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MODELING AND SIMULATION OF MULTICOMPONENT FLOWS

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Abstract.

*Before describing what this paper really is, a few words on **what it is not**. The following description of the main characteristics of multicomponent flows and of some of the models used for their solution is not to be taken as a comprehensive and complete review, provided such a thing were possible in an field as complex and rich in models and variations as the present one. This is only a very brief bird's eye view of a very complex research field. Some of the references given are just to be taken as examples, not as best or first papers in each subject.*

This is a brief introduction to the field of multicomponent flows for people with numerical experience and knowledge of single phase CFD modeling. The most renowned models available in the open literature are classified into four categories, namely Averaging, Surface Tracking, Entity Tracking, and Meso/Microscopic models. The models are briefly described, using not equations, but words and images. The readers are encouraged to consult the references for mathematical and numerical details. Comments on computer power requirements, range of applicability, complexity, etc., are also included in the description of some of the methods.

1 INTRODUCTION

Following definitions given by Drew and Passman in their book *Theory of Multicomponent Fluids*[1] we will call *multicomponent flow* the flow of a *composite fluid*, that is, the flow of non-homogeneous, fluid materials, chemically and or physically distinct, coexisting in more than one phase.

Multicomponent flows are found in many processes, both natural and artificial. Among the natural ones, we may cite: entrainment and transport of air in oceans, lakes and rivers; formation, movement and condensation of clouds; flow of blood in capillaries and small arteries; sedimentation in rivers; etc. On the side of artificial processes, industries are full of examples of multicomponent flows: fluidized beds in chemical reactors; coolant systems in thermal power plants; injection of air in pools for water treatment; recovery of oil and gas in hydrocarbon reservoirs; etc. The present paper is intended to be a bird's eye view on the main characteristics of this type of flow and on the models developed during the last decades in an ongoing effort for simulating and predicting them.

This work is organized as follows. First, we provide a description of multicomponent flows and the basic mass and energy transfer and chemical and mechanical processes involved. Secondly, the mathematical model is described using just a few words. Finally, a classification and a brief description of the most renowned and used models for multicomponent flows is presented, along with results taken from applications reported elsewhere.

2 PHYSICAL DESCRIPTION OF MULTICOMPONENT FLOWS

2.1 Basic definitions

Multicomponent flows are characterized by the presence of continuous regions of matter that may contain other portions of matter in the form of disperse entities (bubbles, droplets, etc.). Note that this classification of a portion of matter as entity or continuous region is rather ambiguous, and that it has relevance only from the point of view of modeling. Both in the continuous regions and inside each entity one may also find gradients of concentration

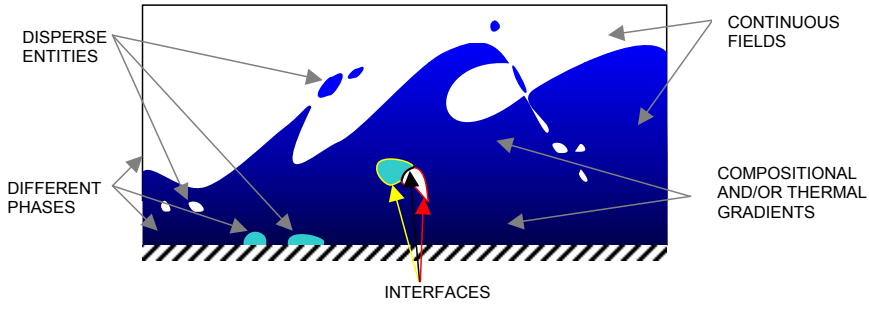


Figure 1: basic definitions

of different chemical species dissolved in the phase. Thermal gradients are also a common feature. Furthermore, many different types of interfaces may be found, both between different phases and between phases and solid walls.

2.2 Chemical, Thermal, and Mass transfer processes

At the interfaces, there may be mass flux due to phase change, along with interfacial chemical reactions and interfacial heat transfer. Heat conduction and chemical reactions between different species may also happen at any point inside the bulk of a phase. The concentration of species is controlled by molecular diffusion and convection.

New entities may be created or destroyed by phase change processes at any time or point in space, the most common examples being the release of bubbles from nucleation sites at solid walls and the complete evaporation of droplets.

