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HR EXCELLENCE IN RESEARCH

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Available CFD models assessment

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"Available CFD models assessment"
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Glossary

aL	Optical thickness
BSL	Baseline *k-ω*
CFD	Computational Fluid Dynamics
COMET	Coupled Ordinates METhod
CPU	Computer Programming Unit
DDES	Delayed-DES
DES	Detached Eddy Simmulation
DNS	Direct Numerical Simulation
DO	Discrete Ordinates
DPM	Discrete Phase Model
DTRM	Discrete Transfer Radiation Model
EMSP	Évora Molten Salts Platform
GIS	Grid-Induced-Separation
Gr	Grashof number
LES	Large Eddy Simulation
MC	Monte Carlo
P-1	P-1 Radiation model
Ra	Rayleigh number
RANS	Reynolds Averaged Navier-Stokes
Re	Reynolds number
RKE	Realizable *k-ε*
RNG	Renormalization Group *k-ε*
RSM	Reynolds Stress Model
RTE	Radiative Transfer Equation
S2S	Surface-to-Surface
S-A	Spalart-Allmaras
SAS	Scale-Adaptive Simulation
SKE	Standard *k-ε*
SKW	Standard *k-ω*
SRS	Scale-Resolving Simulation
SST	Shear-Stress Transport *k-ω*
URANS	Unstable-RANS
V2F	V^2-f model
WSGGM	Weighted-Sum-of-Gray-Gases Model

1. Overview

The partial differential equations that govern fluid flow and heat transfer are not usually amenable to analytical solutions, except for very simple cases. Therefore, in order to analyze fluid flows, flow domains are split into smaller subdomains (made up of geometric primitives like hexahedron and tetrahedron in 3D and quadrilaterals and triangles in 2D). The governing equations are then discretized and solved inside each of these subdomains.

In the present situation, a finite volume method will be used to solve the approximate representation of the equations' system. Care must be taken to ensure proper continuity of solution across the common interfaces between two subdomains, so that the approximate solutions inside various portions can be put together to give a complete picture of fluid flow in the entire domain. The subdomains are often called elements or cells and the collection of all elements or cells is called a mesh or grid. The origin of the term mesh (or grid) goes back to early days of CFD when most analyses were 2D in nature. For 2D analyses, a domain split into elements resembles a wire mesh, hence the name.

The process of obtaining an appropriate mesh (or grid) is termed mesh generation (or grid generation) and has long been considered a bottleneck in the analysis process due to the lack of a fully automatic mesh generation procedure. In this document, the mesh structure and generation will be addressed and some remarks will be produced.

One of the most formidable and complex challenges in the field of classical physics has been, and still remains, the complete and accurate description of fluid flow. For centuries, its complexity has kept it as an unprecedented intellectual challenge. So, what makes the fluid flow such a difficult subject? The answer lies in turbulence, which, despite the vast number of experimental and theoretical studies for its understanding, has proved to be a matter of great difficulty.

There is no definition of turbulence despite the clear manifestation of its presence. Its existence has profound importance in engineering applications, including fluid flow, and the attempt to mathematically describe turbulence has not produced any satisfactory results. The level of complexity is enormous; turbulent flow settings found in practice are an enormously complex subject.

Considering fluid flow over a complex geometry, it is almost impossible to use analytical tools to describe the developing flow field. This is not only for the case of turbulent flows, but even for laminar flows. However, the development and the maturity level of Computational Fluid Dynamics (CFD) has established a very reliable and efficient tool, which can provide a description of turbulent fluid flows around general geometries, like the flow around a pitching submarine, the transonic flow over a wing, the simulation of an explosion event and many others. Therefore, an appropriate turbulence model must be chosen and some remarks on that will be produced.

Knowledge of combined convective and radiative energy transfer in participating media is also crucial for the determination of heat fluxes on the walls of systems in numerous engineering applications. Examples include boilers of power generating equipment, fossil fuel-fired industrial furnaces for materials processing, high-temperature heat recovery equipment, combustors and rocket engines, hypersonic propulsion, entry and re-entry vehicle protection and numerous others.

There are a number of fundamental difficulties introduced by radiation. The first one is related to the treatment of the spectral nature of thermal radiation, i.e. prediction of the spectral absorption coefficient of gases at elevated temperature and the spectral correlation phenomenon which must be accounted for [Zhang et al., 1988]. The second difficulty is related to the "action at a distance" nature of radiation which, in general, requires the calculation of the local volumetric radiation dissipation rate as an integral over space and spectrum. The third problem comes from the nonhomogeneities in temperature and concentration distributions which strongly impact the spectral absorption coefficient in chemically reacting flows. The fourth difficulty comes from the nonlinear relationship between radiation and fluctuating temperature and/or concentration fields in turbulent flows, because the mean radiative fluxes cannot be predicted based on only mean temperature and concentration fields [Song and Viskanta, 1987]. Again, the available radiation models will be addressed, a preferential model for initial attempts will be chosen and some remarks will also be made.

