Applicability of two-phase CFD to nuclear reactor thermalhydraulics and elaboration of Best Practice Guidelines

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Abstract

Two-phase Computational Fluid Dynamics (CFD) is now increasingly applied to some Nuclear Reactor thermalhydraulic investigations. A Writing Group of the OECD-CSNI-GAMA on the "Extension of CFD to two-phase safety issues" has identified a list of Nuclear Reactor Safety (NRS) issues for which the use of 2-phase CFD can bring a real benefit and proposed a general multi-step methodology. Various modelling options were identified and classified and some first Best Practice Guidelines (BPG) were proposed in the final report of the WG3. The purpose of this paper is to specify the methodology in more detail for the selection of model options, to discuss the conditions and limits of applicability of the various options. Four main modelling approaches are considered, the porous body approach, the RANS approach for open medium, the filtered methods, and the pseudo-DNS.

A classification of the modelling approaches is proposed with a nomenclature. The conditions of the consistency between the various choices and steps of the methodology are specified, including the coherence between turbulence and interface filtering, between averaging and formulation of the closure laws, and adequacy of the validation matrix. A list of frequent errors is given. A checklist for application of two-phase CFD to reactor thermalhydraulic issues is proposed.

1 INTRODUCTION

Two-phase Computational Fluid Dynamics (CFD) or Computational Multi-Fluid Dynamics (CMFD) is now increasingly applied to some Nuclear Reactor thermalhydraulic investigations. A Writing Group (WG3) of the OECD-CSNI-GAMA on the "extension of CFD to two-phase safety issues" has identified a list of Nuclear Reactor Safety issues for which the use of 2-phase CFD can bring a real benefit and proposed a general multi-step methodology. The various modeling options were identified and classified and some first Best Practice Guidelines (BPG) were proposed in the final report of the WG3. A progress of this activity was presented at the XCFD4NRS meeting in 2008.

The purpose of this paper is to go farther in the analysis on several points. First the methodology is specified in more detail for the selection of model options. This allows to proposing a classification of modelling approaches with a possible nomenclature. Then, the applicability of the general methodology and of the various model options to each two-phase flow regime is discussed. Four main modeling options are considered, the porous body approach with a homogenization technique, the RANS (Reynolds Averaged Navier Stokes) approach for open medium, the Large Scale Simulation methods (extension of the Large Eddy Simulation concept to two-phase flow simulation), and the pseudo-DNS approaches. Some limitations of each approach are identified and some important non-dimensional numbers are listed which may allow to classify the various situations.

Some pseudo-DNS approaches with Interface Tracking Methods are applied to some basic two-phase flow but CPU cost makes it prohibitive for industrial application. Therefore many attempts to use under-resolved DNS are made in some specific conditions. It is shown that the Large Scale Simulation methods are able to simulate some dispersed flow regimes as well as separate-phase flows, but they encounter many difficulties when trying to apply them to the full range of flow regimes, in particular when there is not a unique interfacial structure and when the associated scales cover a wide range. The RANS like methods can in principle be applied to all flow regimes but have also severe limitations for the most complex flow regimes. A hybrid LES method is also identified which could be applied to all flow regimes with some filtering of the larger interfaces. The porous body approach with a homogenization technique is used in component codes for 3D Core thermalhydraulic simulations. They combine difficulties of the CFD for open medium with the difficulties of the 1D models; they are still used with many simplifications which were not always even identified and listed. For each of these four modeling approaches, attention is drawn on some conditions and limits of applicability.

Some reference to the ERCOFTAC (European Research Community on Flow Turbulence And Combustion) Best Practice Guidelines on Dispersed Turbulent Multi-Phase Flow are made which provide some BPGs. The conditions of the consistency between the various choices and various steps of the methodology are specified, including the coherence between turbulence filtering and interface filtering, between averaging procedure and formulation of the closure laws, and adequacy of the validation matrix with the selected model options. Since non-consistencies in the modeling options are not so rare, a list of frequent errors is given.

A checklist of Best Practice Advice for application of two-phase CFD to reactor thermalhydraulic issues is proposed.

2 METHODOLOGY FOR APPLICATION OF TWO-PHASE-CFD TO NUCLEAER REACTOR SAFETY

2.1 The methodology

The general method of work illustrated in Figure 1 was proposed (Bestion et al., 2006, Bestion et al., 2009a) for using two-phase CFD for safety issues with successive steps:

1. Identification of all important flow processes
2. Main modelling choices

  - 2.1 Selecting a basic model
  - 2.2 Filtering turbulent scales and two-phase intermittency scales
  - 2.3 Treatment of interfaces
3. Selecting closure laws
  - 3.1 Modeling interfacial transfers
  - 3.2 Modeling turbulent transfers
  - 3.3 Modeling wall transfers
4. Verification
5. Validation

If the CFD tool is used in the context of a nuclear reactor safety demonstration using a Best-Estimate approach, one may add a last step:

