This paper will summarize the current state-of-the-art in physical-mathematical modeling and CFD simulation for the prediction of water-vapor multiphase flows through fuel rod bundles and fuel assemblies of nuclear reactors. After a short introduction and motivation for the use of CFD for this particular application in the field of nuclear reactor engineering, the main submodels are discussed, which have been recently developed in CFD software and which are necessary in order to predict multiphase flow through fuel assemblies of nuclear reactors from flow regimes of subcooled fluid flow towards departure of nucleate boiling (DNB). Basic model validation for isolated phenomena experiments will be shown in this paper, while model application for CFD flow prediction in nuclear reactor fuel assemblies will be shown in other papers (e.g. Laurien & Wintterle, Krepper & Koncar, Koncar & Krepper) on the workshop or had been recently published in the open literature (e.g. Dzodzo et al., ICONE-14, Miami, 2006). By discussing the current state-of-the-art in physical-mathematical modeling shortcomings and remaining challenges in the modeling of particular phenomena in CFD simulations of the given kind will be identified and a conclusion on remaining development requirements in the existing CFD software packages will be drawn.
Flow through nuclear reactor fuel assemblies is characterized by very high heat flux applied to the fuel rod walls and their cladding leading to significant boiling of the cooling fluid from the regime of subcooled boiling up to the occurrence of the critical heat flux / boiling crisis at low quality, i.e. Departure of Nucleate Boiling (DNB), where the heat transfer from the fuel rod surface to the coolant flow suddenly decreases. During accidental scenarios a boiling crisis at high quality (dryout) may occur, leading to the disappearance of the liquid film wetting the fuel clad. Obviously, both dryout and DNB (i.e. CHF conditions, more generally) must be avoided by proper design of reactor, safety margins and emergency systems.

So far the design of nuclear reactor fuel assemblies is mainly based on empirical correlations, experimental databases, thermo-hydraulic modelling at subchannel scale and the conduction of very expensive experiments in test facilities like e.g. the test facility in Karlstein, Germany operated by AREVA, where electrically heated nuclear reactor fuel assemblies are experimentally investigated under different operating and accident scenario conditions. Due to the high costs of these experiments it would be highly beneficial and desirable to at least supplement the fuel assembly design by the use of state-of-the-art CFD simulation methods for e.g. the improvement of inflow nozzle performance, spacer grid designs, investigation of thermal stresses and deformations in grid spacer arrangements, fuel rod vibration, the investigation of subchannel cross flows in fuel assemblies and their related effects on coolant fluid boiling and heat transfer.
In order to successfully apply CFD simulation to the prediction of flow through nuclear reactor fuel assemblies a large number of submodels are involved. This starts from the provision of accurate material properties (e.g. steam tables for a wider range of operating conditions for temperature and pressure). Further on submodels are required for single- and multiphase flow turbulence modeling as well as multiphase flow modeling for different flow regimes from liquid flow (subcooled region), bubbly flow (initially subcooled, then saturated), slug flow and annular flow (still saturated). The latter involves further submodels for bulk condensation and evaporation, wall boiling and conjugate heat transfer (CHT) in solids adjacent to the fluid flow domain where thermal boundary conditions have to be applied e.g. at the Uranium core of a fuel rod. High robustness, convergence efficiency and interoperability of all submodels of a certain CFD software code are necessary in order to make CFD simulations applicable to flow prediction for nuclear reactor fuel assembly flows. Finally submodels as well as the whole CFD software package have to be thoroughly validated against data from simplified isolated phenomena experiments and integrated tests.
Material Properties.
Material Properties

- **CFX-11.0:**
  IAPWS-IF97 equation-of-state implemented

The provision of accurate material data especially for water and steam over a wider range of temperature and pressure is an essential requirement for conducting CFD simulations in nuclear engineering thermal hydraulics. Starting from CFX 11.0 the industrial standard IAPWS-IF97 is implemented in the CFX internal material database. Highly accurate material properties have been implemented for subcooled water, supercritical water/steam, superheated steam and saturation data. Error margins for the material properties are specified in the IAPWS standard.
Material Properties

- Equation of state (EOS) types:
  - Ideal gas law
  - Redlich-Kwong EOS
  - Real gas property (RGP) tables
  - User defined equation of state
- Build-in material database
- Connectivity to external material databases (e.g. MatWeb, Matereality, GRANTA MI™)
- User defined materials and material properties → large degree of customizability

In addition to these water and steam properties from IAPWS-IF97 CFX software provides the possibility to use other definitions for material properties and equation of state, like ideal gas law, Redlich-Kwong EOS, RGP tables and fully user defined materials and material properties, e.g. imported from external databases either in tabulated format or implemented as correlations.
Turbulence Modelling.
Turbulent Flows