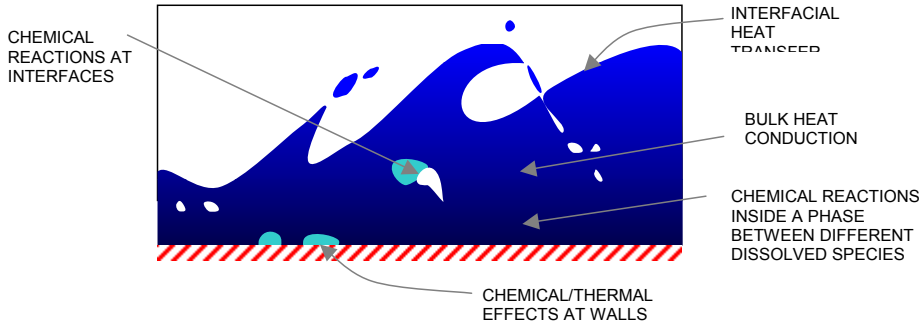


Figure 2: chemical, thermal, and mass transfer processes

2.3 Mechanical processes

Exchange of momentum between phases occur at the interfaces. Surface tension is the main responsible for maintaining the integrity of the disperse entities and keeping the interfacial area from growing unbounded.

Entities may also be created or destroyed by mechanical processes. Two or more entities of the same phase may coalesce if they collide and there is enough time for the film of fluid that keeps the entities apart to disappear before they start to separate. One entity can also break up into two or more new entities due to many physical processes, the most common of which is the interaction of the entity with the turbulent eddies of a surrounding phase.

New entities may also be created by a process called *entrainment*, in which fingers of a phase reenter into the same phase, disturbing the interface and carrying along portions of matter of a second phase that end up as disperse entities inside the bulk of the first phase. The most common example of this process is the entrainment of air bubbles into the ocean by the breaking of waves.

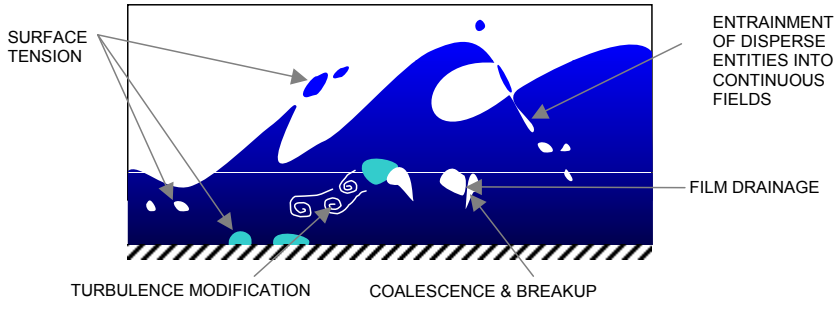


Figure 3: mechanical processes

3 MATHEMATICAL DESCRIPTION OF MULTICOMPONENT FLOWS

A complete mathematical description of this type of flows inside the continuum hypothesis comprises both bulk and interfacial equations, and constitutive relations.

At every point inside each phase, we need:

- Momentum (Navier Stokes) equations
- Mass balances
- Transport/reaction equations for each species
- Thermal transport

At the interfaces, we need:

- Interfacial forces
- Mass transfers
- Chemical reactions
- Heat fluxes

Besides this, constitutive relationships for characterizing the different materials are required. Along with suitable initial and boundary conditions, this set of equations is all we need to fully solve the problem.

We might also write equations at a molecular level. Some special problems are indeed more suited to this approach than to the continuum one.

4 YEAH, BUT ... HOW DO WE SOLVE THEM?

One of the characteristics of MCFs is the wide range of space and time scales involved, even in globally laminar problems. Vortical and usually turbulent flow structures are created by interfacial interactions, mainly around the disperse entities.

In order to capture every minute mechanical, chemical, or thermal detail in these flows, extremely fine grids are needed to properly solve the original set of equations. Trying to solve

problems of engineering interest just by means of this set of equations, therefore, fall well beyond the computing power available in the present and in the near future.

Due to this, a whole hierarchy of models has been developed during the last decades. In this paper, we chose to classify them in four types: *Field (or Averaging) Models, Interface Tracking models, Entity Tracking models,* and *Mesoscopic or Microscopic models.* In the following, we present a **very brief** review of some of the most renowned models (see Figure 4). In some cases, examples of results obtained by this methods taken from the available literature are also presented.

4.1 Field (Averaging) Models

These models are based on a statistical view of the flow. There are really no identifiable entities in these models, but only interpenetrating pseudofluids, each of which fills in the entire domain. At any given point in space, and at any instant in time, we solve for the probability of each phase to be present, and for the average value of that phase's relevant variables (velocity, temperature, etc.). A lot of information is lost during the averaging process, which has to be put back into the models by means of closure laws and additional constitutive equations. A brief description of these models follows.

