SYNTHESIS REPORT

BREU - 0453

BRITE/EURAM PROJECT BE 409S

THE DEVELOPMENT OF VALIDATED PREDICTIVE MODE FOR OPTIMAL DESIGN OF MULTI-PHASE CHEMICAL PROCESSES

Abstract

A computational Fluid Dynamics code has been developed for gas-liquid and liquid-liquid dispersion processes as , encountered in emulsification, chemical reactions, fermentations etc. A two-phase turbulence model has been implemented and extensively tested experimentally. In addition, verified physical models have been developed, which describe the evolution of droplet/bubble sties as a consequence of break-up and coalescence processes. These models have been coupled to the two-phase turbulence model to obtain full coupling between" the two phases. Finally two methods have been developed which allow a detailed calculation of a flow as generated by moving parts such as an impeller" in a stirred , tank. Implementation of all models into the commercial code STAR-CD allowed the successful evaluation of a number of industrial test cases in detail. *Keywords*: multiphase flow, CFD, emulsification; aeration.

1 . INTRODUCTION

The upscaling of multi-phase" processes such as agglomeration, fermentation and emulsification is to a large extent a matter of trial and error. In general several steps are involved in such an exercise and in eases where theoretical guidelines are available these guidelines are often based on empirical correlations. The detailed physics describing the local processes on a microscale is insufficiently developed. Moreover the effect of a second phase on the flow characteristics of the continuous phase has still to be further developed.

To avoid costly and time-consuming upscaling exercises, a promising approach is to use a Computational Fluid Dynamics (CFD) methodology where the basic hydrodynamic equations describing the fluid flow are solved numerically in any geometry, taking into account appropriate boundary conditions. This methodology is already available for one-phase, flow problems comprising laminar and turbulent flows.

1.1 PROJECT OUTLINE

We envisaged to extend the CFD methodology to two-phase processes with particular emphasis on liquid-liquid (emulsification) and gas-liquid (aeration) flows. The objective was to, describe the size arid local volume fraction of bubbles/droplets in a flow as resulting from break-up and coalescence phenomena as they are driven by the local flow characteristics (Fig. 1). The consequence of the presence of 'particles' on these local flow characteristics should be accounted for as well."

The following" approach' has been followed:'

* For the microscopic ('local') physical processes such as droplet break-up, coalescence, local mass transfer, theoretical models were developed based on analytical, first-order theories. Where necessary more in-depth numerical methods were employed. The hydrodynamics naturally enters *into.* these theories via the, *local flow* and *turbulence* characteristics.
* Detailed physics was developed on two-phase turbulence with full, coupling between the two phases; algorithmic aspects for solving the complicated set of equations were addressed..
* Two new methodologies were developed for the calculation of the flow characteristics as generated by moving parts such as the impellers in a baffled tank. .
* All methodologies were incorporated in the commercial CFD code STAR-CD. Various aspects were evaluated first in. a simple CFD code.
* It was the deliberate intention to support all these developments with sufficiently dedicated experimental data.

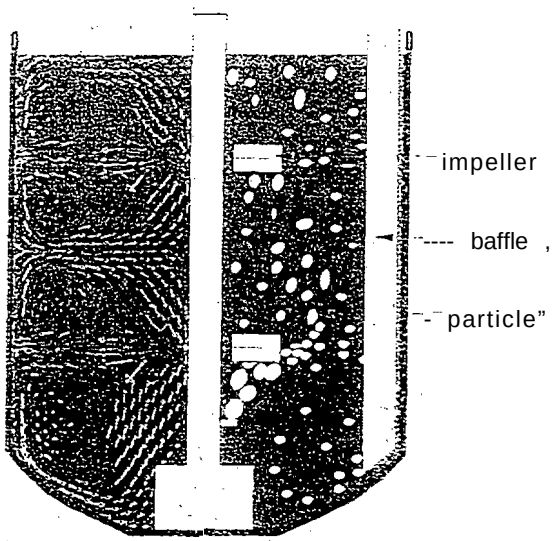

Fig. 1. Interplay of flow field' and bubble size in a stirred vessel.

