LECTURE 16

Computational Fluid Dynamics for Nuclear Systems

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A. CFD Terminology

Computational fluid dynamics (CFD) falls under the broad category of numerical simulation of fluid flow and heat transfer. Numerical simulations can cover a wide variety of theoretical and applied mathematical solutions, many of which have only limited interest for industrial-scale nuclear safety analysis. Nuclear safety-related phenomena typically include turbulent flows with heat transfer in complex geometries. The analyst is commonly faced with modeling phenomena such as mixed convection, thermal radiation, multiple fluids, phase change, and general mixing phenomena at conditions that are at or beyond the limits of experimental data bases.

The term CFD is most commonly associated with solutions of the Reynolds Averaged Navier-Stokes equation set. CFD is also used to describe a wide variety of techniques in which a set of equations based upon the Navier-Stokes equation set is solved numerically on a discrete set of points or volumes that represent the flow domain. There are a multitude of different formulations and solver techniques that form a dizzying array of methods. One high-level method to distinguish between CFD techniques is based on how the turbulence is modeled.

Direct numerical simulations[1] (DNS) solve the governing Navier-Stokes equation set for all significant scales of turbulence. Since no stable, stationary solution exists for turbulent flows, this approach requires time-accurate solutions that must be sampled and analyzed on a statistical basis in order to obtain useful results. The computational effort for DNS scales with the Reynolds number cubed. DNS is an important technique that has been used to demonstrate the legitimacy of the Navier-Stokes equation set for simple geometries at relatively low Reynolds numbers. Although computer performance is constantly rising, analysts are not on the verge of using DNS for reactor-scale problems in the foreseeable future.

Large eddy simulations[2] (LES) reduce the workload required in DNS by only solving directly for the larger scales of turbulence. The smaller scales must be modeled. The method uses a form of low pass filtering on the equations. The result is the elimination of the small length and time scales, which significantly reduces the computational effort. The filtering is commonly a function of the grid size. This makes LES a practical solution for some engineering applications. The impact of the turbulence in the unresolved scales, however, needs to be accounted for with some type of turbulence model. It is suggested that the smaller scales of turbulence are more independent of the overall flow field and are therefore easier to model even though there is still no universally valid turbulence model. A variety of subgrid scale models have been proposed, and LES is gaining in acceptance as computer power continues to increase.

Reynolds Averaged Navier-Stokes[3] (RANS) is an approach that greatly reduces the computational effort required for a solution. The method eliminates turbulent fluctuations through the averaging process, and the equations are formulated in terms of locally averaged flow field quantities. Computational effort for the RANS approach is reduced by many orders of magnitude compared to LES and DNS approaches. The problem, however, is the averaging of nonlinear terms in the Navier-Stokes equations, which results in additional unknowns (the Reynolds stresses). The equation set now has more unknowns than equations and requires additional modeling for closure (turbulence modeling). This problem is referred to as the turbulence closure problem and has been the subject of research for more than 100 years. With RANS, all turbulence is modeled. A major problem is that there is no universal model for turbulent behavior. A given model may be adequate for a specific flow regime but not another. Turbulence models are not based on some fundamental physical law, and the RANS approach misplaces the first principle distinction of DNS. RANS-based turbulence modeling, however, has proven to be efficient and acceptably accurate for a large number of engineering flows. The significantly reduced computational burden of RANS, compared to LES or DNS, allows users to study larger problems or more variables with fewer computational resources. RANS is the most popular approach in use today for nuclear safety analyses, and this trend is expected to continue into the near future.

Detached eddy simulation[4] (DES) is another technique that is becoming more popular in recent years. This is a hybrid LES/RANS approach that uses RANS models in the near-wall locations where it may be more appropriate and relies on the filtered LES approach in the core turbulent region where large turbulent scales are most important. The approach attempts to offer the best of both worlds by reducing computational effort compared to LES and making potential improvements in the turbulent modeling compared to RANS.