Homogeneous models

These are the most simple and probably earlier models; it is not easy to track back in time when was the first time it was used for solving multiphase problems. The whole problem is modeled as a single pseudofluid that somehow represents the average behavior of the multicomponent flow. The only variables, in the case of two phase flows, are the gas (or void) fraction and an average velocity.

The loss of information due to averaging is so high in this type of models, that even with the most elaborate closure laws it is almost impossible to get reasonable results for the majority of the problems of interest, and therefore its use is mainly restricted to some types of bubbly or particle flows in pipes and other simple applications.

Drift flux models

The *Drift Flux* model [2], originally proposed by Zuber & Findlay in 1965 for two phase flows, introduces a drift velocity to account for velocity differences between the phases. Therefore, it is possible for these models to deal with more complex flows in pipes, sedimentation processes, and other flows in which the velocity differences between phases play a significant role. Variations of the original model were proposed later by other authors to extend it to N-component flows.

Two Fluid models

A big step ahead is possible with the *Two Fluid* models, originally developed by Ishii[3], and further improved in the early stages mainly by Lahey, Drew and collaborators. Though rather involved, they are the simplest of the family of RANS models, an acronym for Reynolds

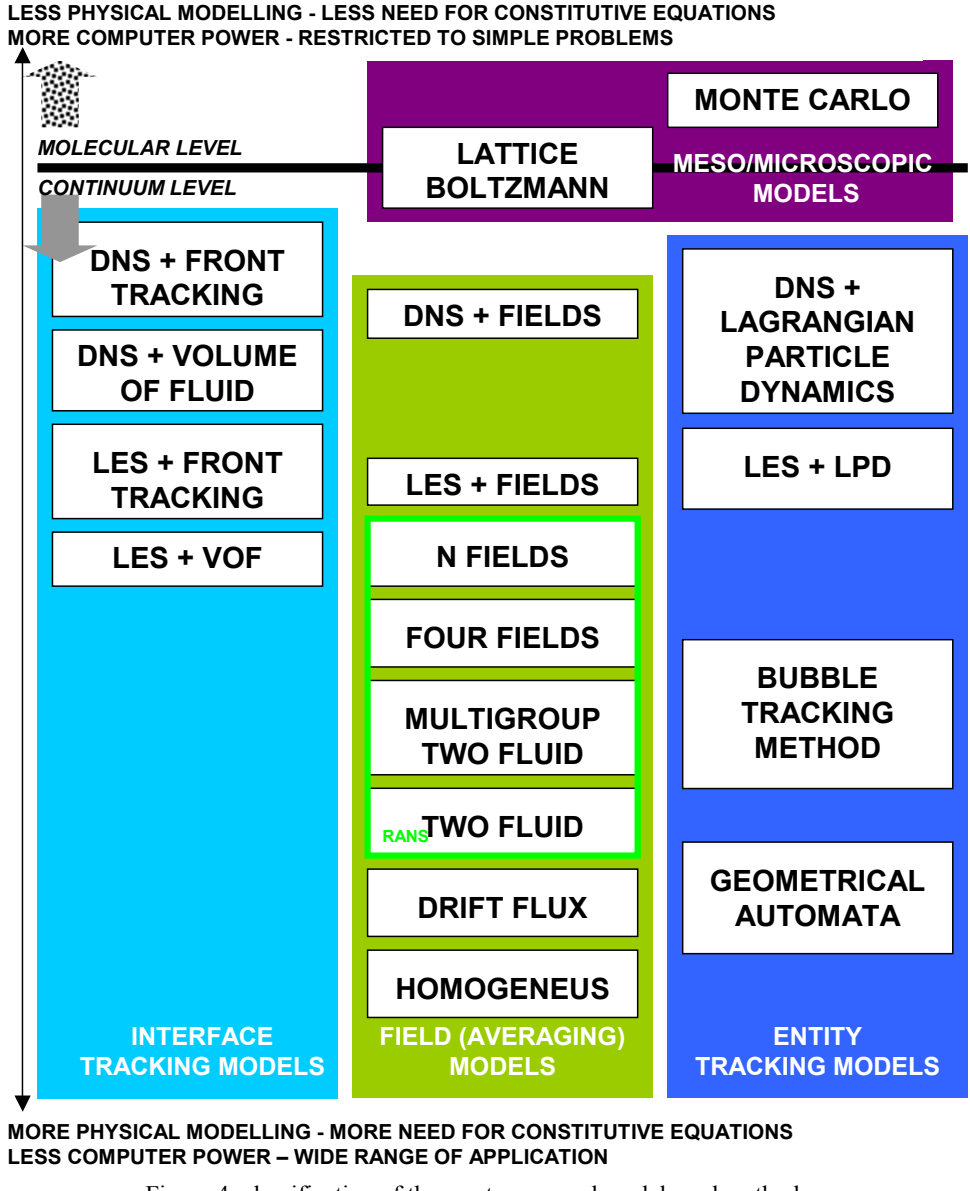


Figure 4: classification of the most renowned models and methods

Averaged Navier Stokes equations. By time, space, or *ensemble* averaging of the instantaneous mass, momentum and energy equations, a set of averaged equations that describe the evolution of two fields (two interpenetrating pseudofluids, namely "gas" and "liquid") is obtained. Additional equations may be added to represent concentrations of chemical species.

The main variables are the gas fraction and the gas and liquid velocities. In particular, there are different approaches to these models that give different values and physical meanings to the gas velocities, mainly differing in the inclusion of the mass diffusion term in the mass balance equation. These models also include in some way coalescence, break-up, and phase change effects.

