be suspected as inadequate, unless clear evidence to the contrary is presented. Secondly, and connected with this, it is clear that the extent of departure from perfect backmixing needs to be quantitatively defined if rigorous reactor designs are to be undertaken. Quantifying this non-perfect backmixing must proceed from detailed understanding of the gas–liquid flow process taking place.

This detailed understanding requires the development of new techniques and methods of observation aimed at describing, for a gas–liquid reactor, the ways in which the gas and liquid circulate within and pass through the reactor as well as the nature and extent of the interfaces formed. It is through these interfaces that the necessary transport processes take place.

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A promising technique in this connection is the use of a neutrally buoyant radio-pill flow follower. Such a flow follower, first developed by Bryant, and subsequently used in a gas–liquid stirred vessel by Middleton, conveniently gives rise to the distribution of times of passage through the impeller region using a loop aerial surrounding the impeller. In principle, the distribution of times of circulation through the impeller contains a complete measure of the liquid flow processes within the vessel. With a proper interpretation, the distribution of circulation times can be related to an exact definition of the vessel internal liquid flow. This is of particular significance, since a simple material balance approach to internal gas–liquid flow, indicates that on the large scale the flow of gas through the reactor can seriously distort the internal recirculation flow of the liquid. Such distortions then lead to changes in chemical yield for certain types of gas–liquid reactions.

Observations of the qualitative behaviour of a flow-follower within a stirred vessel show a specific type of behaviour which emphasises the possible oversimplification of a “zones in loops” description of the internal flow. As Figure 2 indicates, an observation of the passage of the flow-follower through the impeller does not necessarily imply that it has just completed one “circulation” through the vessel as in case A. The nature of the fluid flow structure, which has a primary pumping flow and an associated induced flow, means that the flow-follower may have undergone several circulations without providing a realistic description of the velocity distribution throughout the vessel. Each cell is assumed to be a perfect plug flow element, so that the time of passage of the flow-follower through any particular cell is immediately obtained. In defining a satisfactory throughput distribution amongst the matrix of cell elements, several workers have published experimentally measured fluid velocity profiles for various stirred tank reactor configurations which have been used in conjunction with the Stokes–Einstein equations to derive the pattern of fluid streamlines. For the present model, an example velocity profile similar to the profiles of relative velocities published by Bruxelmame, shown qualitatively in Figure 3, has been employed. This example velocity profile can be used to demonstrate the application of the model, which incorporates a proper conservation of flow through the matrix of cells. The model is depicted in Figure 4 with relative flow throughputs, shown in each i/jth plug flow cell for a $10 \times 10$ set of cells to represent each of the upper and lower circulation zones of the vessel. The choice of a finite number of cells gives rise to the equivalent flow

**Figure 2.** Single and multiple circulations between passages through the impeller

**Figure 3.** Typical velocity profiles

**Figure 4.**
Figure 4. Matrix of flow cells (10 x 10) in upper and lower regions of a stirred vessel
profiles having a series of steps of local flow throughput as shown in Figure 5.

The remaining feature of the model is the incorporation of stochastic switching between adjacent fluid streams which is intended to account for the levels of turbulent mixing which are superimposed upon the general structure of the liquid circulating flow. Due to turbulence, the flow-follower whilst moving along a particular fluid stream can be displaced into an adjacent flow stream. This is achieved in the model by subjecting the flow-follower to a switching probability on exit from each fluid cell. These switching transfers are shown in Figure 4 as dotted lines, with the main flow as a full heavy line. For the purpose of illustration and demonstration, the model assumes equal switching probability for displacement to adjacent flow streams, with these probabilities being equal to the probability of continuing in the present flow stream. In practice this is achieved by a simple logic operation on sets of pseudo-random numbers. This general cell is shown in Figure 6, though the flow vessel incorporates four variants on the general cell which take account of cells giving a change in main flow direction as shown in Figures 7(b), (c), (d) and (e) respectively.

Detailed computation of the model is achieved in the following way. For a cell matrix of size \( N \times N \)

\[
V_{ij} = \frac{V}{2N^2}
\]  

(1)

If the total internal circulation flow generated by the impeller is \( Q \), then the set of \( Q_{ij} \) are to be chosen to describe accurately the internal structure of velocity distributions.

The main flow through the cells is required to obey the material balance in such a way that continuity is preserved. Thus

\[
Q = \sum Q_{ij}
\]  

(2)

with the summation across the appropriate sets of flow cells. The relative flow proportion for an individual cell is then given by

\[
a_{ij} = \frac{Q_{ij}}{Q}
\]  

(3)
Figure 4 shows an example set of $a_{ij}$ for a $10 \times 10$ flow cell matrix with the focus of the internal circulation located off-centre. This reasonably reflects the structure of the velocity profile reported by Bruxelmae. At first, in flowing through and from the impeller, there is a row of four cells representing flow into the upper (and lower) sections of the vessel. This diverges to six cells for the return flow towards the impeller, with a convergence back to four cells at the impeller. Across each row of cells $\sum a_{ij} = 1$, reflecting the conservation of flow implied by equations (2) and (3). This conservation applies also at each of the converging and diverging flow junctions.