6. Uncertainty evaluation

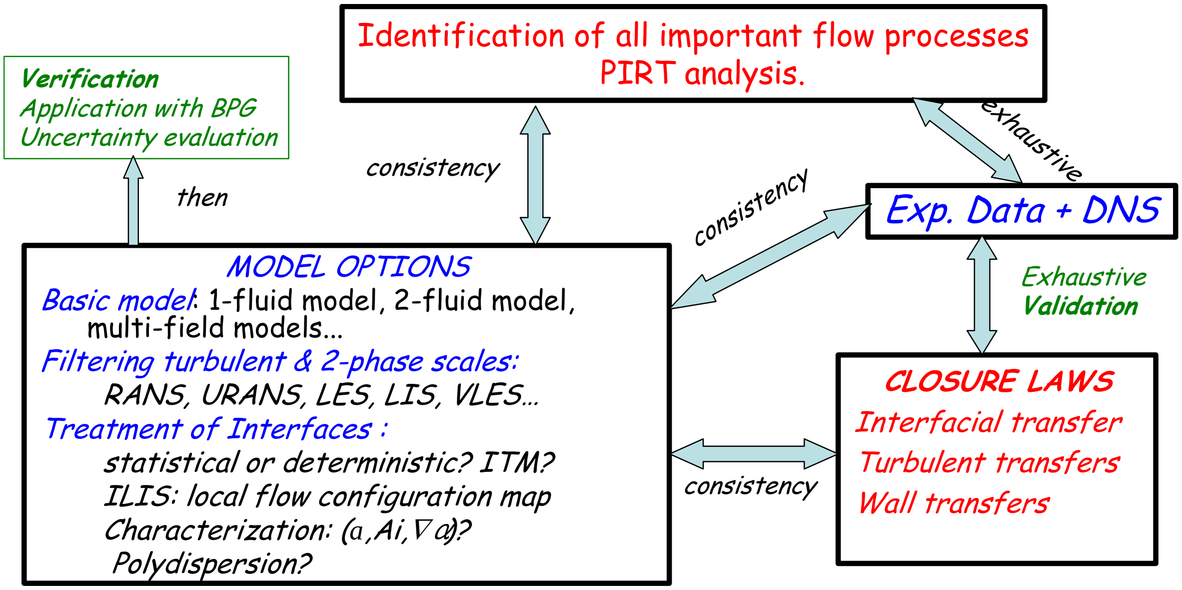


Figure 1: General methodology for two-phase CFD application to nuclear reactor safety

2.2 Identification of all important flow processes

The reasons of this first step are explained by the report of the OECD-CSNI WGAMA WG3 (Bestion et al, 2010). However one must be more specific on the content of this step. The various basic flow processes to be identified may be part of the following non exhaustive list: wall heat transfer, mechanical load on structure, turbulent mixing of momentum, of heat or of another scalar, interfacial friction (or more generally interfacial momentum transfer), interfacial heat and mass transfer by condensation or vaporization, interfacial mass transfer by dissolving or degassing of a noncondensable gas, flow instability, etc. One of the identified processes may be the actual issue of interest but all other processes which may influence the issue have also to be listed.

Then, based on the analysis of some experimental data and on some reflections made in a preliminary brainstorming or during a PIRT exercise, one should try to answer the following questions:

- What kind of two-phase flow regime(s) is (are) likely to be present? In particular, how many separate fields are expected? One may consider two-phase flow regimes as various combinations of continuous liquid field, continuous gas field, and dispersed fields such as bubbles and droplets.
- Is it a steady or transient situation? Since all turbulent flows and two-phase flows have inherent flow parameter variations with time associated to eddies and interface movements, all are somewhat transient but one should identify the time scales of interest. Are there time scales of flow parameter variations which play a role in the process of interest? (For example large scale eddies may play a role in thermal striping and thermal fatigue investigations whereas in many other problems the simple average mixing effect of turbulence has to be considered)
- What is the minimum space scale of interest in the process? This defines the space resolution of the simulation which is required for solving the issue.
- What is the basic phenomenon or physical process of interest?
- What are all the other physical processes which are coupled with or which influence the basic process of interest?
- What are the main non-dimensional numbers which characterize the important flow processes?

3 CLASSIFICATION OF THE TWO-PHASE-CFD MODEL OPTIONS

3.1 Need of a better classification

Some attempts to classify the various model approaches were already proposed in the OECD-CSNI WGAMA WG3 reports (2006, 2010). Classification was made on the following aspects:

- Phase averaging or field averaging:
  - Homogeneous for a two-phase mixture
  - Two-fluid model
  - Multi-field models
- Filtering turbulent scales and two-phase intermittency scales:
  - All turbulent scales are filtered (RANS models)
  - Only some scales are filtered (two-phase LES)
  - All turbulent scales are predicted (DNS)
- Treatment of Interfaces
  - Use of Interface Tracking/Capturing Technique
  - Use of a pure statistical treatment of interfaces
  - Use of an Identification of the Local Interface Structure (ILIS)
  - Characterization of the interfaces through Interfacial area density or other quantities

However one would prefer a classification which shows the successive choices with the arborescence of all possible resulting approaches. One may try to give a more detailed classification by considering (see Table 1) all treatments of the basic local instantaneous equations for mass (continuity equation), momentum (Navier-Stokes equation), and energy, which are used in the various Eulerian modelling approaches. The selection of the respective approaches can be made by considering 5 successive choices:

1. Open medium approach or homogenizing technique for porous body? Is there a multiplication of basic equations by a fluid characteristic function?
2. How many fields are distinguished? Is there a multiplication of basic equations by a phase characteristic function or field characteristic function?

3. Time averaging or ensemble averaging?
4. Space averaging or filtering
5. Deterministic interface, filtered interface or statistical interface?

3.2 Open medium approach and porous body approach

One may distinguish the open medium and porous medium approaches. A simple way to introduce these differences is to consider that local instantaneous equations are first multiplied by fluid/solid characteristic function before any averaging or filtering.

Let χ_f (x,t) be the fluid/solid characteristic function

χ_f (x,t) = 1 when point x is in the fluid at time t

χ_f (x,t) = 0 when point x is in the solid at time t

In case of a flow bounded by non deformable solid structures, χ_F is not function of time.

A Volume average of A is defined as:

$$\boxed{< A > (x,t) \cong \frac{1}{V(x)} \int_{V(x)} A(y,t) dV(y)}$$

A Volume average of χ_f is the so-called porosity factor:

$$\boxed{\phi \cong < \chi_f > = \frac{V_f}{V}}$$

In the classical porous body approach, after multiplication by χ_f, equations are averaged over a fluid volume as follows:

$$\boxed{< A >_f (x,t) \cong \frac{< \chi_f A >}{< \chi_f >} = \frac{1}{V_f(x)} \int_{V(x)} A \chi_f dV}$$

Then every local fluid parameter A may be considered as an average plus a space deviation:

$$\boxed{A \cong < A >_f + \delta A}$$

3.3 The number of fluids or fields

One can separate the two-phase flow in several fields:

- 1-fluid for a model which considers a mixture of the two-phases together
- 2-fluid for a model which considers the two-phases separately
- n-field for a model which splits one or both phases in several fields.

Multi-fields model are commonly on the type 2+nb+nd with two continuous fields (continuous gas and continuous liquid) + one or nb bubble fields and 1 or nd droplet fields.