Multiphase CFD is increasingly referred to as computational multi-fluid dynamics[5] (CMFD). Multiphase (steam-water) flow regimes are common in light-water reactor accidents; therefore, CMFD tools have been the subject of intense research within the light-water reactor (nuclear) safety community. A wide variety of techniques incorporating aspects of DNS, LES, and RANS approaches have been developed for CMFD predictions. This area is beginning to mature for simple flow regimes, but a great deal of work remains. All of the problems of turbulence modeling from single-phase RANS approaches are magnified by the complexities of two-phase turbulence and phase interactions and a critical lack of detailed three-dimensional experiments that would support the closure of such models. Significant improvements in this area have been observed in the past 15 years, and CMFD will remain an area of intense research and development for years to come.

B. Turbulence

The treatment of turbulence is a significant concern for CFD analysts, but turbulence is not always the largest challenge. The nuclear systems analyst also commonly faces challenges such as the lack of adequate validation data, uncertain boundary conditions, complex geometries, and multiphase phenomena. Turbulence, however, is such a fundamental issue for CFD techniques that anyone using or reviewing the results from CFD codes must consider it.

Turbulence modeling is usually associated with the RANS approach, although subgrid scale turbulence modeling for LES is also an important area of research. There is no need for turbulence modeling in a DNS since the Navier-Stokes equation set models the turbulent fluctuations directly. The need for turbulence modeling arises as the Navier-Stokes equations are averaged or filtered to reduce the complexity of the solution. A thorough discussion of turbulence modeling is beyond the scope of this presentation, but a simple overview of turbulence and the Reynolds averaging approach will help illuminate the importance of turbulence modeling in CFD simulations.

The impact of turbulence can be observed by measuring the velocity of a steady turbulent flow with a high-frequency response method such as a hot wire anemometer or a laser Doppler velocimetry system. The measured velocity is observed to have seemingly random fluctuations around an average value. The fluctuations represent the turbulence. Turbulent data of this type can be decomposed into a mean and a fluctuating component whose average value is zero. The turbulence is not random, however, as it can be correlated with other fluctuations in the flow and can be described by structures. It is also noted again that the turbulent fluctuations satisfy the Navier-Stokes equation set.

For most flows of engineering significance, turbulence is present, and there are no stable solutions to the Navier-Stokes equation set. Osborne Reynolds first proposed the idea of decomposing the instantaneous values in the equations into an average and fluctuating component ($u_i = \bar{u}_i + u_i'$). Each variable is written in this manner and substituted into the Navier-Stokes equations, which are subsequently averaged. Since the average of fluctuating components is zero, the averaging process removes many of the extra terms that arise. However, not all terms are eliminated. The average of the product of fluctuating terms is not zero. The RANS equation set contains all of the original variables represented as an average value with the addition of a set of terms representing the nonzero average for products of fluctuating terms. These terms are typically referred to as the Reynolds stresses because they are normally positioned in the equations alongside the standard viscous normal and shear stress terms. Technically, the terms are not stresses. The significance is that new variables have been introduced and the equation set is no longer closed (i.e., there are now more unknowns than equations). This is the turbulence closure problem. The goal for turbulence modeling in this context is to provide a link between the mean flow parameters and the unknown Reynolds stresses that have arisen in the averaging process.

The key benefit of the Reynolds averaging approach and its associated turbulence modeling is a multiple order of magnitude reduction in computational cost compared to a DNS-type solution. A large Reynolds Averaged CFD model could easily require 8 to 10 orders of magnitude fewer computations than its DNS counterpart. Practically speaking, the RANS modeling approach provides a means to obtain CFD predictions for problems of engineering interest that would not be possible using DNS approaches.

The key problem of the RANS approach is the fact that there is no universal turbulence model. The Reynolds stresses represent nine new unknowns in the equations with no fundamental laws left to apply. The new terms must be approximated from empirical methods or untested hypotheses. The first-principles pedigree of the Navier-Stokes equation set is lost in the application of the RANS approach.

Many turbulence modeling approaches have proven to be quite successful thanks to a century of turbulence research. Prandtl's mixing length approach, developed early in the 1920s, is an example of a zero equation model. The Reynolds stresses are found to be related to the product of a mixing length and velocity gradient (squared) with mixing lengths established for various flow types. The approach provides a straightforward way to close the RANS equation set and has some merit under some conditions. Prandtl apparently described the approach as "only a rough approximation." By the 1950s, one-equation, two-equation, and Reynolds stress modeling approaches had been developed. These approaches benefitted greatly from the development of computer technologies that have allowed analysts to make rapid trial-and-error refinements under a variety of conditions. The advent of the modern computer is probably more responsible for the development of turbulence models than any recent revelations about the nature of turbulence itself.