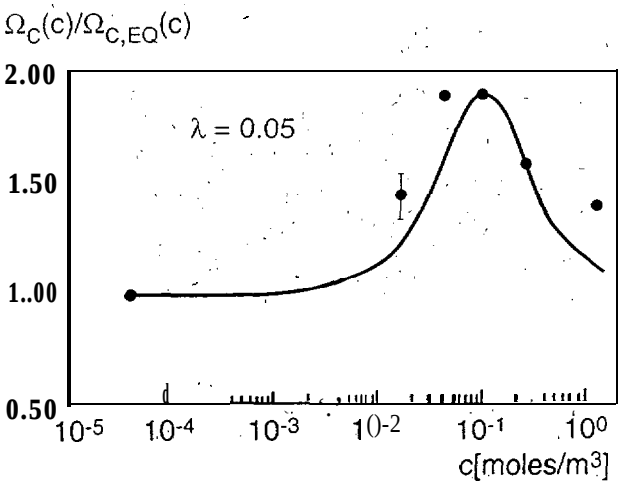

Fig. 2. Critical capillary number for binary break-up of a droplet shear flow as a function of surfactant concentration. , Viscosity ratio of fluids η_d/η_c = 0.05. (•) experiments; (—) , theory.

2. SELECTION OF RESULTS

2.1 LOCAL EFFECTS

In many industrial two-phase processes the 'particle' size is not, uniform' and constant in time during operation. Droplets/bubbles may breakup or they may merge (coalescence) as a consequence of collisions. Control of the processes which determine the final droplet size distribution is of paramount importance. To this end two aspects have to be considered: (i) the physics underlying these processes and how these are coupled to the local flow characteristics, and (ii) the local flow characteristics. Here an example will be highlighted which is related to droplet break-up.

A droplet can break up under various conditions and in various modes. Although the project considered also turbulent 'flows, only' break-up in laminar flows will be considered here', Two break-up modes have been studied extensively with the emphasis on the consequence of the presence of surface active compounds. The example is the break-up of droplets in two daughter droplets, which occurs when the flow is not too intense. In the absence of surfactant the physics was-well. developed. However, surfactants can have a dramatic influence on this process as Fig. 2 depicts. In the intermediate concentration range it is relatively more difficult to break up the droplets compared to the situation at low and high concentration (if the equilibrium interracial tension is taken as a reference). This phenomenon is due to the unequal distribution of the surfactant in the droplet interface, which gives an extra elastic property to the interface. A physical model has been developed to explain this. The phenomena have also been investigated in plane hyperbolic-flow.

Coalescence is affected by surface-active ingredients as well. The experience that they block coalescence, has been substantiated with a quantitative physical model.

Major progress has also been made in the analysis of coalescence in the' presence of inter-phase mass transfer i.e. coalescence while for instance acetone, dissolved in water, transfers 'to the dispersed oleic phase. This mass transfer, as encountered in stirred tanks and bubble columns, can affect the coalescence appreciably. The analysis of this process obtained quite some attention. First order theories have been developed and a full numerical study has been devoted to it. Numerical results are presented in Fig. 3. The increased instability of a bubble column in which mass transfer is taking place from the dispersed to the continuous phase, has been captured by the calculations