The way to introduce these differences is to consider that local instantaneous equations are multiplied by fluid/field characteristic function before any averaging or filtering.

Let χ_k (x,t) be the fluid characteristic function for phase k or field k (k=1,n)

χ_k (x,t) = 1 when point x is in the phase k or field k at time t

χ_k (x,t) = 0 when point x is not in the phase k or field k at time t

One can multiply also by the product χ_k . χ_f for a multi-field model in a porous body approach.

After averaging of the basic equations multiplied by χ_f , or χ_k . χ_f for k = 1, n, the three balance equations (mass, momentum and energy) are written n times one for each phase or field.

3.4 Time averaging and space averaging

Time or ensemble averaging is a common way to derive equations for the so-called RANS (Reynolds Average Navier-Stokes) approach.
Although time averaging and ensemble averaging are different, they can be reasonably considered as equivalent (ergodicity) in steady or quasi-steady flows where the RANS approach is applied.
Time averaging filters all turbulent scales and predicts only a mean velocity field. Time averaging does not allow for the prediction of the space and time position of the interfaces of dispersed droplets and dispersed bubbles. It has also a smearing or diffusive effect on the large interfaces between continuous liquid and continuous gas such as a free surface or the surface of a liquid film along a wall. It is possible to reconstruct a steep large interface by numerical techniques (see Lucas et al., 2009) but waves have disappeared as shown in Figure 2.

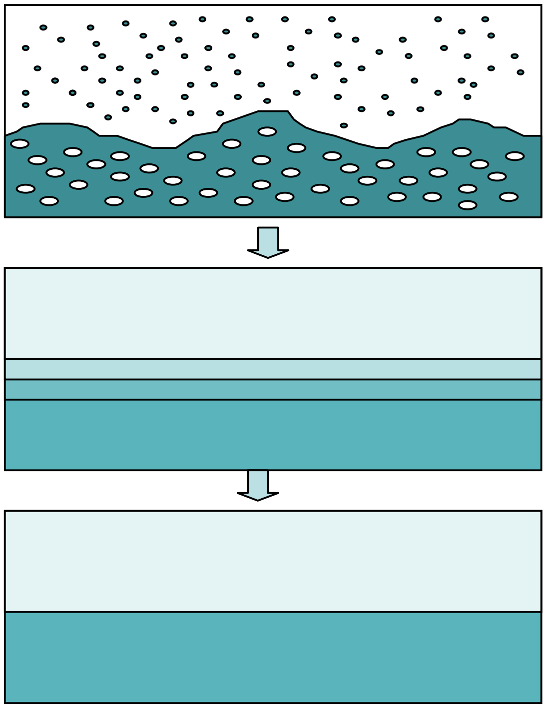


Figure 2: Effect of a time averaging on a two-phase flow: on top the real flow; in the center the averaged flow; at bottom the filtered flow with a reconstructed free surface

Space averaging is necessary in the porous body approach after having multiplied equations by the fluid/solid characteristic function and possibly also by the fluid (or field) characteristic function.
Space averaging or filtering is also used in the so-called Large Eddy Simulation (LES) of turbulent flows in an open medium context. This technique becomes now increasingly applied in single phase CFD to be able to simulate some transient flow or to predict large scale coherent structures. The filter scale defined the part of the turbulence spectrum which is simulated and the part which must be modelled.
Space averaging in two-phase flow filters not only the small eddies but also the interfaces and the density discontinuity is smeared or diffused and replaced by a surface local density gradient. It is possible to reconstruct a steep interface by numerical techniques but small scale deformations of the interface may have disappeared as shown in Figure 3.

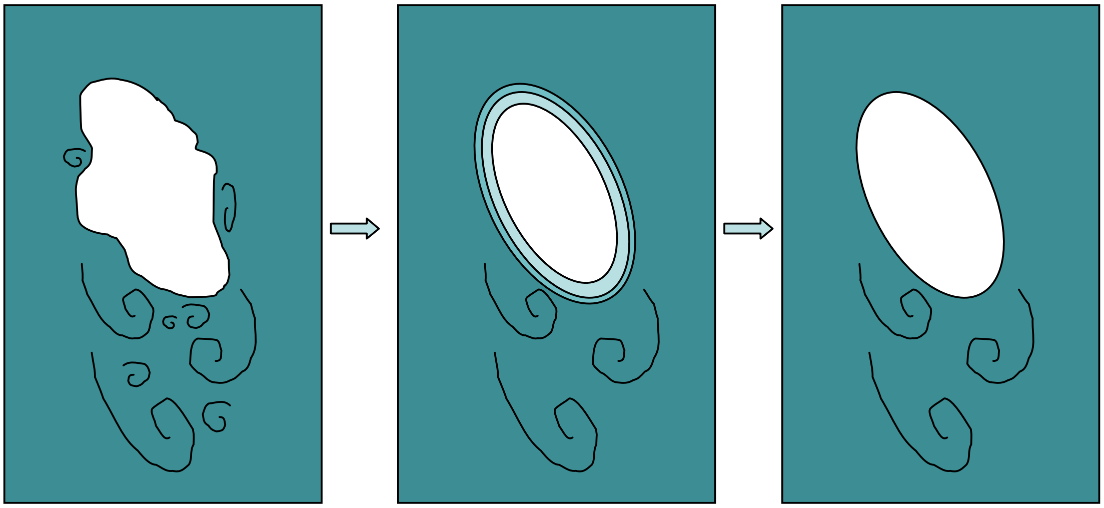


Figure 3: Effect of a space filter on a two-phase flow: on left the real flow, in the center the filtered flow; on right the filtered flow with a reconstructed interface

3.5 Deterministic interface, filtered interface or statistical interface

An interface will be said “**deterministically treated**” when its space and time position is simulated or actually predicted without any simplification. It is clearly the case of a DNS or pseudo-DNS modelling where neither space nor time averaging is used. The flow in the left on Figure 3 is predicted will all eddies and all small deformations of the interface.