Turbulence modeling gets significant attention because of the impact turbulence can have on the diffusion of momentum and energy in a flow field. For a wall-bounded flow, the Reynolds stresses act as a turbulent shear, which greatly increases the stress on the wall compared to a standard viscous shear stress. Similar terms that involve a fluctuating velocity and temperature product show up in the energy equation. These turbulent fluxes are responsible for significant increases in heat transfer.

The variety of turbulence models available can overwhelm a CFD analyst. Many models suffer from limited applicability or numerical instabilities that make them difficult to apply. Keeping track of turbulence modeling issues is a career in and of itself. The good news for the nuclear CFD analyst is that a relatively small number of turbulence models have been optimized, well documented, and benchmarked over a wide range of conditions so that their strengths and weaknesses are relatively well understood. A typical CFD tool can solve a wide variety of flow problems with 10 or fewer major turbulence modeling options.

C. CFD as an Art

On the first page of Patrick Roache's book of more than 600 pages, entitled *Fundamentals of Computational Fluid Dynamics*,[6] the author notes that "in this field, there is at least as much artistry as science." This is difficult for a nonuser to understand when one can point to a variety of published CFD best practice guidelines,[7] CFD verification and validation guides,[8] and many CFD assessment[9] studies. With clear guidelines and standards, it could be argued that CFD methods can be applied in a consistent manner. The validity of results should be a limited only by the quality of the models that are applied. With unlimited time and resources, one could argue that this might be the case.

However, the limitation of resources means that the state of the art for industrial CFD applications still leaves a great deal of room for the "art" of CFD. DNS solutions for industrial applications are simply not possible at this time. Although LES solutions are gaining in popularity, the computational requirements can be 10^3 or more times higher than a RANS approach. RANS methods are still the dominant choice for industrial CFD applications. Referring to the "art" of CFD implies that two experienced CFD users will most likely solve a given application using different options. Depending on the complexity of the application, the users may or may not obtain similar results. This issue is especially true for nuclear safety applications for which specific information about accident conditions might not be available.

A simplified list of major steps in a CFD evaluation is outlined below. These steps assume the use of a code with good documentation and models that have been verified. They also assume that the problems of interest are large industrial CFD applications of the type that can arise in nuclear power plant safety analysis. These four steps highlight some of the choices and compromises that are made and help to illuminate why different users with different experience levels will end up describing a problem in different ways:

(1) Physical Description. All problems start with a physical description. This includes a description of the geometry or domain, the boundary conditions that drive the problem, the fluid of interest, and possibly the initial conditions at the start of the simulation. The analyst sometimes makes simplifications at this point in order to make the problem feasible or to fill in missing details. A two-dimensional or axisymmetric simplification is sometimes used. This assumption makes the problem less expensive to solve since three-dimensional problems require significant resources. It is common for the CFD modeler to describe the geometry in a simplified manner, ignoring small details such as fasteners, gaps, filets, or small supporting structures. The size of the domain is also a consideration. There is a tendency to make the domain as small as possible in order to focus resources on a limited region. This approach leads to the application of boundary conditions positioned too close to the region of interest. Boundary conditions drive the solution, and, unless they are known precisely, they should be moved far from the region of interest so that their influence can be diminished. Wall boundary conditions include heat transfer and roughness conditions, which are commonly applied as constants because of a lack of detailed information. Inlet conditions include turbulence, velocity, temperature, and pressure conditions. These conditions, which are normally part of the solution, are difficult to specify in detail at a boundary.

(2) Model Development or Selection. Once a physical description of the problem is established, the analyst must create a computational mesh that is used to solve the equations of interest. This step is closely associated with the development of the physical description described above.