A key issue on these and the following models in this section is the need for constitutive equations for the interfacial forces, that is for the momentum exchange between phases, in terms of the main variables of the model. Terms like *virtual mass, turbulent dispersion, lift,* etc., had to be modeled in order to account for the many different forces that appear in the averaged equations. This is the most controversial and difficult point, and has been in the past and still is in the present subject of strong research efforts.

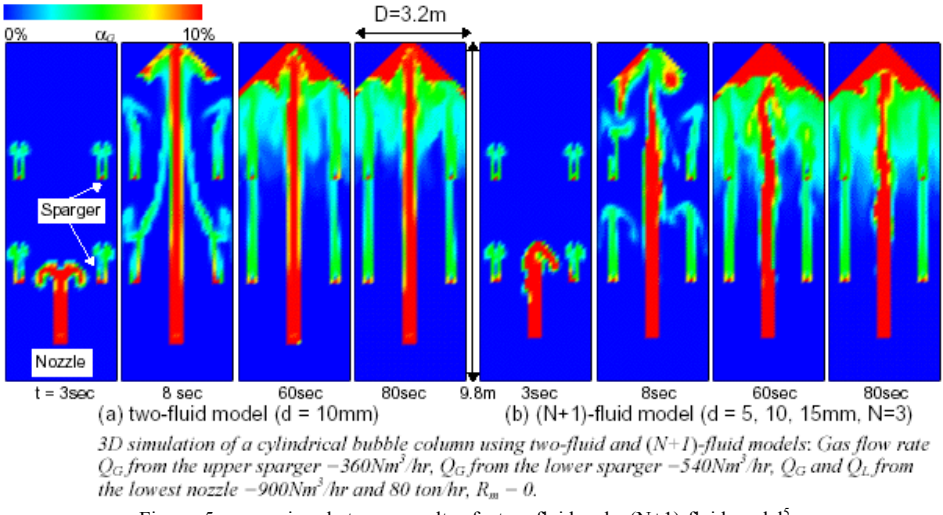
Another important subject to be taken into account in this and the rest of the averaged models is the one-way vs. two-way coupling issue. By one-way we mean that the effect of one phase into another given phase is considered, but the opposite is not. This approach is commonly applied, for example, to low gas concentration bubbly two-phase flows, in which the bubbles are transported by the surrounding liquid, but the effect of these bubbles on the liquid is neglected. Two-way coupling, on the other hand, means considering all of the effects that any phase produces in any other phase, which includes interfacial forces, interfacial heat transfer, reduction or increase of turbulence, etc. The standard Two Fluid model and all of the models presented below have been reported in the literature with both one-way and two-way coupling implementations.

Multigroup Two Fluid models (or N+1 Fluid models)

In many liquid-gas flows (water-air, or water-vapor) in which the gas is the disperse phase, the strong dependence of interfacial forces, break-up/coalescence rates, dissolution rates, etc., on the size of the bubbles makes it unreasonable to treat all bubbles as if they had a unique size on average. A natural extension to the Two Fluid model has then been to introduce additional "gas phases", usually called *groups*, that group bubbles in families of sizes that collectively span all the sizes expected in a given problem. The total number of phases is no longer 2 but N+1, with N being the number of bubble groups.