The residence time in a particular $ij$th cell is given by

$$\tau_{ij} = \frac{V_{ij}}{Q_{ij}} = \frac{V}{2a_{ij} Q N^2} \quad (4)$$

The probability of the flow-follower remaining in the main flow stream is designated by $P_{mf}$. If the switching probability is $P_s$, with an equal probability of switching to adjacent flow streams (except for the special cases of edge and corner cells, see Figure 7), then

$$P_{mf} + 2P_s = 1 \quad (5)$$

Thus, specifying the probability of continuance in the main flow automatically defines the magnitude of the switching probability.

The time taken by the flow-follower between passages through the impeller cells (10,4 for the upper part of the vessel, 11,4 for the lower) is calculated from the summation of individual cell residence times along the path traced out by the flow-follower, so that

$$\tau_{ff} = \sum \tau_{ij} \quad (6)$$

The dimensionless mean turnover time is $\tau_c$ and the number of dimensionless mean turnover times elapsed between consecutive passages through the impeller cells (where the loop aerial detects the flow-follower) is then given by

$$n_{tc} = \frac{\tau_{ff}}{\tau_c} \quad (7)$$

This structural flow model with random switching gives rise to a stochastic simulation of the pathways of the flow-follower through the vessel. As a multi-cell model it bears a resemblance to the models of Tavlarides and Kopp, but it differs in the sense that it has been constructed to simulate the random meanderings of a flow-follower. Direct theoretical simulation of large numbers of random meanderings will give rise to an estimate of the distribution of passage times through the impeller, and the model therefore offers a means of diagnosis of flow-follower experiments.

**PREDICTIONS OF THE MODEL**

Because the model is based upon a close physical description of the internal flow processes taking place in a stirred vessel, it gives rise to a surprising number of predictions of phenomena over and above the potential for simply correlating passage times through the impeller zone. However, these passage times have traditionally been observed in flow-follower experiments and the passage time distribution predicted from the parameters of Figure 5 are presented in Figure 8. The ordinate on Figure 8 is a normalisation of the number frequency distribution function of passage time $f_d(t)$ which is defined such that $f_d(t)dt$ is the number fraction of the passage times which lie between $t$ and $t + dt$. The curve depicted in Figure 8 was derived from the model for 5000 simulated
passes through the impeller region. The abscissa of Figure 8 is also normalised using the ratio:

$$\frac{Q}{V} = \frac{\text{total internal flow induced by impeller}}{\text{vessel volume}} = \tau_c$$

(8)

where $\tau_c$ is the mean vessel turnover time. The abscissa is therefore in units of dimensionless vessel turnover time.

The cumulative curve in Figure 8 is composed of circulation passages which involve either single or multiple flow passes through the upper and lower circulation regions. The multiple passes could involve movements through both the upper and lower regions before being detected at the impeller. The result of these multiple passages is to skew the passage time function towards longer times relative to the mean. The mean dimensionless turnover times is (by definition) unity, but the mean passage time in Figure 8 is 2.75 times larger. A good proportion of the passage times are therefore more than mean turnover times. The passage time distribution function is shown decomposed into its basic components in Figure 9. Single circulations in the upper region are in Figure 9(a), with as expected a dimensionless passage time mean close to unity. It is essentially identical to Figure 9(b) which is for single circulations before passage through the impeller in the lower region. Figures 9(c) and (d) are for multiple passes only through the upper region and only through the lower region respectively, whilst Figure 9(e) is for multiple passes involving more than just the upper or lower regions.

The model is also capable of generating information relating to the random pathways traced out successively by the flow-follower. Correspondingly it can predict the frequency of appearance at any particular location. Figure 10 gives examples of two pathways, one of which involves a single circulation through the upper zone, whilst the movement through the lower zone before returning to the impeller involves two nominal circu-

![Figure 9](image-url) Components of the distribution of passage times through impeller

![Figure 10](image-url) Two example stochastic pathways.
lations. The set of pathways for five passages through the impeller region (selected at random from the 5000 simulations) appear in Figure 11.

The predicted relative frequency of appearance at each location (i.e. each flow cell element) is presented in Figure 12 which has been constructed on the basis of a maximum of 1000 appearances occurring at some cell in the network. In this instance this maximum occurs in cell 14,7 (in the lower circulation region) and it can be seen that the model predicts the greatest frequencies of appearance around the centres of circulation. The frequency of appearance in the two impeller zones, where the loop aerial is taken to be located, is however only marginally lower at 843 and 885. This map of frequency of appearance means that the model can be further studied by moving the loop aerial around the vessel. As might be expected, the frequency of appearance becomes quite low towards the farthest "corners" of the vessel.