Creating a computational mesh is typically an optimization problem with many approaches and possible outcomes. Best practice guidelines instruct the user that square elements aligned with the flow are optimal. Change in element size and element angles must be limited. Wall treatments typically require very thin elements along boundaries. The analyst is faced with resource limitations and typically will have some upper limit to the number of computational elements that are practical. In addition, the complex geometries encountered with industrial applications result in mesh elements that are not ideal. The user must decide how much to size, stretch, grow, and skew the elements in order to end up with a reasonably sized mesh that conforms to the physical domain. Many options are available, and each user will end up with a different mesh design.

In addition to the computational mesh, the user must select the equations as well as any optional terms to be solved. The turbulence model is a major selection, but there are additional terms that can be selected for the energy and momentum equations, such as buoyancy, wall treatments, source terms, and material property options. In many cases, the analyst makes simplifications.

(3) Solution Procedure. The solution of the differential equations on the computational mesh is a time-consuming process that must be carefully monitored. Depending upon the physical models selected, the solution can be unstable and require adjustments to the numerical scheme to avoid code failure. Examples of flows that can be difficult include buoyancy-driven flows, compressible flows with shock waves, and many two-phase flows with phase change. Many of the solvers rely on schemes that have inner iterations that

must converge before moving to the next step. The level of convergence at each step is also a consideration. The differencing scheme is another important component. First-order differencing schemes, although more stable, are known to be less accurate for many flows and are unacceptable for many applications. Attention to details is needed to ensure that the code does an adequate job of predicting the solution to the equations of interest.

(4) Sensitivity Studies and Validation. The complexities of industrial CFD problems make it difficult to rely on a single solution. The set of assumptions and possible compromises impact the predictions, and this impact should be quantified. It is common to perform a set of sensitivity studies and perhaps a validation of the solution. Sensitivity studies are typically carried out for the major assumptions made during the steps in the process. The analyst should consider the sensitivity of key assumptions, simplifications, or modeling choices. Turbulence model and grid size sensitivities are commonly analyzed. The grid convergence index[10] is one method that is gaining in popularity for quantifying the grid-size sensitivity.

Validation involves using properly instrumented experiments to determine whether the model selections (physical models selected) are appropriate for the problem under consideration. This is a costly and time-consuming process that is not typically attempted on something on the scale of an industrial CFD problem. Validation is more likely to involve well-defined separate effects tests. Many CFD problems in the nuclear industry involve multiple types of flow physics for which the code may need to be validated. For instance, a single application may involve buoyancy-driven flows, mixed convection, stratified flows, forced convection, and free jets or plumes all within the same model. A common approach is to validate the code for a large problem by using small separate effects tests for each of the important phenomena.

D. Methods and Codes

Because of the widespread use of this technology and the number of universities, corporations, and research organizations that have developed their own custom CFD tools, CFD codes and methods are too numerous to list. A large number of codes use specific solvers that are customized for a certain type of flow, such as compressible flow over an airfoil or incompressible flow in a pump. Model selection and solver methodologies are limited in these problem-specific tools to what has been proven to be most effective for the intended application. These types of tools are best used only for their intended applications.

The most widely used codes in the nuclear safety community include the commercial codes ANSYS/Fluent and ANSYS/CFX, as well as CD-Adapco's starccm+ code. These codes fall into the category of general-purpose CFD tools and provide well-documented options for several of the most widely used CFD approaches within a single code interface. Open Field Operation and Manipulation (OpenFOAM) is a general-purpose CFD tool that is gaining in popularity because the source code is freely available and the user can become a developer if needed. This type of code requires more effort and knowledge of computer systems than the commercial tools. At a recent workshop sponsored by the Organisation for Economic Co-operation and Development/Nuclear Energy Agency (OECD/NEA), "CFD for Nuclear Reactor Safety

Applications (CFD4NRS-3)," 29 participants from around the world submitted results for a blind CFD benchmark study. More than half of the participants used one of the ANSYS commercial CFD codes, and another 25 percent used either starccm+ or OpenFOAM. The submissions were ranked by comparing the predictions to measured particle image velocimetry data. The top 10 ranked submissions included nine using either ANSYS (seven), starccm+ (one), or OpenFOAM (one).

Some key options or features available in the general-purpose CFD codes include the following.