2. Mesh

In computational solutions of partial differential equations, meshing is a discrete representation of the geometry that is involved in the problem. Essentially, a mesh is the partition of space into elements (or cells) over which the equations can be approximated.

Zone boundaries can be free to create computationally best shaped zones, or they can be fixed to represent internal or external boundaries within a model.

Common cell shapes

There are two types of 2-dimensional cell shapes that are commonly used: the triangle and the quadrilateral. They are computationally poor elements, mainly because they will have sharp internal angles or short edges or both.

- **Triangle:** This cell shape consists of 3 sides and is one of the simplest types of mesh. A triangular surface mesh is always quick and easy to create. It is most common in unstructured grids.
- **Quadrilateral:** This cell shape is a basic 4 sided cell. It is most common in structured grids. Quadrilateral elements are usually excluded from being or becoming concave.

The basic 3-dimensional elements are the tetrahedron, the quadrilateral pyramid, the triangular prism, and the hexahedron. They all have triangular and quadrilateral faces. However, extruded 2-dimensional models may be represented entirely by prisms and hexahedron as extruded triangles and quadrilaterals.

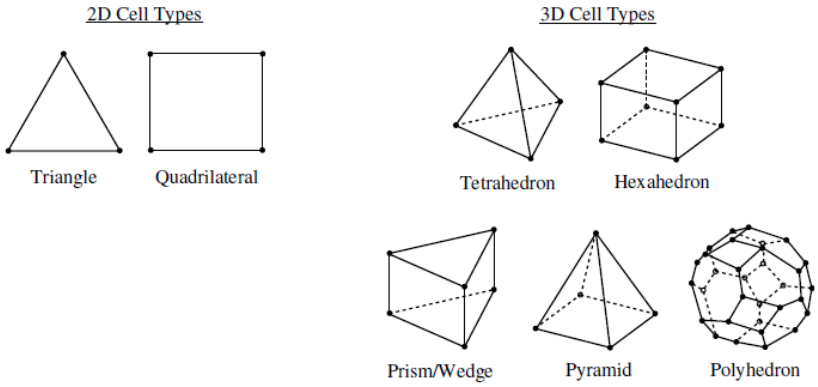

Figure 1: Cell Types.

In general, quadrilateral faces in 3-dimensions may not be perfectly planar. A non-planar quadrilateral face can be considered a thin tetrahedron volume that is shared by two neighboring elements.

- **Tetrahedron:** A tetrahedron has 4 vertices, 6 edges, and is bounded by 4 triangular faces. In most cases a tetrahedron volume mesh can be generated automatically;
- **Pyramid:** A quadrilateral-based pyramid has 5 vertices, 8 edges, bounded by 4 triangular faces and 1 quadrilateral face. These are effectively used as transition elements between square and triangular faced elements and other in hybrid meshes and grids;
- **Triangular prism:** A triangular prism has 6 vertices, 9 edges, bounded by 2 triangular faces and 3 quadrilateral faces. The advantage with this type of element is that it resolves boundary layer efficiently;
- **Hexahedron:** A hexahedron, a topological cube, has 8 vertices, 12 edges, bounded by 6 quadrilateral faces. It is also called a hex or a brick. For the same cell elements count, the accuracy of solutions in hexahedron meshes is the highest;
- **Polyhedral:** There is no explicit face and node numbering for polyhedral cells as with the other cell types. Although, they are expected to have more vertices, edges and faces than a hexahedron. Polyhedral cells are supposed to decrease significantly the number of cells count in a case, however, they are not the best approach in an irregular geometry or near irregular parts of the geometry.

Pyramid and triangular prism zones can be considered computationally as degenerated hexahedrons, where some edges have been reduced to zero and the connecting vertices merged.

Choosing the appropriate mesh type

In 2D geometries, a mesh can be comprised of triangular or quadrilateral cells (or a combination of both) and, in 3D geometries, a mesh can be created using tetrahedron, hexahedron, polyhedral, pyramid or wedge cells (or a combination of some or all of them). Additionally, cells can be arranged in structured, unstructured and hybrid grids, whereas:

- Structured meshes are identified by regular connectivity. The possible element choices are quadrilateral in 2D and hexahedron in 3D. This type of mesh is highly space efficient, considering that the neighborhood relationships are defined by storage arrangement. Some other advantages of structured over unstructured grids are improved convergence and higher resolution;
- An unstructured mesh is identified by irregular connectivity. It cannot easily be expressed as a 2-dimensional or 3-dimensional array in computer memory. This allows for any possible element that a solver might be able to use. Compared to structured meshes, this model can be highly space inefficient since it calls for explicit storage of neighborhood relationships. These grids typically employ triangles in 2D and tetrahedron in 3D;
- A hybrid mesh contains a mixture of structured portions and unstructured portions. It integrates the structured meshes and the unstructured meshes in an efficient manner. The parts of the geometry that are regular can have structured grids and those that have much complex geometry can have unstructured grids. These grids can be non-conformal which means that grid lines don't need to match at block boundaries.