An interface can also be considered as “deterministically treated” after a space filtering if the reconstructed interface (see figure 3) is not degraded compared to the real interface. A “deterministic interface” requires that all phenomena having an influence on space and time position of the interface, are also simulated. The conditions for this are specified below in the section on LES with Deterministic Interfaces.

An interface will be said “**Statistically treated**” when an averaging or filtering procedure does not allow to predict its space and time position. Only statistical or averaged information on several interfaces may be predicted through quantities such as a void fraction, or an Interfacial area density. Such a statistical treatment may result from time averaging or from space averaging.

An interface will be considered as “**Filtered Interface**” when its space and time position is predicted with some filtering of the smaller scale deformations. Cases illustrated in Figures 2 and 3 are filtered interfaces. This filtering may result either from space filter or from time averaging.

3.6 A possible terminology for Eulerian Two-phase CFD approaches

Following the 5 choices above one may propose a terminology for Eulerian two-phase CFD approaches.

The nomenclature is a series of 4 groups of characters: **MM-nF-TT-II**

MM can be:

- **OM** for Open medium approach
  - **PM** for 3D porous medium approach
  - **1D** for area-averaged 1D models in ducts, channels, sub-channels
  - **2D** for 2D models using a space averaging in the 3rd direction

The latter case does not apply to 2D models which use some symmetry in a 3D flow to reduce the dimension to 2. It applies for example to a 2D modelling of an annular dowcomer of a reactor vessel when equations are averaged over the radial direction, keeping a 2D problem in vertical and azimuthal directions (Z, θ).

- **nF** is the number of fluids or fields**:**

  - **2F** for the classical two-fluid approach
  - **nF** for a n-field model
  - **nG/pL** for n gas fields and p liquid fields (if one wants) to be more precise on the number of fields in each phase
- **TT to characterize the filtering of turbulent scale:**
  - **DN** for Direct simulation of the whole turbulence spectrum
  - **RA** for Reynolds Average approach
  - **FT** for filtered turbulence like LES, DES, …
- **II to characterize the treatment of interfaces:**
  - **DI** for Deterministic Interface using an Interface Tracking Technique
  - **SI** for Statistical treatment of Interfaces
  - **FI** for filtered Interfaces: an Interface Tracking or reconstruction Technique is used but it does not predict smaller scale deformations of this interface
  - **FI/SI** for hybrid methods where the larger scale interfaces are known by an Interface Tracking or reconstruction Technique and the smaller scale interfaces are only statistically treated

Table 1: Classification of Eulerian Fluid Dynamic Simulation approaches for Two-Phase Flow

OM: Open medium approach PM: Porous medium approach 1F: one-fluid 2F: two-fluid DS: Direct Simulation FT: Filtered turbulence
FI: Filtered Interface DI: Deterministic Interface SI: Statistical Interface RA: Reynolds Averaged

	Treatment of local equations	**Pseudo DNS**	**Filtered approaches**			**RANS 2-fluid**	**Component codes System codes**		
Open medium/ Porous medium	Multiplied by fluid/solid characteristic functions	No	No	No	No	No	Yes	No	No
Nb of fields	Multiplication by field characteristic functions	No	No	Yes 2-fluid n-field	Yes 2-fluid n-field	Yes 2-fluid n-field	Yes 2-fluid n-field	Yes 2-fluid n-field	Yes 2-fluid n-field
RANS?	Time or ensemble averaging	No	No	No	No	Yes	Yes	Yes	Yes
LES?	Space averaging	No	Yes	Yes	Yes	No	Yes Volume averaging	Yes Space averaging	Yes 1D averaging
LIS? Statistical/ deterministic/ filtered Interfaces	ITM or Interface Recognition	Yes	Yes ITM	Yes IR	No	No	No	No	No
Type of CFD	Possible terminology with Acronyms	**OM-1F-DS-DI**	**OM-1F-FT-DI**	**OM-2F-FT-FI/SI** **OM-nF-FT-FI/SI**	**OM-2F-FT-SI** **OM-nF-FT-SI**	**OM-2F-RA** **OM-nF-RA**	**PM-2F** **PM-nF**	**1D-2F** **1D-nF**	**PM-2D-2F** **PM-2D-nF**
		Pseudo DNS	**LES with deterministic interfaces**	**Hybrid LES With filtered & statistical interfaces**	**LES with statistical interfaces**	**RANS**	**Porous medium approach**	**1D**	**2D**

4 THE PSEUDO-DNS APPROACH OM-1F-DS-DI

The DNS or pseudo-DNS does not apply any space or time averaging of the equations. However some additional equation or numerical treatment is required to track the interface and to add the physics of the liquid-solid interface or of a triple line (liquid-solid-gas). There is no need to solve equations for several fields and a 1-fluid approach is generally used with some additional equation or technique to track the interface position. Additional models are often required for example for implementing a film splitting criterion when two bubbles coalesce or for the contact angles at a triple line solid-liquid-gas. Such additional models are the reason why in two-phase flow the word DNS must be replaced by pseudo-DNS since some very small scale physics is not solved but only modelled.

Since no averaging or filtering is used, pseudo-DNS should be able to predict the smaller scale eddies (up to the Kolmogorov dissipative scale), the smaller scale interface deformations and smaller scale distance between interfaces. This would be extremely difficult for liquid films between two bubbles when they collide before coalescence since it would require mesh sizes in the order of the micrometer. Therefore such very thin films are often not predicted to allow larger mesh sizes. It may affect the prediction of some phenomena such as coalescence or break up phenomena but we will still consider that such extension still belongs to the pseudo-DNS approach.

Pure DNS solving only exact equations without any modelling does not exist in two-phase flow and pseudo-DNS techniques also have to be validated against experimental data to see how the models and the simplifications affect the predictions.

Since even pseudo-DNS require extremely expensive CPU cost, its use is restricted to the investigation of very small scale flow processes as a complement to experimental investigations and as a support for the modelling and validation of more macroscopic approaches.

5 THE RANS APPROACH

This is the most simple, the cheapest (in terms of CPU), the most advanced and the most used available two-phase CFD method. The RANS approach for two-phase flow consists in applying an ensemble averaging or a time averaging which filters all turbulent scales and all two-phase intermittency scales. The method is applied to steady flows or quasi-steady flows when the time scales of variation of mean variables are larger than the largest time scales of turbulence and two-phase intermittency.