- custom interface for geometry and mesh design as well as postprocessing
- steady-state or transient solvers
- incompressible or compressible flow solvers
- laminar or turbulent flow options
- turbulent RANS, DES, or LES options
- RANS one equation, two equation, and Reynolds stress turbulent models
- density- or pressure-based solvers
- coupled heat transfer with solids
- segregated or coupled solvers
- multigrid approach
- radiation exchange
- chemical reactions
- multiple species tracking
- multiphase modeling options

The theory manual of any one of the commercial codes, such as that for ANSYS,[11] will more thoroughly explain the options available.

E. Single-Phase Examples

Mixing at T-Junction. Mixing two flows of different temperatures at a pipe junction can lead to temperature fluctuations and ultimately to thermal fatigue of the pipe walls. Industrial plants have a history of thermal fatigue-generated pipe failures. CFD methods are one way to study these phenomena and the impact of possible design solutions such as static mixing vanes. RANS-based CFD approaches do not predict the temperature fluctuations because of the averaging process and the turbulence models involved. Methods such as LES or DES have been applied with some success.[12]

OECD/NEA sponsored a blind benchmark exercise for mixing at a pipe junction.[13] The exercise involved detailed measurements of boundary conditions and mixing phenomena related to thermal mixing from two flows at different temperatures intersecting at a pipe junction. More than 30 researchers from various countries participated in the benchmark exercise, and 29 final results were submitted for comparison with the test data. The U.S. Nuclear Regulatory Commission (NRC) Office of Nuclear Regulatory Research participated in this exercise to support the validation of the codes used by the NRC staff and to develop and maintain expertise in CFD applications. The basic model used by the NRC included the following features:

- LES turbulence approach, dynamic Smagorinsky-Lilly subgrid turbulence
- variable material properties
- bounded central difference for energy equation
- second-order spatial derivatives
- second-order implicit time scheme
- time step equal to 0.0005 second
- 34 million computational volumes
- 0.2 millimeter wall cell thickness
- 0.1-meter-diameter branch pipe connected to 0.14-meter-diameter pipe

The NRC submission was ranked second out of 29 total submissions for the accuracy of the velocity-associated turbulence profiles. For the predictions of a limited set of thermocouple data, the NRC submission was ranked eighth. The majority of the velocity profile comparisons showed that the highest ranked CFD predictions were within the experimental uncertainty. Specific turbulence profiles were also predicted well, especially in directions where the fluctuations were large. In directions where the turbulent fluctuations were small, the predictions did not match as well, in part because of an asymmetry in the data that was most likely the result of an undocumented asymmetry in the facility. The temperature fluctuations near the wall were not predicted as well as the velocity profiles.

This exercise was designed as a CFD benchmark. Boundary conditions were carefully measured, and the domain of interest was relatively small (0.14-meter pipe with 0.1-meter side pipe). The results are indicative of what is possible with CFD using the LES method. The significant computer resources needed to obtain a single set of results for essentially a single flow rate highlight the difficulty with using LES for industrial-scale problems. LES is demonstrated to be a reliable tool, but its application to domains that are orders of magnitude larger is a challenge.

The NRC staff first executed the model using a steady RANS method to establish a crude initial condition. Next, the LES model was executed until the turbulent statistics became established (about 4–8 seconds of flow time). Finally, the staff collected a set of data at 0.0005-second intervals for 20 seconds in order to compute average and root mean square values for the velocity, temperature, and turbulence parameters. This entire process required approximately 5 to 6 weeks running on a 64-bit Linux cluster using 140 3.2-gigahertz processor cores. The mesh size was appropriate in the central region of the model for the LES approach at these conditions. At the wall, however, the cell thickness was approximately five times the recommended value. Using an ideal mesh at the wall would have required additional computer resources and time.

For this particular exercise, the LES approach was warranted because the thermal fatigue issue is related to the magnitude and frequency of temperature fluctuations. A RANS approach could easily obtain steady solutions for the mixing T-junction problem in less than 1 percent of the time, but these solutions would lack the turbulent fluctuations of interest. This example illustrates an ideal application of LES while highlighting the large computational expense.