There are subtle issues to be accounted for in this kind of models, such as if grouping bubbles by geometrical size or by mass, approaches with their own advantages and disadvantages.

It is not clear to the authors who was the first to implement and use a multigroup two fluid approach; the reader is encouraged to read the work of Carrica et al.[4] for an example application to bubbly flows around surface ships.



3D simulation of a cylindrical bubble column using two-fluid and (N+1)-fluid models: Gas flow rate Q_G from the upper sparger −360Nm^3/hr, Q_G from the lower sparger −540Nm^3/hr, Q_G and Q_L from the lowest nozzle −900Nm^3/hr and 80 ton/hr, R_m − 0.

Figure 5: comparison between results of a two-fluid and a (N+1)-fluid model[5]

Four Fields models

The first contributions to these models are probably due to Kelly[6] and Siebert et al.[7]. The driving force for devising such models is the fact that in many situations of interest in two phase flows, the gas and liquid phases interchange their roles as continuous and disperse phases in different places of the domain, or even in different times at the same point in space. Therefore, it is necessary to include this feature in the models by introducing two continuous and two disperse "phases", namely *continuous liquid, continuous gas, disperse liquid,* and *disperse gas*.

These models have proven to be very powerful at dealing with multiphase flows in heated channels, and also in other types of problems.

Multigroup Four Fields models

A natural extension of the previous models, the multigroup version allows for the grouping of bubbles (disperse gas) or droplets (disperse liquid) into groups of different sizes or masses, thus adding to the model the capability of dealing with problems in which size distribution of at least one of the disperse phases is relevant per se or through its effect on other phases. The price to pay is, of course, more memory and CPU needs. With the addition of thermal and/or chemical equations, these models are the end of the line for the RANS family of models. Being involved enough so as to capture the flow in reasonable detail, but simple enough so as to not require a huge computational effort, these models represent the most powerful tool available in the present days for dealing with complex engineering problems.

Large Eddy Simulation (LES) + concentration fields

In these models, the continuous fluid is solved via a LES approach, while the disperse material (gas, fluid, or solid) is solved in an averaged way via a concentration equation, obtained from the original equations via some suitable averaging process.

In the LES approach, the scales of turbulence are resolved by the computational grid down to a given scale, below which they are modeled in some way, the most widespread of which is the Smagorinsky sub-grid Reynolds stress model[8].

These somehow hybrid models have proven to be very successful in dealing with flows in which the transport of the disperse phases is mainly due to the large scale structures of the flow. However, physical interpretation of the results obtained is open to discussion, due to the fact that while the fluid is modeled in a deterministic way (at least over the subgrid scale) the transported quantities are statistical in nature (the result of an averaging process). The results may then only recover a clear meaning once they have been averaged out at the end of the simulation.

Direct Numerical Simulation (DNS) + concentration fields

This approach is in fact similar to the previous one, the only difference being that the grid is fine enough so as to capture the smallest scales of the problem, thus making it unnecessary to use sub-grid stress models. Models like this are avid consumers of memory and CPU and are therefore restricted in most of the cases to simple geometries, serving mainly as a tool for getting detailed information for improving the constitutive equations used in RANS and LES models.

4.2 Interface tracking models

These family of models tries to maintain information about position and velocity of interfaces. The different phases are no longer treated as interpenetrating pseudofluids that span the entire domain, but as distinct phases enclosed inside interfaces.

Some hybrid methods, however, do consider a field that spans over the entire domain: an indicator functions whose values are used to detect the position of the interfaces. Examples of those are the LES+VOF and DNS+VOF, explained below.

LES or DNS + Volume of Fluid (VOF)

These models use LES or DNS to compute the carrying fluid and define a volume-of-fluid indicator which accounts, as its name states, for the volume of fluid that is really present inside each computational cell. This indicator function is then used to estimate the position of the interfaces. The original method has been proposed by Hirt and Nicholls[16]. Many improvements, including conservative forms of the method, have also been proposed in the literature (see for example the work of Johansen[17]).