The Figure 4 below illustrates how a two-phase flow is simplified by a RANS like approach.

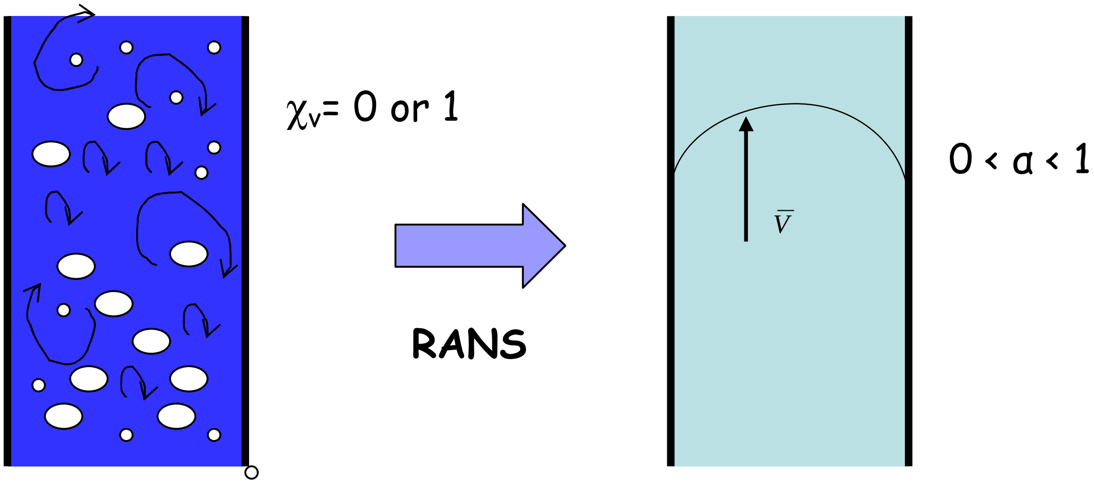


Figure 4: Illustration how a RANS like approach simplifies a two-phase flow

No velocity fluctuation is predicted and only time averaged velocities are solved. The presence of interfaces is treated statistically by averaged parameters such as the void fraction or the interfacial area density.

Compatibility of RANS with flow regimes

RANS is in principle compatible with all two-phase flow regimes provided that they are steady or quasi-steady. The condition is that the time scale of mean flow variations is significantly larger than the time scales of turbulence and two-phase intermittency (time between passage of two interfaces at a given point).

For dispersed bubbly flow (see Bestion, Anglart et al., 2009b) or dispersed droplet flow, the condition is easy to satisfy.

For separate-phase flows (stratified flow, annular flow), the averaging filters interfacial waves in a way which is not fully clear: although the modelling of turbulent diffusion prevents simulation of large eddies it does not prevent irrotational waves to be predicted resulting from Kelvin-Helmholtz instability.

For slug and churn flow regimes with large bubbles (either Taylor bubbles in slug flows or distorted large bubbles) the intermittency due to the passage of these bubbles corresponds to rather large time scales. Since the RANS filters even these large scales it is not able to predict this intermittency.

Compatibility of RANS with the number of fields

RANS is compatible with all the possible choices for the number of fields, including single-fluid, two-fluid and all kinds of multi-field models.

Compatibility of RANS with interface treatments

Due to the time (or ensemble) averaging, RANS is not compatible with a deterministic treatment of interfaces since interface movements and deformations are influenced by eddies which are not simulated by the RANS approach.

RANS is fully compatible with the statistical treatment of interfaces.

RANS is also compatible with some “Filtered Interface” for some large interfaces as shown in Figure 2 with a free surface which is parallel to the mean flow velocity (Coste et al. 2008).

6 THE LES WITH DETERMINISTIC INTERFACES

The LES with Deterministic interface (OM-1F-FT-DI) combines a filtering of turbulent fluctuations with an Interface Tracking method used for all interfaces. This method was developed and used by Bois et al (2010), Toutant et al. (2009a, 2009b), Magdeleine (2010), Lakehal (2008a, 2008b), in both dispersed flow and free surface flows.

A “deterministic interface” requires that all phenomena having an influence on space and time position of the interface are also simulated. The smaller scale deformations of the interfaces are influenced by the turbulent fluctuations and the surface tension.

A limiting value of a Weber number should define the limits of applicability of LES together with a Deterministic Interface.

$$We = \frac{\rho\, v(l)^2\, l}{\sigma} \le We_{\lim}$$

$v(l)$ is the velocity scale of turbulent fluctuations for eddies of size equal to l.

For a given turbulence spectrum it may give a maximum value of the filter scale lfliter:

$$l_{filter} \le We_{\lim} \frac{\sigma\, v(l_{filter})^2}{\rho}$$

For a given filter scale l_{fliter} the maximum value of the turbulent fluctuating velocity $v(l)$ at scale l_{fliter} is:

$$v(l_{filter}) \leq \sqrt{We_{\lim} \frac{\sigma}{\rho\, l_{filter}}}$$

Another limit, which is often less restrictive, is related to the Laplace scale:

$$l_{filter} \leq \frac{1}{n} \sqrt{\frac{\sigma}{g\, \Delta\rho}}$$

This Laplace scale is related to the smallest wavelength of free surface waves (capillary waves) or film waves when there is no high turbulence intensity. The required value of n (probably in the range 5 to 10) should be determined.

Finally, if there are very small bubbles much smaller than the Laplace scale, e;g. in boiling flow, the filter scale should allow a good description of the interfaces of these smallest bubbles of diameter d_{min}, which results in a severe limitation:

$$l_{filter} \leq \frac{1}{m} d_{\min}$$

According to Magdeleine (2010), m can be taken as 6 at best without degrading the results.