- Turbulence is an irregular 3D unsteady fluid motion
- Resolution of turbulence in time and space requires excessive computing resources
  → Turbulence modeling
- Simplification ⇔ accuracy
- Turbulence occurs in almost all technical flows
- Turbulence has important effects on engineering quantities, e.g.:
  → all transport phenomena
  → heat transfer
  → volume fraction distribution

Turbulent flow behind a cylinder in crossflow at a Reynolds number of ~4 million shows the complexity of turbulent flows, and the involvement of many different scales in time and space. A Direct Numerical Simulation (DNS) of turbulence is not possible in most technical flows. It can only be achieved for very simple geometries and very low Reynolds numbers. Further Large Eddy Simulation (LES) is also very costly in case of wall bounded flows, as near the wall the resolution requirements of LES are close to DNS.

Therefore turbulence modeling using two-equation or higher order turbulence models derived from RANS (Reynolds averaged Navier-Stokes) equations is required for flow simulation in technical applications.
### Turbulence Models in CFX

- **One Equation Models:**
  - Spalart-Allmaras
  - KE1E (Menter)

- **Two Equation Models**
  - \(k-\varepsilon\), RNG, \(k-\omega\), BSL, SST
  - EARSM based on \(\omega\)-equation

- **Reynolds Stress Models**
  - Launder-Reece Rodi
  - Speziale-Sarkar-Gatski
  - SMC-\(\omega\) (based on \(\omega\)-equation)
  - SMC-BSL

- **Unsteady Models:**
  - URANS (all models)
  - Scale-Adaptive Simulation (SAS, based on SST model)
  - Detached Eddy Simulation (DES, based on SST model)
  - Hybrid RANS-LES \(\alpha\)-version
  - LES
    - Smagorinsky
    - Dynamic (\(\alpha\)-version)

ANSYS CFX is providing a large number of turbulence models, ranging from 1-equation models to unsteady scale-resolving turbulence models like LES (Large Eddy Simulation), DES (Detached Eddy Simulation) and SAS (Scale-adaptive Simulation). In one-equation models the second turbulent scale is replaced by the local shear strain rate. Under such conditions, only one transport equation is needed for the eddy-viscosity. Two-equation turbulence models provide one turbulent length scale and one turbulent time scale by solving two independent transport equations for two different turbulence properties. And finally, in unsteady scale-resolving turbulence models an entire spectrum of turbulent length and time scales are resolved, while modeling is applied only to the isotropic part of the turbulent length scale spectrum (i.e. the small scale turbulence). The list provides an overview over most of the turbulence models available in CFX. Most popular turbulence models are SST, \(k-\varepsilon\), EARSM (Explicit Algebraic Reynolds-Stress Model) and the \(k-\omega\) based RSM-models (e.g. SMC-BSL), also with increasing computational capabilities the SAS turbulence model becomes more and more attractive in many applications.
There are many effects which standard models cannot handle, as they have not been calibrated for them. They are introduced by modifications/enhancements as appropriate. Some of the corrections listed above are standard, others (like reattachment modification, automatic wall treatment, transition model) are specific and exclusively available in the ANSYS CFX software. Another emphasis in the ANSYS CFX software is on the interoperability of physical models, so that the user is able to use almost any turbulence model in combination with other physical models as well, e.g. in the context of a multiphase flow simulation. Accuracy and grid independence of flow simulation results on sufficiently refined numerical grids is another design and implementation paradigm in the ANSYS CFX software.
Multiphase Flow Modeling.
Even for simple flow geometries like a vertical pipe flow multiphase flows show a wide variety of different flow regimes and flow morphologies. Unfortunately current CFD methods are not able to handle transition between different flow morphologies, e.g. from slug flow to annular flow, automatically. In current state-of-the-art multiphase flow models in CFD codes the user has to provide additional information about the applicable flow regime for modeling and flow simulation.
Multiphase flow modeling is further complicated if interfacial heat and mass transfer due to evaporation and condensation has to be taken into account. Virtual side view projections from wire-mesh sensor measurements in water-vapor flows through a DN=200mm vertical pipe (TOPFLOW test facility at FZR, Rossendorf, Germany) show the change in multiphase flow pattern and vapor bubble sizes for two experiments carried out without and with subcooling of the carrier water flow, while superficial water and vapor velocities as well as the pressure level had been kept constant. Especially the influence of a polydisperse bubble size distribution is still a challenge for Eulerian-Eulerian multiphase flow modeling.
If we consider flow conditions in a pipe or channel with heated walls, then we observe a change from single-phase subcooled liquid flow, to bubbly flow (ONB – Onset of Nucleate Boiling, OSB – Onset of Significant Boiling), slug flow regime with nucleate boiling, annular flow and finally the formation of droplet flow under dry-out conditions. The lower schematic diagram shows the behavior of wall and mean fluid temperature in comparison to the fluid saturation temperature in correspondence to the changing flow regimes.
Multiphase Flow Modeling -
Levels of Simplification

• Current focus on flow regimes without sudden change in flow morphology, e.g. slug flow \(\rightarrow\) annular flow

• Simplifications & additional assumptions due to unknown detailed & local physics, e.g. transport of interfacial area, flow regime transition, etc.