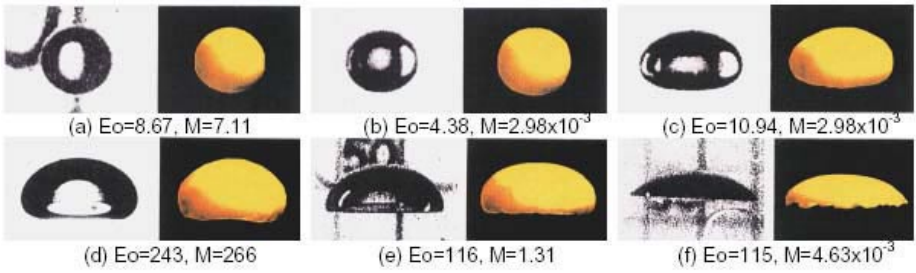


Figure 6: measured and predicted bubble shapes (VOF method)[5]

LES or DNS + Front Tracking

This is a more complex approach that allows, in principle, to track down directly the true position of the interfaces, at least down to grid accuracy. It is more involved and time consuming than the VOF models, specially in 3D problems, in which hard topological difficulties may arise. A good example of a conservative version of this algorithm can be found in the work of Manservisi et al.[9].

A regular "marker and cell" grid is used in most cases, although there are examples of front tracking schemes using step by step regridding of unstructured grids. These unstructured methods are very expensive and only suitable for dealing with low *Re* flows with tens or hundreds of disperse entities at most.

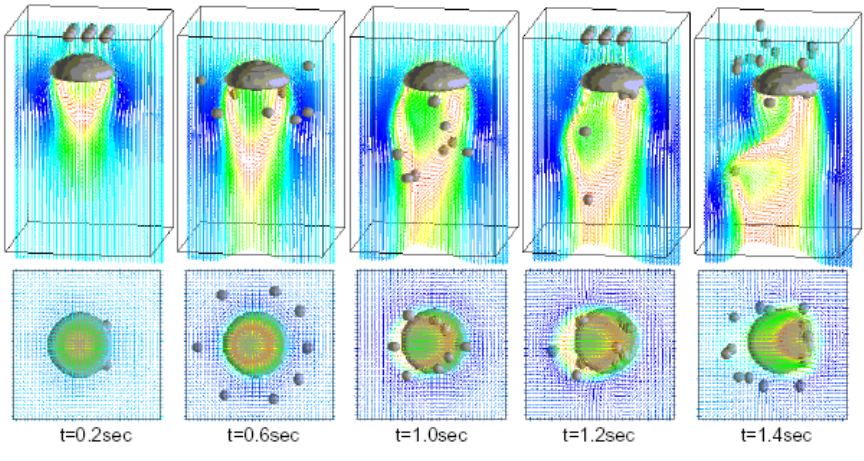


Figure 7: predicted time evolution of interacting bubbles via an interface tracking method[5]

4.3 Entity tracking models

As the name states, these models treat the separate parts of some or all of the disperse phases as individual entities. These entities (particles, clusters of particles, droplets, etc.) are somehow tracked down during the evolution of the process. They may disappear as individuals by breaking up into two or more new entities or by loosing all of their mass due to phase change, and also by combining with other entities due to coalescence during collisions.

The most time consuming phenomenon to model into entity tracking methods is coalescence, since it implies considering at each time step the possible interaction of every entity with (in principle) every other entity present in the flow field. The time required for simulating this phenomenon is of order N^2, with N being the number of entities in the field, unless some special implementation is devised.

Geometrical Automata

This is one of the simplest approaches to entity tracking. The entities, usually bubbles or particles, are considered rigid spheres (or circles in 2D pseudo-problems) and are treated as automata that posses a set of states and are subject to a set of rules for changing those states. The parameters that define the state of a geometrical automaton are position, velocity, and size. The automata interact with other automata and with the boundaries of the domain though a set of simple rules that model the processes of transport, break-up, coalescence, bouncing into walls, dissolution, etc. At each time step, the state of each automaton is updated according to these rules.

The fluid movement is usually calculated based on very simple models, and turbulence is added only as a random velocity perturbation at each point in space. The main application of these models is in generating statistical results of, for example, collision rates, or for simulating simple flows in channels. A very interesting example of this method can be found in the work of Herrero et al.[10].

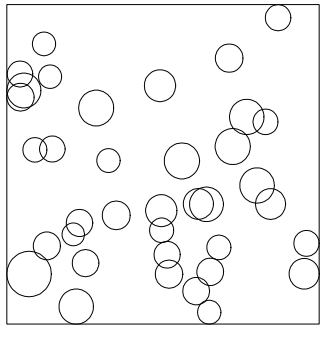


Figure 8: snapshot of an agitated tank with bubbles modeled by geometrical automata[11].