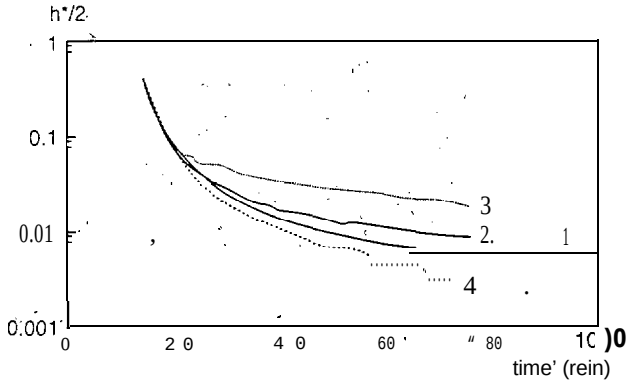

Fig. 3. Film thickness as a function of" time for coalescing droplets. (1) without mass transfer; (2) AC = 10"³(C→D); (3) ΔC = 5 . 1 0 "³ (C→D); (4) ΔC = - 1 0 "³ (D→C)

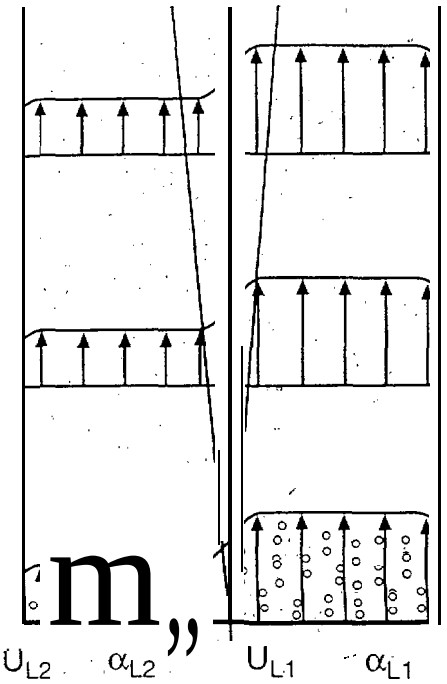

Fig. 4. Schematic representation of mixing layer experiment.

2.2 TWO-PHASE TURBULENCE

In the modelling of two-phase turbulent flows several equations have to be solved at the same time: two momentum equations and two continuity equations which have to be coupled to a turbulence model (in this case the κ-ϵ). In doing.' . so several terms in these equations have to be modelled separately. The coupling "between the two phases is taken-into account through the force that one phase exerts on the other. This comprises three contributions: the drag force, the . virtual mass force and. the. lift force. These forces turned out to be essential for obtaining a, good comparison between simulation and experiment. As an example the 'ducted plane shear layer' will be discussed (Fig. 4). Two fluid streams at different velocities and at different bubble fractions enter a duct and mix in a shear layer. The local volume fraction and velocities were measured at several axial positions along the test section. A good agreement has been obtained between the experimental results and the simulations for the void fraction (Fig. 5). The two-phase mixing layer which develops downstream is characterised by a span-wise distribution of mean velocity and void fraction. The presence of a peak' and trough in the distribution within the shear layer is attributable to dominating lift forces acting on the hubbies; The layer ' expansion was found to be much greater than in single phase flows. . .