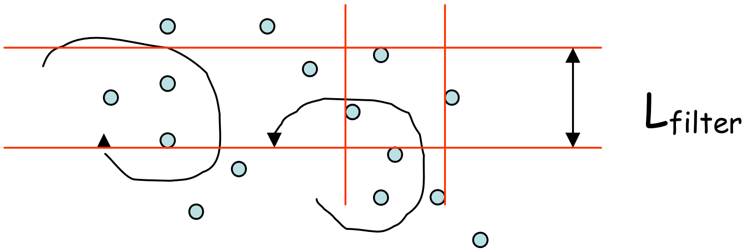
All these limitations make this “LES with Deterministic Interface“ method less CPU consuming that pseudo-DNS (up to 1 or 2 orders of magnitude) but still rather expensive. It is still used as a research tool as a support for the modelling and validation of more macroscopic approaches and cannot address a real industrial problem.

7 THE LES WITH STATISTICAL INTERFACES

When the largest two-phase intermittency scale is rather short and significantly shorter that the largest turbulent eddies (see Figure 5), a LES method is applicable with a filters scale smaller than the larger eddies but larger than the two-phase scale to allow a statistical treatment (OM-nF-FT-SI). This was already applied with some success to some turbulent dispersed flow by Dhotre et al. (2007) and Niceno et al. (2009).

These authors have applied the so-called Milleli criterion about the smallest l_{filter} scale, d_{min} being the smallest bubble or droplet size.

$$l_{filter} > 1.5\, d_{\min}$$



Figurer 5: A dispersed flow treated by a LES with statistical Interfaces

Such a method is clearly much less CPU consuming than the pseudo-DNS and the LES with deterministic interface but it is restricted to some flow situations, typically the dispersed bubble or dispersed drops where the large eddies are much larger than the largest bubbles or eddies. In slug or churn flow where the largest bubbles and the largest eddies are of the size of the geometrical dimensions of the flow (such as a Hydraulic diameter) this method is clearly not applicable.

This method is compatible with the two-fluid model and multi-field models where the dispersed bubbles or droplets may be treated by size groups.

8 THE HYBRID LES METHOD WITH BOTH FILTERED AND STATISTICAL INTERFACES

Looking for a method which may address all flow regimes with a more reasonable CPU cost than the pseudo-DNS and the LES methods above, one may imagine a hybrid method which filters the smaller eddies and treats statistically the small droplets or bubbles while the other interfaces are simply filtered (OM-nF-FT-FI-SI). This is illustrated in Figure 6. the space filter eliminates the smaller bubbles which are treated statistically, and it thickens and filters the interface of the large bubble which may be reconstructed with a simplification of the shape as on the right side view.

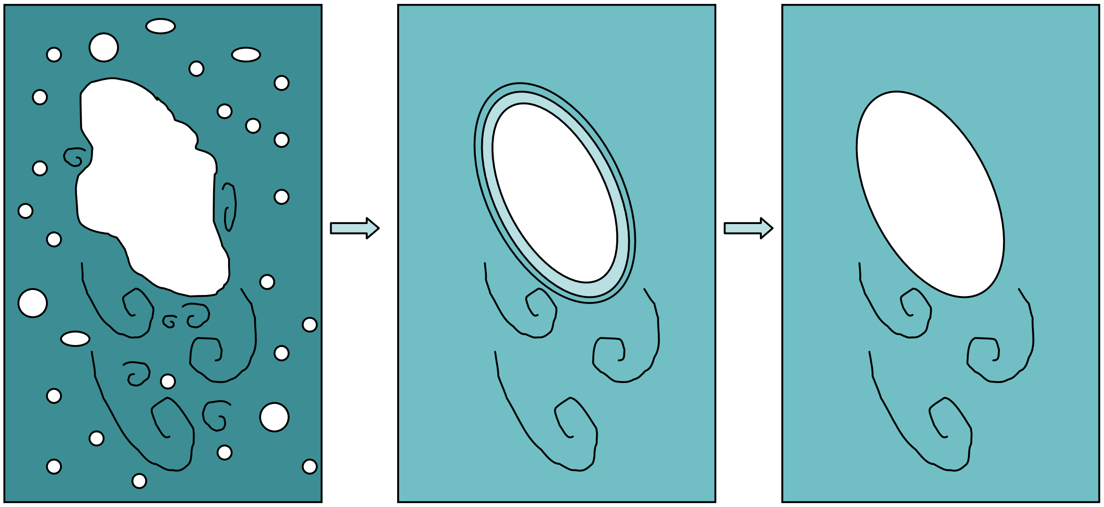


Figure 6: Treatment of a two phase flow with a hybrid LES method

Although this method has not been clearly defined and applied, some analyses with a two-fluid model without any turbulence model may be somewhat similar to it (Bartosiewicz et al., 2007, 2008).

It may be a promising way of modelling the most complex two-phase flow (such as churn or slug flow) at a reasonable CPU cost without filtering the two-phase structures like RANS does. However the closure issue is rather complex and the present state of the art is not very well advanced.

This method is compatible with the two-fluid approach and with multi-field models. A 4-field model with a continuous gas field, a continuous liquid field, a dispersed bubble field and dispersed droplet field may be help to reconstruct the large filtered interfaces.

9 THE CFD IN POROUS MEDIUM APPROACH

The CFD in porous medium approach uses a space averaging or filtering of time averaged basic equations multiplied by χ_f or by the product $\chi_k \cdot \chi_f$ as defined in section 3.2 above. It is adapted to the macroscopic 3D description of two-phase flow in reactor components such as the Core or the Steam Generator. The minimum filter scale in such components is the subchannel scale. This approach is used with some simplifying assumptions in the component codes for Core and SGs.

Due to the time averaging, additional terms such as Reynolds stresses $\overline{u'_i u'_j}$ or turbulent diffusion of heat $\overline{u'_i \theta'}$ appear in balance equations. Due to space filtering, dispersion terms of momentum and energy (related to <δui δuj> and <δui δθ>) appear in the equations which would require some modelling.

In the present state of the art, no modelling of dispersion terms exists and only very simple turbulent diffusion models are used.

This method is compatible with the single-fluid model, the two-fluid model, and any kind of multi-field model. In the nuclear community, the most complex models are using the 3-field model with a gas field a continuous liquid and a droplet field, which is adequate for annular mist flows.