• Simplifications for reducing computational effort, e.g. two-phase flow model (2 N.-S. eq.) or inhomogeneous MUSIG (N+1 N.-S. eq.)

Due to the remaining challenges in automatic multiphase flow regime detection in CFD the current focus in multiphase flow simulation is on flow regimes without sudden changes in flow morphology. Another motivation for different levels of applied simplifying assumptions in multiphase flow modeling arises from the related computational effort, which is involved for resolving more and more details of detailed and local physical processes in multiphase flows. An example is the reduction of the physics in bubbly flows to the solution of a two-phase flow model by assuming, that all bubbles of the disperse phase are moving with a single velocity field. More details of a polydisperse bubbly flow like e.g. lateral demixing of differently sized bubbles can be resolved by the so-called inhomogeneous MUSIG model. The accuracy of simulation results can be substantially improved by the latter modeling approach, but for the price of a larger computational effort.
In recently published CFD simulations for flow prediction in nuclear reactor fuel assemblies either of the two following approaches had been used. In the first approach a quite restrictive simplifying assumption has been made, that the two-phase flow is quasi monodisperse. In this modeling approach the local bubble diameter is evaluated from experimentally obtained correlations and is related to the local properties of the carrier fluid (pressure, temperature, etc.). In this case only two sets of Navier-Stokes equations have to be solved, which reduces the necessary computational effort significantly.

But in reality a boiling water-vapor flow is polydisperse, i.e. shows a wider distribution of bubble sizes in any location of the flow geometry downstream from the ONB. Due to different response of small and larger bubbles to fluid turbulence and fluid velocity gradients (bubble deformation and resulting lateral bubble lift) it seems necessary to take bubble size distribution and different bubble velocities into account in order to achieve necessary level of accuracy in multiphase flow CFD simulations. Furthermore bulk condensation of the vapor phase might be significantly affected by changes in local interfacial area due to a wider and locally changing bubble size spectrum. A combination of the inhomogeneous MUSIG model derived by FZR and ANSYS with a wall boiling model seems to be the next step forward in detailed and accurate modeling of the physics in flow simulation for nuclear reactor fuel assemblies.
Eulerian MPF Modeling - The Particle Model

Mass weighted averaged conservation equations

- Mass, momentum, energy transport equations for each phase

\[
\frac{\partial}{\partial t}(\rho_k r_k) + \nabla \cdot (\rho_k r_k U_k) = \sum_{l=1}^{N} \Gamma_{kl}
\]

\[
\frac{\partial}{\partial t}(\rho_k r_k U_k) + \nabla \cdot (\rho_k r_k U_k U_k) = -r_k \nabla P - \nabla \cdot (r_k \Pi_k) + F_k + I_k
\]

\[
I_k = F_{I} + F_{D} + F_{L} + F_{WL} + F_{TD} + F_{VM}
\]

- turbulence models for each phase (e.g. k-ε / k-ω SST model, 0-eq. disp. phase turb. model)
- heat transfer equations for each phase with interfacial transfer closure
- interfacial forces need empirical closure
- high void fraction effects, bubble induced turbulence, etc.

The main governing multiphase flow equations for mass and momentum transport in a full N-phase multiphase flow framework are presented. The RHS of the momentum transport equations contain additional interfacial momentum transfer terms, which require additional closure. The mass and momentum transfer equations have to be accompanied by at least two turbulence model equations for the continuous phase and heat transfer equations for each of the phases, providing additional closure laws for interfacial heat and mass transfer (bulk condensation/evaporation) and turbulence modification due to the presence of the disperse phase (e.g. by the Sato model).
Lift force, Wall lubrication force & turbulent dispersion

**Lift force:**
- due to asymmetric wake and deformed asymmetric particle shape
  
  \[ \text{Tomiyama } C_L \text{ correlation} \]
  
  \[ F_L = C_L r G \rho_L (U_L - U_G) \times \nabla \times U_L \]
  
  \[ C_L = C_L (Re_p, Re_v, Eo) \]

**Wall lubrication force:**
- surface tension prevents bubbles from approaching solid walls
  
  \[ \text{Antal, Tomiyama & Frank W.L.F. models} \]
  
  \[ F_{WL} = -C_{wall} r G \rho_L \left| \mathbf{U}_{rel} - (\mathbf{U}_{rel} \cdot \mathbf{n}_W) \mathbf{n}_W \right|^2 \mathbf{n}_W \]
  
  \[ C_{wall} = C_W (Eo, y/d_p) \]