Bubble Tracking Method (BTM)

Following Tomiyama[5], bubbles are classified due to their shapes into five types: spherical, ellipsoidal, spherical-cap, semi-Taylor, and Taylor bubbles. The shape transition sizes are determined based on available empirical information on shape regimes. In this one-way coupling method, the individual bubbles are tracked using a simple *force=mass* × *acceleration* equation. Constitutive equations suitable for each type of bubble are used for computing forces over the bubbles. This rather simple method has proven useful for predicting developing flows in ducts.

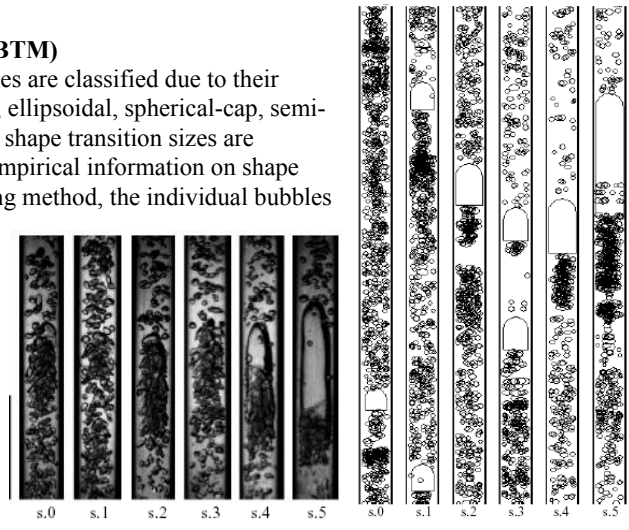


Figure 9: experimental vs. BTM simulations of two-phase upflow in a pipe[5]

LES + Lagrangian Particle Dynamics (LPD)

A huge step ahead from the previous model is the LES+LPD approach. In this model, the carrier phase is modeled via LES, and the entities are tracked down by a Lagrangian approach. The forces on a particle have to be calculated using constitutive equations for Drag, Lift, etc., and the LES solution in the vicinity of the particle. Two-way coupling may be modeled as concentrated forces on the fluid in the point where the particle is located, converted into body forces in the corresponding grid cell for computational purposes.

An example of this approach as applied to bubbly flow in the wake of a surface ship, including clustering and coalescence effects, can be found in the work of Smirnov et al.[12].

DNS + Lagrangian Particle Dynamics

These models are just like the LES+LPD but with no subgrid scale model for turbulence. Again, the grid is assumed to be fine enough so as to capture even the smallest scales of the problem.

The applicability of these models to real engineering problems is almost impossible for now, due to the huge amount of computing power that they demand. Currently, the main use of these models is as substitutes of real multiphase experiments; they are usually less expensive to carry on (provided the computer power is already available) and provide enormous amounts of data, extremely useful for helping develop constitutive equations for other, more general, models.

Due to the fact that in LES models sub-grid scales of turbulence are only taken into account in a statistical sense, care should be taken when trying to simulate flows with very small particles, because the path taken by the particles would not be accurately simulated. In those

cases, full DNS simulations are to be preferred.

4.4 Mesoscopic or Microscopic models

Lattice Boltzmann Equations (LBE)

This method, due to McNamara & Zanetti[13], originates from the kinetic theory of gases. It can be classified as a mesoscopic approach, lying in between microscopic molecular dynamics and conventional macroscopic fluid dynamics methods. It is not to be considered a molecular approach, since the transported thing is not real molecules but a continuous molecular population function.

An analog of the integro-differential Boltzmann equation for particle dynamics is solved in a regular grid or lattice. Only discrete velocities in well defined spatial directions are allowed. Physical quantities of the macroscopic flow, such as the fluid density, are defined as moments of the molecular population function. Non-local interaction mechanisms may be introduced to model non-ideal gas equations of state.

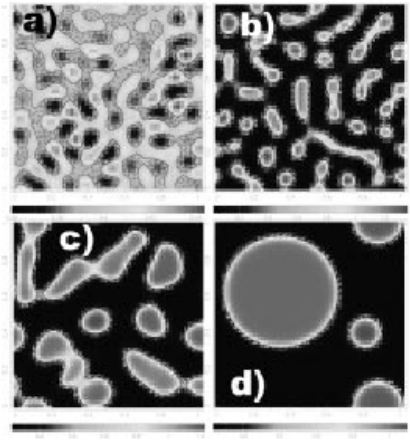


Figure 10: Fluid segregation process using an LBE model. Nourgaliev et al [14]

Monte Carlo Models

These models are based on the well known Monte Carlo method (see for example the work of Meiburg[15]). This is a probabilistic microscopic method that requires the averaging of many simulated experiments or realizations in order to get the solution to the macroscopic problem. Due to the requirements of computing power, these models are only adequate for simulating simple multicomponent flows.