<u>Severe Accident Natural Circulation Flows</u>. The NRC has been studying thermal-hydraulic phenomena related to low-probability induced-failure scenarios in pressurized-water reactors (PWRs) using CFD tools. A set of predictions is completed for use as a numerical experiment to

determine mixing and entrainment in the hot leg, surge line, and steam generator inlet plenum during specific severe accident natural circulation flow conditions in a PWR. These results are used to determine the distribution of temperatures for the flows entering the steam generator tube bundle, which is needed for an accurate prediction of the potential for thermally induced steam generator tube failures. The results are also used to adjust severe accident system code models to account for the three-dimensional nature of the natural circulation flows during certain periods of the severe accident scenarios. A challenge presented by the work is the extension of a limited set of available test data at $1/7^{th}$ scale to the full-scale conditions. The large scale and complexity of the domain, which includes the entire primary side of a steam generator, the hot leg, and part of the vessel upper plenum, also creates modeling challenges. This type of CFD analysis has more uncertainty than the the T-junction benchmark outlined because of the size and complexity of the issue. The following are some of the challenges and sources of uncertainty:

- The domain too large to mesh using best practice guidelines.
- Thousands of steam generator tubes need to be simplified (reduced in number).
- Details of the severe accident boundary conditions are only best estimates.
- The available integral test is not instrumented sufficiently for CFD validation.
- There are limited or no separate effects data under some of the conditions encountered.

The first step of the analysis was a benchmark study at $1/7^{th}$ scale, which is documented in NUREG-1781, “CFD Analysis of 1/7th Scale Steam Generator Inlet Plenum Mixing During a PWR Severe Accident,” issued October 2003.[14] CFD was used to predict the available data from a test facility designed to establish the natural circulation conditions of interest during a severe accident. The CFD predictions matched the tube bundle flow rates and temperatures very closely, and these predictions provide a valuable confirmation of the ability of the code to predict bulk natural circulation flows and overall mixing for natural circulation flows of this type. The test data are limited to a single inlet plenum design that turns out to be atypical of the designs in operation. In addition, there are concerns related to the scaling of the tube bundle heat transfer rates and overall scaling during the test. Further testing is estimated to be a multimillion dollar effort, so further studies were planned using CFD at full-scale conditions.

A full-scale CFD model[15] with a more detailed tube bundle was created. The model included 1/4 of the vessel upper plenum region, along with a hot leg and the primary side of a steam generator. The vessel region is highly simplified because the resources were not available to model all of the reactor internals. The inlet plenum and hot leg lack some detail at corners and transitions but generally represent the full-scale plant. The model also includes the option for a pressurizer surge line. In order to make the model small enough to become useable for a wide range of sensitivity studies, the more than 3,300 tubes in the bundle are reduced in number. The tube bundle in the model consists of 371 full-height tubes with a total flow area equal to the full-scale plant. Each steam generator tube in the model roughly represents the flow area of nine (a 3x3 grouping) prototypical steam generator tubes. Loss coefficients and a thermal property adjustment are added to the model in the tube bundle region to account for the differences in pressure drop and heat transfer caused by the reduced surface area of the simplified tube bundle.

The CFD modeling approach has the following basic features:

- time-dependent RANS, 0.05-second time step, steady boundary conditions
- ¼ symmetry simplified vessel and upper plenum model
- Reynolds stress turbulence, full buoyancy effects on turbulence
- nonequilibrium wall functions
- temperature-dependent properties (steam and hydrogen) at constant pressure
- hydrogen species tracking
- gravity
- segregated solver with second-order differencing on momentum and energy
- porous media flow loss coefficients in vessel region and simplified steam generator tubes

The finite volume mesh consists of 7.8 million computational volumes (cells) composed mainly of hexagonal elements. Approximately 1 million cells are used for the inlet plenum region where the most complex flows are expected. The tube bundle contains about 6 million hexagonal cells. Special attention was paid to cell quality as outlined in the "NEA/CSNI Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications," issued 2007.[7] The mesh used is significantly improved compared to that used for the 1/7th-scale benchmark study. Where flow direction is known, the hexagonal mesh is flow aligned. Grid angles and grid-density changes are also controlled. The choice of the second-order root mean square turbulence model carries over from the initial studies, in which this option was selected because of the nonisotropic nature of the expected turbulence in the counter-current hot leg flows and the rising plume. This selection is consistent with the recommendations for RANS modeling of counter-current flows.