**Turbulent dispersion force:**
- turbulent dispersion = action of turb. eddies via interphase drag
  
  \[ F_{ID} = \frac{3}{4} \rho_F \frac{C_D}{d_p} \frac{V_F}{\sigma_{rF}} \left| U_F - U_F \right| \frac{\left( \nabla \tilde{r} - \nabla \tilde{r} \right)}{r_p - r_F} \]
  
  \[ \text{FAD model by} \]
  
  \[ \text{Burns et al. (ICMF’04)} \]

For the interfacial momentum transfer additional closure laws for the lift force, the wall lubrication force and the turbulent dispersion force have to be provided. For bubbly flows these can be specified by using Tomiyama’s correlation for the lift force coefficient, Frank’s generalized correlation for the wall lubrication force coefficient and by using the Favre averaged drag (FAD) turbulent dispersion force model by Burns et al.
For gas-liquid flows of higher volume fraction the bubble size distribution is establishing in a balance between a) bubble breakup and coalescence processes and b) bulk condensation or evaporation taking place at the interface between the gaseous and liquid phase. Due to different lift exerted on bubbles of different size, small bubbles are driven to the geometry walls while large bubbles move to the geometry center like it can be observed e.g. in pipe and channel flows. This leads to further changes in the radial volume fraction distribution enhancing either bubble fragmentation or coalescence in dependence on local fluid velocity gradients and turbulence. In order to take these physical effects into account the inhomogeneous MUSIG model has been developed by FZ Rossendorf and ANSYS.
In the inhomogeneous MUSIG model the gaseous phase (either a gas like air or the vapor of a fluid phase) is subdivided in \( N \) so-called velocity groups. It is assumed, that bubbles belonging to the same velocity group are moving with the same velocity field. For most applications a smaller number of 2-4 velocity groups will be sufficient in order to cover the main demixing effects for small and large bubbles. Furthermore each velocity group is further subdivided into \( M \) bubble size classes leading to a representation of the overall bubble size distribution with \( N \times M \) discrete bubble size classes.
The Inhomogeneous MUSIG Model

Inhomogeneous MUSIG model solves for:

- N volume fraction equations
- N+1 momentum equations
- (> 2) turbulence model equations
- NxM size fraction equations

\[
\frac{\partial}{\partial t} \left( \rho_d r_{dg} \right) + \frac{\partial}{\partial x^i} \left( \rho_d r_{dg} u_{g,j}^i \right) = S_g \quad g = 1, \ldots, N \times M \quad j = 1, \ldots, N
\]

\[
r_d = \sum_{g=1}^{N \times M} r_{dg} \quad f_{dg} = \frac{r_{dg}}{r_d} \quad g = 1, \ldots, N \times M \quad \sum_{g=1}^{N \times M} f_{dg} = 1 \quad \sum_{g=1}^{N \times M} S_g = 0
\]

In terms of transport equations the subdivision of the disperse gaseous phase into N velocity groups and NxM bubble size classes leads to following equation system to be solved (see listed equations above). In case of a water-vapor flow with heat and mass transfer additionally N heat transfer equations would have to be solved. In that case the source term on the RHS of the size fraction equations has not only to include the description for bubble breakup & coalescence processes but furthermore the description of bubble size distribution changes due to condensation and evaporation.
The Inhomogeneous MUSIG Model

\[ S_g = \rho_d \sum_{h=g+1}^{N_x M} B_{gh} r_{dh} \]

breakup birth

\[-\rho_d r_{dg} \sum_{h=1}^{g-1} B_{gh} \]
breakup death

\[+ \frac{1}{2} \rho_d \sum_{h=1}^{g} \sum_{i=1}^{g} C_{hi} r_{dh} r_{di} X_{g \leftarrow hi} \frac{m_h + m_i}{m_h m_i} \]
coalescence birth

\[-\rho_d r_{dg} \sum_{h=1}^{N_x M} C_{gh} r_{dh} \frac{m_h}{m_i} \]
coalescence death

For the simplified case without heat and mass transfer this source term in the NxM size fraction equations \( S_g \) consists of 4 separate terms for positive and negative contributions to the size fraction of a given bubble size class due to bubble breakup and coalescence respectively. The birth and death rates for both processes have to be modeled accordingly based on local fluid flow properties.
Bulk Condensation/Evaporation and Wall Boiling
Thermal Phase Change Model – Bulk Condensation & Evaporation

- Interfacial mass transfer =
  Mass transfer rate per unit area ×
  Interfacial area/unit volume

\[ \Gamma_{lv} = \dot{m}_{lv} A_{lv} \]