10 THE CLOSURE ISSUE AND THE SELECTION OF THE VALIDATION MATRIX

10.1 The wall transfers

Momentum and energy transfers at the wall have to be modelled for all CFD approaches except for the pseudo-DNS. The number of models is multiplied by the number of fields.

The so-called wall function approach is generally used to avoid the use of too fine nodes in the boundary layer close to the wall. Such wall functions exist for single phase and some progress was made to extend to two-phase situations (see Koncar et al., 2008).

10.2 The interfacial transfers

A two-fluid model requires a modelling of mass, momentum and energy interfacial transfers.
A multi-field model requires a modelling of mass, momentum and energy interfacial transfers for all types of interfaces. In a 2+nb+nd model there are 1 + nb + nd interfaces:

- 1 interface between continuous liquid and continuous gas
- nb bubble interfaces (1 interface between each bubble field and the continuous liquid)
- nd droplet interfaces (1 interface between each droplet field and the continuous gas)

For interfaces of dispersed fields (bubbles and droplets), some models exist which have a reasonable degree of reliability (see some information in ERCOFTAC 2007 document). For large interfaces like a free surface some models were also developed (Coste et al, 2008, Lakehal et al. 2008).

10.3 The inter-field mass transfers

In case of a multi-field model mass transfers between the fields belonging to the same phase are needed.

In a 4-field model with a continuous gas field, a continuous liquid field, a dispersed bubble field and dispersed droplet field there are only two possible transfers:

- between continuous liquid and droplet field by entrainment and deposition
- between continuous gas and bubble field by bubble capture and bubble bust at a free surface

In a 2+nb+nd model there are nb! + nd! possible mass transfers. This includes the same transfers as above for each dispersed field plus the mass transfers between each couple of droplet field and between each couple of bubble fields by coalescence and break up.

There is some experience in modelling of such mass transfers in the MUSIG method applied to polydispersed bubbly flow (see Krepper et al., 2009, Morel et al., 2009) with a rather large number of bubble fields.

There is also some experience in the modelling of entrainment and deposition of droplets in annular-mist flow described with a 3-field model.

10.4 The turbulent transfers

Both time (or ensemble) averaging in the RANS approach and space averaging in the LES approaches require a modelling of second order moments of fluctuations such as $\overline{u'_i u'_j}$ or $\overline{u'_i \theta'}$. All the existing types of turbulence modelling developed for single phase flow (k-ϵ, Rij- ϵ, LES,…) haven been extended to two-phase flow with a lower maturity and a lower degree of reliability. Some information is available for dispersed flow in the ERCOFTAC (2007) document.

10.5 Additional models for filtered interfaces

In the filtered interface approach such as used in a RANS modelling of stratified flow (see Figure 2), or in the hybrid LES method illustrated in Figure 6, a large interface can be reconstructed from the available information (void fraction, void fraction gradient, …) but many possible processes related to the interface are not predicted which require some modelling:

- Waves at the interface created by filtered pressure and velocity fluctuation
- Capture of bubbles by some phenomena like the breaking waves
- Entrainment of droplets by splitting of the large filtered interface

For example the presence of waves at a free surface which are not seen by the filtered interface must be taken into account for their effects on the momentum transfers and heat and mass transfers. The waviness acts as a roughness which increases interfacial friction and enhances also heat and mass transfers (see Coste et al, 2010).

10.6 Identification of the Local Interfacial Structure (ILIS)

The formulation of interfacial transfers depends on the local structure of interfaces. If we consider the point M at location x at time t, the local interfacial structure in the vicinity of M may be:

1 Dispersed bubbles
2 Dispersed droplets
3 Presence of a large interface between continuous liquid and continuous gas
4 Same as 3 + droplets in continuous gas and or bubbles in continuous liquid

In case of a 4 field or 2+nb+nd multi-field model, the knowledge of the local volume fraction of each field is sufficient to know the local structure at M(x,t) and there is no ambiguity to select the adequate interfacial transfer models.

In the case of a two-fluid approach or even a single-fluid approach, the local structure has to be determined from the more limited available local information, void fraction, interfacial area, void fraction gradient. An ILIS is required which is the equivalent of the flow regime map for 1D models. No reliable published ILIS exists for the two-fluid model with an automatic recognition of all possible local interfacial structures and this may be a difficulty for some specific cases such as a plunging jet (see Schmidtke & Lucas, 2008).

10.7 Selection of the validation matrix

Both Separate Effect Tests (SET) and Mixed Effect Tests (MET) are required for the validation of a CFD model applied to a safety issue.

The SET and MET validation matrix should cover all important flow processes identified during the first step of the methodology.

The SET validation matrix should ideally be able to validate each important closure law in a separate effect way. The number of measured flow parameters in SET should be sufficient to allow a validation of each important closure law.

The SET and MET validation experiments should cover ideally the range of the non-dimensional numbers which are expected to play an important role.

The instrumentation in the validation tests should provide enough information to get initial conditions and boundary conditions for the simulation.

11 CONSISTENCY IN APPLICATION OF THE METHODOLOGY

11.1 Consistency checks

During the successive steps of the general methodology, several choices are made which require some consistency. One can list a few required consistency checks:

- This basic choice of the number of fields must be adapted to the physical situation or to an acceptable degree of simplification of the situation. In particular, if the specific behavior of two fields plays an important role according to the PIRT, they must be treated separately.
- The experimental SET validation matrix should be exhaustive with respect to all identified flow processes.
- The experimental SET validation matrix should be able to validate all the interfacial turbulent and wall transfers.
- In the ideal case the number of measured flow parameters in the validation experiments should be consistent with the complexity of the selected model to validate. A model defined by a set of n equations having a set of principal variables Xi (i = 1, n) can be said “validable” when one can measure n parameters giving the n principal variables.
- The averaging procedure must be specified to give a clear definition of the principal variables and of the closure terms in the equations. The filtering of the turbulent scales and of two-phase intermittency must be fully consistent.
- The averaging of measured variables must be consistent with the averaging of the equations.
- A Deterministic Interface using an Interface Tracking Method requires that all phenomena having an influence on the interface are also simulated or deterministically treated.
- The choice of an adequate interfacial transfer formulation must be consistent with the interface treatment (deterministic, filtered, statistical), and with the ILIS.