The set of CFD predictions provides insights into the natural circulation flows that are at the extreme conditions associated with a severe accident. CFD is important in this evaluation because of the three-dimensional nature of the flows and thermal loadings and because of the lack of full-scale experiments. The predictions are used like a numerical experiment to develop an updated mixing model, a hot leg flow model, a surge-line-flow split model, and a distribution of the tube temperatures. The results are used to adjust the flow and mixing parameters in the NRC's one-dimensional severe accident system codes SCDAP/RELAP5 and MELCOR. Challenges still remain in this area because of the lack of available data for proper CFD validation. The work relies on creative modeling to develop the vessel and steam generator models, and CFD best practice guidelines help produce a robust solution for the given set of assumptions. Although the results are far from a final solution, they significantly enhance the understanding of this important phenomenon and help to identify areas for further evaluations or experiments in the future. This problem is an example of the type of large-scale industrial CFD problem that the nuclear safety analyst can encounter.

F. Multiphase CFD—Pressurized Thermal Shock

Multiphase or two-phase CFD techniques are still in a period of rapid development. The number and complexity of empirical correlations involved with these methods make them much more difficult to apply than single-phase CFD techniques. In addition, the correlations available are typically tailored to a specific flow regime (not universal) and suffer from a lack of detailed experimental data for validation. OECD/NEA recently published a survey of multiphase CFD applications for nuclear safety.[16] This document notes that "two-phase CFD is still not very mature" and that best practice guidelines should be updated.

Pressurized thermal shock (PTS) has received a great deal of attention in Europe over the past 15 years, and efforts have focused on developing multiphase CFD techniques for this issue. PTS is a good topic to consider in order to determine what is possible with multiphase CFD tools for reactor-scale problems.

PTS is ultimately a materials issue, and the root cause is radiation embrittlement of the reactor vessel steel and weld material. The embrittlement results in a lack of fracture toughness at lower temperatures that can occur in a PWR system during cooldown transients. The ultimate concern is a reactor pressure vessel failure. A common type of PTS scenario involves a loss-of-coolant accident and the associated injection of relatively cold safety injection flows into the cold leg of the reactor coolant system. System codes such as TRACE or RELAP5 are typically used to predict the system behavior, but these codes cannot model the details of the three-dimensional mixing, heat transfer, and condensation that affect the thermal conditions in the vessel downcomer region. Analysts must rely on experimental investigations, regional engineering models, and more recently three-dimensional CFD codes to more accurately predict the conditions leading to PTS.

An international comparative assessment study[17] in the late 1990s included a thermal-hydraulic portion to help gauge the state of the art in the thermal-hydraulic analysis of PTS events within the nuclear safety community. This study challenged nuclear thermal-hydraulic analysts from around the world to predict downcomer temperatures, condensation rates, and heat transfer coefficients during a postulated PTS event. One scenario of interest involved the injection of cold water into a steam-filled cold leg while the overall system water level was a few meters below the cold leg. Although many of the participants were CFD users who provided CFD predictions for the single-phase portion of the study, none of the participants attempted the multiphase PTS scenario with CFD. Generally speaking, CFD tools in the late 1990s were not considered adequate for this type of problem. Participants relied on regional mixing tools or engineering correlations to predict the flows, heat transfer, and condensation rates. Temperature predictions in the critical downcomer region were scattered over 100 degrees Celsius during parts of the scenario. The reactor vessel wall heat transfer predictions also showed as much as 10,000 $W/m^2/K$ difference between participants. The results of this study highlighted the fact that the prediction of two-phase PTS conditions is a difficult task and the need for improvements in this area.

In 2002, the EUROFASTNET program identified PTS as a key safety issue with significant areas for further research. Follow-on programs such as NURESIM[18] and NURISP,[19] which both highlighted the PTS issue, focused significant resources on improving the ability of multiphase CFD techniques to solve this problem. These efforts involved experimental programs and model development in several countries. Conferences sponsored by OECD/NEA, XCFD4NRS (2008) and CFD4NRS-3 (2010), held dedicated PTS sessions with numerous CFD papers. The recent work demonstrates a trend toward improving capabilities and methods.