- Heat transfer coefficient from Ranz-Marshall correlation

Bulk condensation and evaporation in e.g. a water-vapor two phase flow is modeled by the so-called thermal phase change model. Here the interfacial mass transfer is related to a mass transfer rate per unit volume and the interfacial area density. The latter requires an additional assumption about the flow morphology, i.e. for the assumption of spherical bubbles in the disperse phase this quantity can be computed from the bubble diameter and the gas volume fraction. Further the condensation/evaporation rate can be related to the liquid subcooling and the latent heat, while for the interfacial enthalpy some closure has to be applied (e.g. the Ranz-Marshall correlation for the heat transfer coefficient).
In case of coolant flow through a geometry with heated walls the bulk condensation/evaporation model is not enough in order to cover the wall boiling heat and mass transfer, since the ONB starts even if the coolant fluid is still subcooled. Additional processes like quenching at the wall occur, leading to changes in the heat flux from the hot wall to the liquid. This leads to the development of a wall boiling model.
The Rensselaer Polytechnical Institute (RPI) developed the so-called RPI wall boiling or heat partitioning model. In this model the overall heat flux from the heated wall to the two-phase flow (the subcooled liquid) is divided into 3 parts: a convective, quenching and evaporation heat flux. Furthermore the heat flux partitioning model associates each of the heat flux contributions with a dimensionless wall area ratio in order to define the ratio between heat flux contributions.
Originally the RPI wall boiling model has been developed for 1-dimensional flow modeling and relates the convective and quenching heat flux contribution to the bulk liquid temperature. But in the framework of a CFD algorithm this value is locally (at the wall nearest mesh cell) not available. If the required liquid temperature value is nevertheless taken from the wall-nearest grid cell, then the model becomes grid dependent and inaccurate and the quenching heat flux will reduce with increased near wall resolution. Thereby the heat flux partitioning becomes inaccurate in favor of the evaporation and convective heat fluxes.
Grid dependent correlations

• Evaporation heat flux

\[ \dot{q}_E = \dot{m} \cdot (h_G - h_L) \]

\[ \dot{m} = \frac{\pi d_w^3}{6} \rho_G f \cdot n \]

\[ d_w = \min \left\{ 1.4\,\text{mm}, 0.6\,\text{mm} \cdot \exp \left( -\frac{T_S [K] - T_L [K]}{45 [K]} \right) \right\} \]

\[ d_w \quad \text{– bubble departure diameter} \]

\[ n \quad \text{– nucleation site density per m}^2 \]

\[ f \quad \text{– bubble departure frequency} \]

• small quenching & overestimated evaporation on fine grids
• wrong heat flux partitioning

Trends to film boiling on fine grids (due to \( T_L \to T_W \))

The same issue appears in some of the closure correlations of the model, e.g. for the bubble departure diameter used in the evaporation heat flux. The use of the wall nearest grid cell value of the liquid temperature instead of the non-available bulk liquid temperature leads to the tendency of too high vapor production and therefore to film boiling.
Revisited RPI Boiling Model

- grid invariance of the model required
- determine $T_L$ from temperature wall function (Kader, 1981)

$$T^+ = Pr \cdot y^+ e^{(-\Gamma)} + \left[ 2.12 \cdot \ln(y^+) + \beta \right] \cdot e^{(-1/\Gamma)}$$

$$y^+ = \frac{\rho_L \cdot \Delta y \cdot u_\tau}{\mu}$$

- from definition:

$$T^+ = \frac{\rho \cdot c_{PL} \cdot u_\tau}{\dot{q}_W} (T_W - T_L)$$

→ evaluating $T^+$ at 2 different locations

In ANSYS CFX 5.7.1 the wall boiling model has been revisited. The determination of the near wall liquid temperature was based on the temperature wall function of Kader (1981) and by evaluating $T^+$ at two different locations.
Revisited RPI Boiling Model

- heat flux in boundary layer identical at both locations

\[
\hat{q}_{w, y^+ = \text{first cell}} = \frac{\rho \cdot c_{PL}}{T_{y^+ = \text{first cell}}} (T_W - T_L)_{y^+ = \text{first cell}}
\]

\[
\hat{q}_{w, y^+ = \text{const}} = \frac{\rho \cdot c_{PL}}{T_{y^+ = \text{const}}} (T_W - T_L)_{y^+ = \text{const}}
\]

heat fluxes are equal

\[
(T_W - T_L)_{y^+ = \text{const}} = \frac{T_{y^+ = \text{const}}}{T_{y^+ = \text{first cell}}} \cdot (T_W - T_L)_{y^+ = \text{first cell}}
\]

- additional factor in correlations for \( d_w, \hat{q}_F, \hat{q}_Q \)
- assumption of \( y^+ \)\text{const}=250; model parameter

Since the heat flux in the boundary layer should be equal for both evaluated wall distances (in the first grid cell and at a constant \( y^+ \)), the resulting two heat fluxes from the above expressions can be equalized. From the resulting equation we can now determine the difference between the wall temperature and the bulk liquid temperature in dependency on the given values of the wall temperature and the liquid temperature in the wall nearest grid cell. An additional pre-factor occurs in this relation. The wall distance of heat flux evaluation is a model parameter and was set to \( y^+ = 250 \).
Conjugate Heat Transfer (CHT).
Grid Connections, Multiple Meshes