5 CONCLUSIONS AND COMMENTS

A bird's eye view on the subject of modeling and simulation of multicomponent flows has been presented. The main features of this complex type of flows, and the most common models for simulating them, have been enumerated and briefly described. A global classification of the models into four categories, namely *Averaging*, *Surface Tracking*, *Entity Tracking*, and *Meso/Microscopic* models, has also been proposed. Some example applications due to other authors are also shown for some of the models. The 0-equation, descriptive approach to multicomponent models taken in the present work is not to be taken as a comprehensive review but as a first introduction to the subject for people with numerical experience but not specialized in multiphase or multicomponent flows.

6 REFERENCES

[1] Drew, D.A., Passman, S.L., *Theory of Multicomponent Fluids*, App. Math. Sci. vol 135, Springer-Verlag, 1999.

[2] Zuber, N., Findlay, J.A., *Average volumetric concentration in two-phase flow systems*, Journal of Heat Transfer, 453, 1965.

[3] Ishii, M., *Thermo-fluid dynamics theory of two-phase flow*, Eyrolles, 1975.

[4] Carrica P. M., Drew D., Bonetto F. & Lahey Jr. R. T., *A Polydisperse Model for Bubbly Two–Phase Flow Around a Surface Ship*, Int. J. Multiphase Flow, **25**. 257-305, 1999.

[5] Tomiyama A., *Struggle with computational bubble dynamics*, Third Intl. Conf. on Multiphase Flows, Lyon, France, June 8-12, 1998.

[6] Kelly, J.M., *A four-field approach toward developing a mechanistic model for multiphase flow*, Battelle, Pacific Northwest National Laboratories Report PNL-SA-18878, 1993.

[7] Siebert, B.W., Maneri, C.C., Kunz, R.F., Edwards, D.P., *A four-field model and CFD implementation for multidimensional, heated two-phase flows*, in Proceedings of the Second International Conference in Multiphase Flows, Kyoto, 1995.

[8] Smagorinsky, J., *General circulation experiments with the primitive equations: Part I. The basic experiment*, Mon. Weather Rev., 91, pp. 99-164, 1963.

[9] Manservisi, S., Popinet, S., Scardovelli, R., Zaleski, S., *Two front-tracking algorithms for 2D interface problems*, Third Intl. Conf. on Multiphase Flows, Lyon, France, June 8-12, 1998.

[10] Herrero, V., Guido Lavalle, G., Clausse, A., *Simulation of boiling environments using geometrical automata*, 1st Intl. Conf. on Heat Transfer, Fluid Mechanics, and Thermodynamics, Kruger Park, South Africa, April 8-10, 2002.

[11] Larreteguy A., Clausse A., *Properties of a 2D Field of Bubble-Resembling Geometrical Automata*, presented at MECOM'96, Tucumán, Argentina, September 10-13, 1996.

[12] Smirnov, A., Shi, S., Celik, I., *LES of a bubbly shipwake flow*, ASME 2001 Fluids Engineering Division Summer Meeting, , New Orleans, LA, USA, May 29th-June 1st

2001.
[13] Mc Namara, G.R., Zanetti, G., *Use of the Boltzmann equation to simulate lattice-gas automata*, Phys. Rev. Lett., v 61, 20, pp. 2332-2335, 1988.
[14] Nourgaliev, R.R., Dinh, T.N., Sehgal, B.R., *Numerical simulation of droplet deformation and break-up by a Lattice-Boltzmann Method*, Third Intl. Conf. on Multiphase Flows, Lyon, France, June 8-12, 1998.
[15] Meiburg, E., *Comparison of the molecular dynamics method and the direct simulation Monte Carlo technique for flows around simple geometries*, Phys. Fluids, v.29, p.3107.
[16] Hirt, C.W., Nicholls, B.D., *Volume of Fluid Method for the Dynamics of Free Boundaries*, J. Comp. Phys., 39, pp. 201-225, 1981.
[17] Johansen, S.T., *Large Scale Simulation of Separated Multiphase Flows*, Third Intl. Conf. on Multiphase Flows, Lyon, France, June 8-12, 1998.