The final NURESIM project report[18] outlines several conclusions on PTS modeling. The report recommends a general two-fluid model for PTS simulations but notes that enhancements should be possible in the near future to improve on the existing state of the art. The report recommends RANS codes (steady and unsteady) but notes the potential benefits of LES methods in the future. The modeling of interfacial transfers is another key aspect of the predictions, and different techniques are needed for different flow regimes. In some flow regimes, the interfacial transfer problems remain unresolved. For the wall transfers, none of the available experiments provide a proper validation database. Several new and promising techniques are attempted, but many of the new techniques are simply not mature enough for widespread use. The NURESIM project significantly improved the understanding of the thermal-hydraulic issues associated with the PTS problem and provided a logical framework in which issues were identified and resolved, if possible.

The documents published by OECD/NEA CFD Writing Group 3 provide another view of the state of the art for multiphase PTS analyses. The initial best practice guide (NEA/CSNI/R(2007)5)[7] focused on single-phase CFD techniques. In referring to the PTS example, the concluding remarks noted that further "work is needed in nodalization and model studies to resolve serious discrepancies in results within the downcomer." This study demonstrates that, even for single-phase CFD, for which the models are relatively mature and best practice guidelines are available, good results are not guaranteed. The follow-on CFD assessment report (NEA/CSNI/R(2007)13)[9] includes an assessment of the state of the art for CFD analyses of PTS. The paper provides a good summary of the situation by stating that, "although the single-phase CFD applications seem mature enough to be used, reported attempts were not all successful." This report does not provide details on two-phase CFD predictions but notes that these types of simulations are still "just beginning." A followup report on two-phase CFD applications (NEA/CSNI/R(2010)2)[16] outlines a thorough summary of the important phenomena related to two-phase PTS evaluations. The report notes that two-phase PTS problems are difficult to model because of the variety of two-phase flow conditions in the system. Multiple flow regions are identified, and the important phenomena for each are noted. The report notes that a significant limitation is the need for improved experiments that use sufficient instrumentation to make validation and benchmarking exercises possible. The report makes clear that great strides have been made in the area of two-phase CFD modeling for PTS events, but some phenomena still require significant modeling improvements.

The conclusions drawn from the PTS experience summarized above are that multiphase CFD applications require a significant effort to complete, and the methods are still not robust under many conditions. The tools are nowhere near the maturity level of single-phase CFD techniques. Significant developments are still underway, and multiphase CFD applications are still an area for research.

G. Summary

Modern CFD methods include a wide range of techniques for both single-phase and multiphase flows. Single-phase CFD methods are at an advanced state of maturity but still suffer from a lack of a universal treatment for turbulence. Although DNS techniques are still impractical for industrial CFD evaluations, techniques such as DES and LES are increasing in popularity because of the ever increasing capabilities of modern computer systems. RANS methods are still the most widely used approach because of the efficiency of these techniques and the demonstrated capability to compute realistic solutions under many conditions. The widespread use of RANS means that there will be a continued focus on turbulence modeling approaches.

The complexity and numerous options for CFD application, along with the simplifications and compromises that are commonly made, make the application of CFD as much art as science. Experienced users are still much more likely to obtain realistic solutions than a novice with the same code. Even among experienced users, differences in approach are common. For many large industrial problems, analysts simply cannot strictly adhere to the best practice guidelines that are available. In many cases, simplifications to the geometry or boundary conditions or both are more critical than any mesh design or turbulence modeling approach.

The number of CFD codes and methods available is too large to list. New techniques and codes are added all the time. Fortunately for the user, many of the most promising approaches have become somewhat standardized and are available in general-purpose CFD codes. The common methods have been subjected to a wide variety of benchmark and validation studies, and they have well-documented strengths and deficiencies. The nonlinear Navier-Stokes equation set precludes any general statements, however, and careful attention to validation and testing is still required for each new problem. The field of multiphase CFD is still in a period of rapid development. General-purpose multiphase CFD is still more of an area of research than an application. Methods for some of the simpler multiphase flow regimes have advanced to a high degree of sophistication and have a large number of successful benchmarks. The most successful approaches are usually tied to flow regimes for which an abundance of separate effects test data are available. Moving forward, the reliance of analysts on CFD tools to provide insights in the field of nuclear safety analysis is expected to continue to increase.

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