- GGI to connect unmatched meshes
- Topology change, physical shape change, physical gaps and interference
- Several frame change options
- Automatic, robust, accurate, fully implicit coupled connection

In some cases thermal boundary conditions can not be formulated on the boundary of the flow domain but only on the outer boundary of an adjacent solid. In that case the inner wall temperature is part of the solution of heat transfer in both the fluid and solid domains. A prerequisite for such a model capability is the solver capability to solve the heat transfer equation in both domains and to deal with unequally resolved numerical meshes on both sides of the solid-liquid interface (GGI – General Grid Interface).
Accurate numerical interpolation is shown in the above example, where no deformation of the pressure shock can be observed across a GGI with different mesh resolution on both sides.
The same can be proven for fluid-solid interfaces in a conjugate heat transfer application. In the above simulation the grid resolution in the solid is much coarser than in the fluid flow domain. Nevertheless, temperature distributions in the fluid and solid domain are physically reasonable and show the right temperature decrease at the tip of the solid blunt body and the temperature increase at the location, where the shock wave hits the solid surface.
The above slide shows the result of a coupled CHT simulation for a nuclear reactor rod bundle geometry using ANSYS Fluent Vers. 6.3.
Applications: Boiling flow in nuclear reactor core

- Wall temperature is defined by bisection method from flux partitioning
- Turbulent dispersion force and bubble induced turbulence stabilize solution

Comparison with experiment for area averaged vapor void fraction for different zones

Comparison with experiment for lateral vapor void fraction


In a first simulation the boiling water-vapor flow has been simulated with a similar RPI wall boiling model implementation and a two-phase flow setup. The lateral vapor volume fraction profiles and circumferentially averaged vapor volume fractions have been compared to available experimental data, but which were unfortunately due to the applied measurement technique subject to larger error margins. Having this fact in mind, the simulation data compare quit well to the experiments.
In another simulation the thermal boundary condition (heat source) has been applied as a volumetric heat source in the Uranium cores of the fuel rods and by taking the Zirkonium cladding into account. Pictures show the axial and radial temperature distributions in the symmetry sector of the fuel rod bundle for both fluid and solids.
FSI: Stresses and Deformations.
Latest software releases of ANSYS software allow for the either 1-way or 2-way coupling of CFD (Computational Fluid Dynamics) and CSM (Computational Structural Mechanics) simulations in order to predict thermal and mechanical fluid-structure interaction. ANSYS Workbench can be used for the generation of a single geometry representation of the fluid as well as the solids domains in the computation and for control of the simulation process. In a 1-way FSI simulation the properties of the CFD simulation are transferred at the domain boundaries to a CSM simulation, e.g. as thermal or mechanical loads and the deformations and stresses in the solids are computed. In this case it is assumed, that the deformations are small enough in order to neglect there influence on the fluid flow. In a 2-way coupled FSI simulation resulting deformations of solid boundaries are large, so that they can not fairly neglected for the CFD simulation. In this case the solution process includes a 2-way coupled iteration procedure, where the geometric boundaries of the fluid domain are deformed in accordance with the results of the CSM simulation.
Finally the ANSYS software provides the capability of a unified post-processing of both the CFD and CSM simulation results.
Applications: Fluid-Structure Interaction for Fuel Rod Grid

- Demonstration problem for 3X3 bundle
- Rods are stiff, grid is flexible
- FLUENT and ABAQUS communicate via MPCCI force and motion communication
- FLUENT uses Detached Eddy Simulation (DES) turbulence model

ANSYS Fluent 6.3 provides a less integrated FSI capability by using standardized MPCCI interface for coupling with external CSM products. In a demonstration case for a 3x3 bundle with spacer grid the resulting stresses in the solids material of the spacer grid had been predicted.
In the DES (Detached Eddy Simulation) large scale turbulence structures develop from the edges of the spacer grid leading to its agitation. The resulting time dependent lateral and axial displacements of the spacer grid and vortex generator elements have been predicted in the CSM simulation.
Model Validation against Experiments.
Model verification and validation is one of the most important steps in model development and implementation. In validating physical-mathematical models it is of special importance that the validation simulations are carried out in accordance to highest CFD standards, as they are outlined in the so-called Best Practice Guidelines (ERCOFTAC, ECORA), in order to clearly differentiate between sources of numerical errors (which has to be minimized by all means in a validation study) and remaining model errors. Furthermore it has to made sure, that suitable, high-resolution and high-quality experimental data are finally used for results comparison in order to avoid wrong judgment about the model accuracy.