11.2 Some frequent errors or defaults

Due to the availability of many modelling options in commercial CFD codes such as FLUENT, STAR-CD, CFX, or in CFD codes specific to the nuclear community such as NEPTUNE_CFD (Bestion & Guelfi, 2005, Guelfi & Bestion, 2007), it may happen that some non-consistent choices are made. Most errors are relative to non consistent choices of space and/or time resolution for interfacial, wall, and turbulent transfer modelling. A few examples of frequent errors are given here:

1. *Use of a 1D model for modelling interfacial transfer in CFD approaches*

The interfacial transfer formulation in a 3D modelling relates a local flux F_x of a quantity X to a difference between local phase variable X_k multiplied by a local transfer coefficient : C_x

$$F_x^i = C_{x3D}^i \left[X_l - X_v \right]$$

The interfacial transfer formulation in a 1D modelling relates an area averaged flux F_x of a quantity X to a difference between area averaged phase variable X_k multiplied by a global transfer coefficient C_x:

$$\left\langle F_x^i \right\rangle = C_{x1D}^i \left[\left\langle X_l \right\rangle - \left\langle X_v \right\rangle \right]$$

Even if the flow remains unidirectional, e.g. in a pipe, there is no reason that $C_{x3D}^i = C_{x1D}^i$ and the difference between them can of several orders of magnitude. It would be exact only in case of uniform fields of X_l and X_v which cannot be the case in a 1D model since area averaging contains boundary layers along walls in which all variables have generally strong gradients.

2. *Use of interfacial transfers of porous medium model in a open medium approach*

This is the same type of errors as for the previous case. In the porous medium approach, the transfer is volume averaged in a space domain which contains boundary layers along solid structures in which all variables have generally strong gradients.

3. *Use of wall transfers of porous medium model in a open medium approach*

This is a similar error to the previous one. In the porous medium approach, the wall transfer terms are homogenized due to the volume averaging in a space domain which contains solid structures. In an open medium approach transfers with walls generally use the wall function approach.
The wall transfer formulation in an open medium approach relates a wall flux Fwx of a quantity X to a difference between local variable Xk and the value at the wall Xk multiplied by a local transfer coefficient: Cx

$$F_x^w = C_x^w \left[X - X_w \right]$$

The wall transfer formulation in a porous medium approach relates a volume averaged flux Fx of a quantity X to a difference between volume averaged phase variable <Xk> and the value at the wall multiplied by a global transfer coefficient Cx:

$$\left\langle F_x^w \right\rangle = C_x^w \left[\left\langle X \right\rangle - X_w \right]$$

Here again the difference between the two transfer coefficients can be of several orders of magnitude both wall friction and wall heat transfers.

4. *Use a 3D two-fluid model without any turbulence modelling*

The two-fluid model includes a time averaging over a long period of time covering all two-phase intermittency scales. Therefore all or part of the turbulence spectrum is filtered by this averaging process and this results in additional terms in momentum and energy equations for turbulent stresses (Reynolds stresses) and for turbulent diffusion which require adequate modelling.
In the case of a heated pipe with a two-phase flow, only the fluid meshes along the wall could be heated correctly by the wall but the transfer to the core flow can only be correctly described by a turbulent transfer model in energy equations.

5. *Use of averaged interfacial transfer coefficients in a DNS or LES approach*

This is the same inconsistency as the previous one but in a different context. The intention is here to have a fine resolution simulation with an Interface Tracking Technique for a deterministic treatment of interfaces. In absence of adequate modelling of interfacial friction of interfacial heat transfer,

12 CHECKLIST FOR APPLICATION OF TWO-PHASE CFD TO REACTOR THERMALHYDRAULIC ISSUES

The following checklist is proposed for application of two-phase-CFD to a nuclear reactor issue. They correspond to the successive steps of the methodology presented in section 2 and they can be grouped in the following way.

A: Identification of important flow processes

1. What is the basic process of interest in my reactor issue that I would like to predict by CFD (e.g. fluid temperature field in a component, clad temperature, a local heat transfer, a mechanical load on some structure, a velocity field in a component, a system peak pressure…)?
2. What are all the other important basic processes which are coupled to the process of interest?
3. What are the main non-dimensional numbers which characterize the important flow processes?
4. What is the space and time domain of interest for the coupled processes?
5. What kind of two-phase flow regime(s) is (are) likely to be present in the domain of interest? In particular, how many separate fields are expected?
6. Is it a steady or transient situation? In case of a transient what is the minimum time scale of interest?
7. What is the minimum space scale of interest in the process?

B: Selecting basic model options

8. Specify the time and space resolution of the simulation according to answers to questions 5 and 6
9. Choice of a number of fields according to answer to question 4
10. List of wall transfers (mass, momentum and energy) which may play a significant role in the whole process
11. List of interfacial transfers (mass, momentum and energy) which may play a significant role in the whole process
12. List of turbulent transfers (mass, momentum and energy) which may play a significant role in the whole process

C: Review of experimental data for validation

13. Check that the available experimental data cover all basic flow processes identified in 2. If required, plan and design new experiments to cover all processes.
14. Check that the available experimental data cover all important wall transfers, interfacial transfers and turbulent transfers identified in 9, 10, and 11. Check that they can be used to validate all important transfer models in a separate effect way. If required, plan and design new experimental programs in order to be more exhaustive.
15. Check that the instrumentation and the experimental tests provide enough information to get initial conditions and boundary conditions for the simulation.
16. Check that the instrumentation and the experimental tests provide sufficient local information on flow parameters of interest to validate closure laws for wall, interfacial, and turbulent transfers identified in 9, 10, and 11.

NOMENCLATURE

BPG	Best Practice Guidelines
CFD	Computational Fluid Dynamics
CMFD	Computational Multi-Fluid Dynamics
DNS	Direct Numerical Simulation
ERCOFTAC	European Research Community on Flow Turbulence And Combustion
ITM	Interface Tracking Method
LES	Large Eddy Simulation
LIS	Large Interface Simulation
RANS	Reynolds Averaged Navier Stokes

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