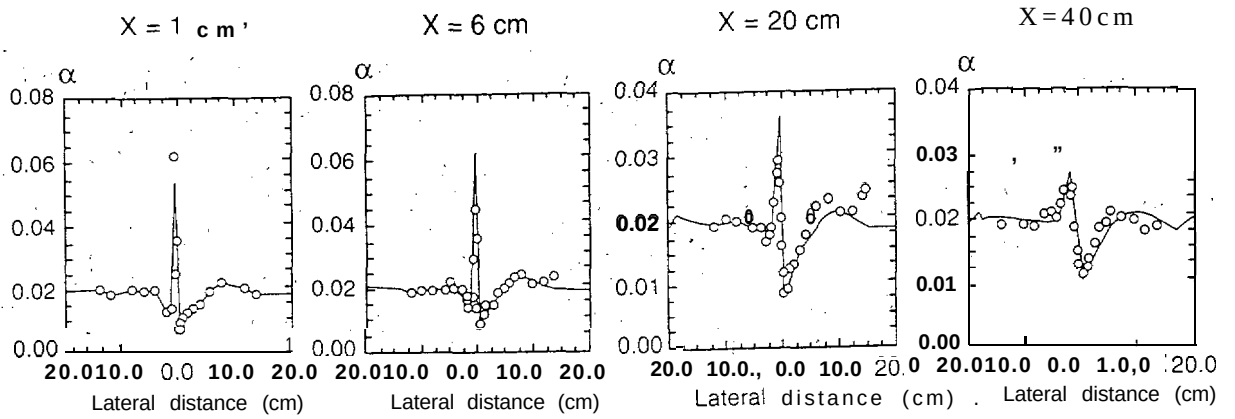

Fig. 5. Two phase flow in a plane shear layer(o) experiments; (—) simulations.'

2.3 IMPELLER MODELLING

Many industrial processes are executed under agitated conditions where the flow is generated by impellers. For prediction of the flow characteristics in the vessel the momentum transfer from the impeller to the fluid has to be modelled Properly" Until recently the impeller was considered to be a rotating cylindrical box with boundary conditions which were obtained from local 'LDA measurements. Changing to another impeller meant that other boundary conditions had to be obtained from experimental data. This situation had to be improved in the sense that the fiow within the impeller region had to be simulated simultaneously with the rest of the fluid in the vesseL_In the project two new methodologies have been designed and incorporated into STAR-CD, both appropriate for single and two-phase flows

In the 'Sliding Mesh': method, which allows time dependent calculations, the solution domain is divided into two sections, the first being attached to the impeller, the second to the stationary outer wall and remains static. At the interface the two meshes move relative to each other as time progresses. The coupling between the cells on either side of the interface is treated implicitly taking into account that the mesh cell connectivity changes due to the sliding motion.

The 'Multiple Frame of Reference' (MFR) method utilises separated but connected mesh regions, on each of which the flow is analyzed as a steady-state problem. The first frame rotates at the impeller speed and is used to calculate the flow within the impeller domain; the 'second frame is stationary and is used to compute the flow outside the impeller region. At the interface the two computational regimes are matched implicitly by appropriate velocity transformation from one frame to the other. Fig. 6 depicts a detailed plot of the turbulent energy dissipation in the impeller regime of a Rushton agitator as obtained using the MFR method. The zones of high dissipation behind the blades are clearly visible. A proper simulation of these zones is essential when local processes in that region have to be calculated.

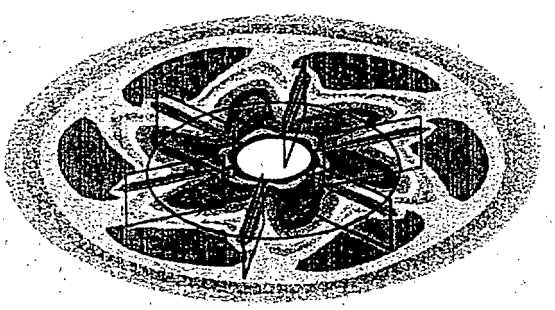

Fig. 6. Turbulent kinetic energy dissipation in Rushton impeller region as obtained by CFD analysis using the 'Multiple Frame of Reference' methodology.

2.4 TEST CASES

All models and methods discussed above, have been amalgamated and incorporated into the commercial CFD code STAR-CD which in this way obtained a two-phase version. As the code supports unstructured meshes flow simulations in any geometry can be executed.

Gas/liquid Stirred Vessel Flow. For validation purposes we used a data set from Literature for air-water systems including dispersed phase velocities, bubble diameters and local phase fractions in a tank with a standard Rushton impeller (Fischer and Lübbert, Chem. Eng. Techn. 15 (1992) 309). The plot in Fig. 7 shows the local phase fraction as a, function of radial position at various heights in the tank. The sparger was located at Z/H = 0.08, the impeller at 0.31. As the measuring techniques show quite different results in places, it can be stated that the simulation results are probably in agreement with the data to within experimental error. *This is as good* a result as one can expect.