Model verification and validation is carried out on very different levels, starting from very simple configurations which allow under certain circumstances even analytical flow solutions. Next validation steps are undertaken for isolated phenomena tests, where special experiments are conducted in simplified geometries to reduce the level of flow complexity and phenomena interaction, e.g. by setting up quasi 1-dimensional experiments. Finally more combinations of physical models are validated in so-called demonstration tests, where flow complexity and physical phenomena interaction is comparable to the industrial size flow application.

For the validation of the multiphase flow models FZ Rossendorf has established a large database of wire-mesh sensor measurements for air-water and vapor-water vertical pipe flows of different inner diameter (DN=55mm and DN=198mm). On the slide above the test matrix of the MT-Loop test facility is outlined, where the colored combinations of superficial air and water velocities mark the experiments for which cross-sectional velocity and gas volume fraction profiles are available. Numerical validation tests with ANSYS CFX have been carried out for the test conditions marked in red frames and results are compared to the experimental data.
Only a few results of this extensive validation study can be shown here. Further results are available in technical reports and publications. After verification tests aimed to minimization of numerical errors (grid refinement studies, investigations on proper convergence level, integration time scale and discretization scheme for advection terms and time derivatives), different closure assumptions and correlations for the non-drag forces on bubbles have been compared to each other. It was found, that the lateral gas volume fraction distribution at the upper most measurement cross section in the MT-Loop test facility depends not only on the lift force, but to a large degree on the formulation of the so-called wall lubrication force too. It could further been shown, that the popular and widely used Antal correlation fails for a wide range of flow conditions, while the Tomiyama correlation and the generalized formulation by Frank was in good agreement to data.
In CFD simulations using the Antal correlation for the wall lubrication force the gas volume fraction reached non physical high values close to the pipe wall, since the wall lubrication force amplitude predicted by the Antal correlation was too small in order to balance the lift force directed towards the wall as predicted by Tomiyama’s law.
Above pictures show the numerically predicted lateral gas volume fraction profiles for 4 test case conditions in direct comparison to experimental data showing error margins from the measurements. It can be seen, that the derived physical models for air-water bubbly flows are in good agreement with the experiments.
Validation of 3x7 Inhomogeneous MUSIG Model on TOPFLOW-074

- Good agreement at levels A, L through R
- Too fast spreading of the bubble plume from inlet

For the TOPFLOW (DN=198mm) test facility the gas/vapor inlet boundary conditions are different from MT-Loop, since the gaseous phase enters the flow domain through ring-shaped wall nozzles. Different levels of gas injection allow for the variation of the distance between gas injection and the measurement plane without changing the sensor location, which is difficult and time consuming in a high-pressure and high-temperature environment (as for water-vapor experiments). But in the result the two-phase flow can no longer be regarded as monodisperse, since the gas volume fractions at least in the vicinity of the gas injection location can exceed 25-30% leading to strong bubble coalescence. Therefore the inhomogeneous MUSIG model has been applied for the validation against TOPFLOW data in order to account for the polydisperse character of the bubbly flow. The above diagram shows the comparison of lateral gas volume fraction profiles from a 3x7 inhomogeneous MUSIG model simulation to wire-mesh sensor data. From the data it can be seen, that the inhomogeneous MUSIG model is able to predict the flow transition from a strong near wall peak in the lateral gas volume fraction profile (A-level injection) to a flow with a core peak for the largest distance between gas injection and the measurement plane (R-level injection).
The comparison for air and water velocity profiles show a similar good agreement to the available gas velocity measurement data from the wire-mesh sensors. Data comparison is shown for the 4 largest distances between gas injection and measurement plane (I- through R-level injection). It can be seen, that for I-level injection tests the velocity profile still shows strong deformation in the vicinity of the pipe wall, which is induced by the strong buoyancy effects of the near wall gas bubble plume from the wall nozzle injection. With flow regime transformation to a core peak in the lateral gas volume fraction profile the velocity profiles of both the gaseous and liquid phases become more and more fully developed.
Basic validation tests have been carried out for the revisited formulation of the RPI wall boiling model using temperature wall functions. Two test cases have been selected from the open literature for the flow through a circular pipe and a rectangular channel with heated walls.
Flow conditions and wall heat flux are given for the test case. The gray area marks the range of +/-5% from the linear mean vapor volume fraction increase with height in the vertical pipe. Simulations had been carried out on numerical meshes with different wall refinement showing, that the revisited formulation of the RPI wall boiling model gives almost grid independent results for the axial increase in cross-sectional averaged vapor volume fraction. The agreement with the experimental data is within the range of +/-5% error (or even less).
The same comparison of predicted mean water temperature over the height in the pipe gives similar grid independent result.
Results for the flow in a rectangular channel with heated walls under the flow conditions given on the above slide are in comparable good agreement as for the circular pipe flow. Again the CFD results are independent from the near-wall grid resolution and in good agreement to data.
More detailed comparison is based on radial vapor volume fraction distribution in comparison to experimental data. Again the CFD solutions on differently refined numerical meshes do not differ very much and show grid independency of results from the CFD model. For the smallest distance between measurement plane and the inlet cross section the comparison to data is fairly good, since the water-vapor flow is here still fairly monodisperse and dilute. The fluid in the channel core is still subcooled leading to strong bubble recondensation in a certain distance from the heated wall.
Next level of data comparison is in a distance of X=36m from the inlet cross section. CFD results and experimental data show a further increase in near wall vapor volume fraction with increased axial distance from the inlet. First vapor bubbles are able to reach the center line of the channel despite recondensation.
At $x=0.51 \text{m}$ flow regime transition can be observed from the experimental data. The vapor volume fraction profile shows a change from a near-wall maximum towards a core peak. The two-phase flow model used for this simulation was based on the monodisperse bubbly flow assumption using a correlation for the local bubble diameter and did not include the Tomiyama lift force on the vapor bubbles. Therefore, the transition in the vapor volume fraction profile towards a core peak can not be observed in the CFD results, also the cross-sectional averaged vapor volume fraction is still in good agreement to data.
Finally at x=0.67m the flow regime transitions to slug flow with a pronounced core peak in the vapor volume fraction profile. Without taking into account the non-drag forces acting on vapor bubbles and without accounting for the correct change in bubble diameter due to wall boiling, recondensation, bulk evaporation and coalescence, this flow behavior cannot be predicted by the CFD model.
Further investigations on model validation and application of the outlined CFD simulation capabilities of ANSYS CFX to flow prediction in nuclear reactor fuel assemblies can be found in a number of recent publications, e.g.:


   - Detailed geometrical modeling of a 17x17 rod fuel assembly including the nozzle inlet from the lower core support plate and spacer grids
   - Prediction of single phase turbulent flow through the fuel assembly and assessment of axial and lateral water velocity distributions for optimization of inlet nozzle performance
   - Figures show axial and lateral velocity distributions after 500mm downstream of the inlet


   - Investigation of spacer grid induced swirling flow on the vapor volume fraction distribution on rod surfaces
Further investigations on model validation and application of the outlined CFD simulation capabilities of ANSYS CFX to flow prediction in nuclear reactor fuel assemblies can be found in a number of recent publications, e.g.:

   - Validation of revisited RPI wall boiling model on refrigerant R-113 boiling flow in a vertical annulus

   - Application of ANSYS CFX wall boiling model to flow prediction in a fuel assembly of a High Performance Light Water Reactor (HPLWR)
   - Evaluation of void fraction and water temperature distributions in sub-channels
Main required model capabilities in CFD simulation for nuclear reactor fuel assemblies and the current state-of-the-art of physical-mathematical modeling have been summarized in this presentation. So finally the question arises: Can contemporary CFD software accurately predict the occurrence of CHF in nuclear reactor fuel assemblies?

The answer is currently: No, not yet. But CFD already provides a very detailed and accurate insight into flow conditions and flow phenomena, which either enhance or mitigate the occurrence of CHF on a later stage of axial flow development in a fuel assembly. Thereby CFD can be used as a valuable tool to get additional information for flow analysis and optimizing fuel assembly designs. In this way CFD can contribute to the further reduction of fuel assembly design and development costs.

In order to make CFD simulations an even more reliable tool for fuel assembly design, the outlined development requirements for future model and CFD software development can be identified. Hereby an emphasis is on the further increase in model interoperability and in validation of the resulting very complex flow setups including a large number of interacting physical models. Furthermore a currently unresolved issue is the flow regime transition in multiphase flows, if they are accompanied by strong flow morphology changes.
Summary & Outlook

- **Overview on state-of-the-art modeling & simulation for flows through nuclear reactor fuel assemblies**
- **Methodology:**
  - Experiment → Model Development → Validation
  - High interoperability of physical models
- **Result:**
  - Geometry & Grid independent modeling
  - Models applicable to complex design & NRS studies
- **Outlook:**
  - Multiphase CFD remains a challenge in many details
  - Ongoing & customer driven CFD model development
  - Research cooperation with Academia & Industry

The given presentation summarizes the current state-of-the-art in different fields of physical-mathematical modeling for CFD simulations for nuclear reactor fuel assemblies. The underlying methodology of CFD model development from special conducted experiments to model formulation & implementation and finally to model validation has been outlined. In all the development process high importance is given to a maximum model interoperability and compatibility by maintaining the high level of model accuracy and numerical efficiency.

In the result CFD provides a geometry and - at least asymptotically - numerical grid independent form of flow and physical phenomena modeling, which is a main advantage over other simulation techniques. Thereby derived and validated physical models can be applied to complex nuclear reactor engineering designs and nuclear reactor safety scenarios.