![Figure 11 Stochastic pathways for 5 passages through impeller.](image1)

![Figure 12 Frequency of appearance of flow follower.](image2)

![Figure 13 Influence of variation of switching parameter](image3)

So far, the model has been examined with respect to a particular set of parameters in order to illustrate its capability for use in assessing flow-follower experiments. A parameter of the model which is particularly prone to uncertainty is the magnitude of the switching probability \( P_s \) relative to the probability of remaining in the main flow \( P_{mf} \). The previous demonstrations of the model are based on \( P_s = P_{mf} = 0.333 \). Somewhat remarkably, the passage time distribution is fairly insensitive to this parameter and Figure 13 compares the equal switching probability case with \( P_s = 0.333 \) with the case for \( P_{mf} = 0.600 \) and \( P_s = 0.200 \). The switching tendency is significantly re-

INTERPRETING FLOW-FOLLOWER DATA FROM A STIRRED VESSEL

Figure 14. Comparison with "4-zones-in-loops" model

duced, but as Figure 13 demonstrates, no appreciable change in the passage time distribution function is observed. It would seem therefore that variations in the stochastic switching parameter are not important in determining the overall properties of the system in relation to flow-follower observations where a large number of observations are compounded (of the order of several thousand). It is likely to influence the nature of the distribution of intervals of appearance at a given location where the short-term details are closely observed, though this remains to be undertaken. Also of course, in extending the switching concept in terms of local exchanges of fluid, the switching parameter would almost certainly exert an influence upon concentration fields in chemically reacting systems. This also remains to be done.

Figure 15. Comparison of theory with a set of experimental observations

Indeed it can be safely said that the presently proposed and partially explored "structured flow model with stochastic switching" merely offers the hope of an improved quantitative description of the undoubtedly complex mixing and flow behaviour of the typical stirred vessel.

Figure 14 is intended to provide a comparison with the expected passage time distribution function using four backmixed zones in each of the upper and lower circu-

lation regions as previously used\(^1\) and shown in Figure 1. Four zones in loops give a much sharper distribution curve with no detectable skew towards longer passage times. A preponderance of longer intervals of passage through the impeller is invariably observed when logging a flow follower in practice. The general suitability of the present model can be judged from Figure 15 which compares a set of experimental observations (numbering 376) with a set predicted from the model corresponding to the parameters of Figure 4. It is clear that there is a remarkable convergence of model and actual experimental results which leads to the conclusion that the model as presently conceived can claim to be a possible improved basis for studying passage time data generated by the flow-follower technique.

A major practical potential for the model is in determining the distortion of the liquid phase circulation pattern in a stirred gas–liquid reactor from which time of passage and frequency of appearance data are available. In the single phase case, the flow rates into the upper and lower regions are equal when the impeller is at the mid position, but if a substantial gas flow is introduced this cannot be the case. In a previous analysis\(^1\), it was suggested that for a large-scale vessel with a specific gas input rate, the liquid flow would be expected to split into the proportions 0.85:0.15. The consequences of altering this balance of liquid flow shows up clearly in the passage time distribution function and this is shown in Figure 16. Hence the flow-follower technique in conjunction with the current stochastic flow model appears to be a promising basis for studying the interaction between gas and liquid flow in a stirred vessel type reactor. This should lead to improved design methods likely to give rise to chemically more efficient reactor designs in the future.

SYMBOLS USED

\(a_{ij}\) dimensionless proportion of flow through cell element \(i\), \(j\)

\(i\) row position of a cell in the matrix of flow cells

MANN, MAVROS AND MIDDLETON

\[ j \] row position of a cell in the matrix of flow cells
\[ N \] square matrix size of cells in half vessel
\[ n_{m} \] number of dimensionless mean internal turnover times
\[ P_{mf} \] probability of flow-follower remaining in main flow stream
\[ P_{s} \] probability of flow-follower switching to adjacent flow stream
\[ Q \] total flow rate produced by impeller rotation
\[ Q_{ij} \] flow rate through cell element \( i, j \)
\[ V \] total liquid volume in vessel
\[ V_{ij} \] volume of cell element \( i, j \)
\[ \tau_{ij} \] residence time in cell element \( i, j \)
\[ \tau_{c} \] dimensionless mean internal turnover time
\[ \tau_{ff} \] time elapsed between passages through the impeller cells

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ADDRESSES

Correspondence should be addressed to Dr R. Mann, Department of Chemical Engineering, UMIST, PO Box 88, Manchester. P. P. MAVROS is serving with the Greek armed forces and Dr J. C. MIDDLETON is at ICI Corporate Laboratory, The Heath, Runcorn, Cheshire

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