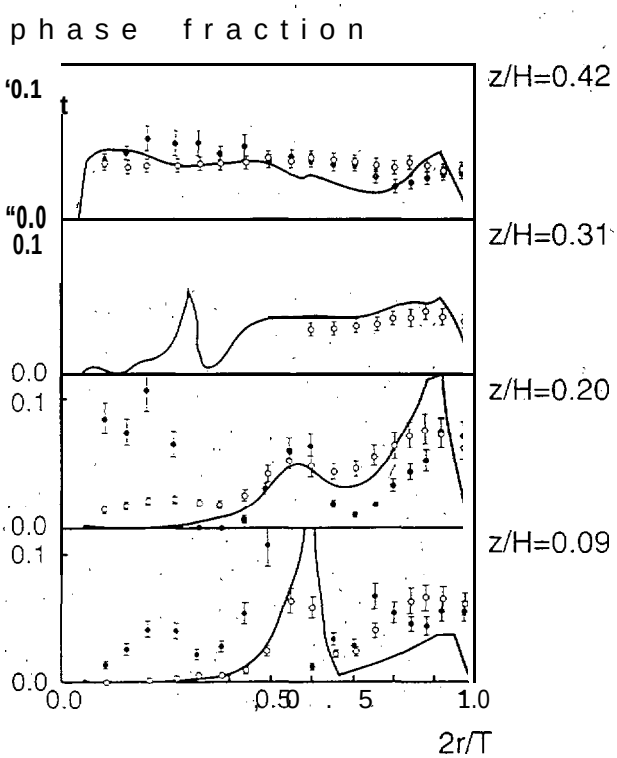

Fig. 7. Comparison between computed local phase fraction and experimental data for gas/liquid flow in a stirred tank with Rushton impeller. (•) ultrasound; (○) conductivity (—) simulation.

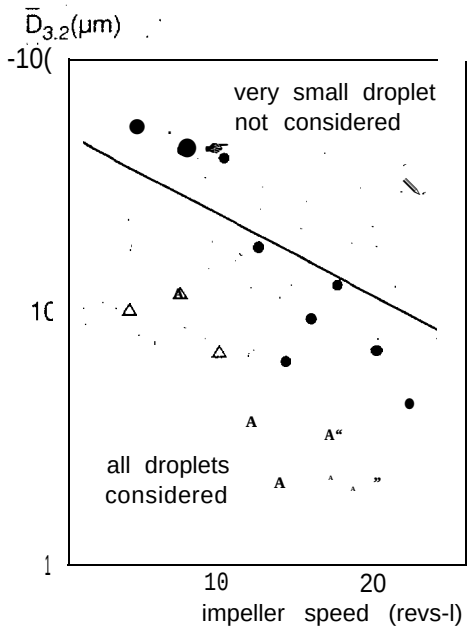

Fig. 8. Emulsification in a stirred "vessel. Experiments: (•) droplets of the coarse part of the binodal distribution; (A) for the full size distribution; (—) simulation.

Emulsification. An o/w emulsion was prepared in a 'standard stirred tank agitated by a standard Rushton turbine. The line in Fig. 8 represents the simulation results as obtained using the MFR method and corresponds very well with the coarse part of the bimodal distribution as analysed microscopically. The fatter comparison is the most relevant one as it tests the break-up model which has been incorporated into the code. The small droplets *in* the distribution originate from a special break-up mode, called tip-streaming.

3. CONCLUSIONS

This project accomplished what it has been set out to do: to develop a commercial two-phase CFD code which ean cope with varying droplet/bubble size and size distributions. An advanced two phase turbulence model has been developed and incorporated as well. The models are based on detailed experimental data, acquired in the project as well as from literature.

This achievement is a major step forward to arrive at a reliable prediction of multi-phase processes. Partners consider this approach and further developments in this direction vital for the future competitive edge of Europe.

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