A rule of thumb recommends to use the following configurations:

- For simple geometries use quadrilateral/hexahedron meshes;
- For moderately complex geometries use triangular/tetrahedron meshes with wedge elements in the boundary layer;
- For fairly complex geometries use pure triangular/tetrahedron angular meshes.

The choice of which mesh type to use will depend on the intended application. When choosing the mesh type, a good approach is to consider the following parameters:

- Setup time;
- Computational expense;
- Numerical diffusion.

Setup time

Many flow problems solved in engineering practice involve complex geometries. The creation of structured or block-structured meshes (consisting of quadrilateral or hexahedron elements) for

such problems can be extremely time-consuming if not impossible. Therefore, setup time for complex geometries is the major motivation for using unstructured meshes employing triangular or tetrahedron cells. However, if the geometry is relatively simple, there may be no saving in setup time with either approach.

Other risks of using structured or block-structured meshes with complicated geometries include the oversimplification of the geometry, mesh quality issues, and a less efficient mesh distribution (e.g., fine resolution in areas of less importance) that results in a high cell count.

Computational expense

When geometries are complex or the range of length scales of the flow is large, a triangular/tetrahedron mesh can be created with far fewer cells than the equivalent mesh consisting of quadrilateral/hexahedron elements. This is because a triangular/tetrahedron mesh allows clustering of cells in selected regions of the flow domain. Structured quadrilateral/hexahedron meshes will generally force cells to be placed in regions where they are not needed. Unstructured quadrilateral/hexahedron meshes offer many of the advantages of triangular/tetrahedron meshes for moderately complex geometries.

A characteristic of quadrilateral/hexahedron elements that might make them more economical in some situations is that they allow for a much larger aspect ratio than triangular/tetrahedron cells. A large aspect ratio in a triangular/tetrahedron cell will invariably affect the skewness of the cell, which is undesirable as it may prevent accuracy and convergence. Therefore, if a relatively simple geometry is considered in which the flow conforms well to the shape of the geometry, such as a long thin duct, a mesh of high aspect ratio with quadrilateral/hexahedron cells should be used. The mesh is likely to have far fewer cells than if triangular/tetrahedron cells are used.

Converting the entire domain of the (tetrahedron) mesh to a polyhedral mesh will result in a lower cell count than the original mesh. Although the result is a coarser mesh, convergence will generally be faster, possibly saving some computational expense.

In summary, the following practices are generally recommended:

- For simple geometries, use structured quadrilateral/hexahedron meshes;
- For moderately complex geometries, use unstructured quadrilateral/hexahedron meshes;
- For fairly complex geometries, use triangular/tetrahedron meshes with prism layers;
- For extremely complex geometries, use pure triangular/tetrahedron meshes.

Numerical diffusion

A dominant source of error in multidimensional situations is numerical diffusion (false diffusion). The term false diffusion is used because “this” diffusion is not a real phenomenon, yet its effect on a flow calculation is analogous to that of increasing the real diffusion coefficient. The following comments can be made about numerical diffusion:

- Numerical diffusion is most noticeable when the real diffusion is small, that is, when the situation is convection-dominated;
- All practical numerical schemes for solving fluid flow contain a finite amount of numerical diffusion. This is because numerical diffusion arises from truncation errors that are a consequence of representing the fluid flow equations in a discrete form;
- The amount of numerical diffusion is inversely related to the resolution of the mesh. Therefore, one way of dealing with numerical diffusion is to refine the mesh;
- Numerical diffusion is minimized when the flow is aligned with the mesh.

This is the most relevant to the choice of the mesh. If a triangular/tetrahedron mesh is used, the flow can never be aligned with the mesh. If a quadrilateral/hexahedron mesh is used, this situation might occur, but not for complex flows. It is only in a simple flow, such as the flow through a long duct, in which a quadrilateral/hexahedron mesh is reliable to minimize numerical diffusion. In such situations, it is advantageous to use a quadrilateral/hexahedron mesh, since a better solution will be achieved with fewer cells than with a triangular/tetrahedron mesh.

- If higher resolution for a gradient that is perpendicular to a wall is preferable, prism layers with higher aspect ratios near the wall can be created.

Mesh quality

The quality of the mesh plays a significant role in the accuracy and stability of the numerical computation. The attributes associated with mesh quality are node point distribution, smoothness, and skewness.

Regardless of the type of mesh used in the domain, checking the quality of the mesh is essential. Depending on the cell types used in the mesh (tetrahedron, hexahedron, polyhedral, etc.), different quality criteria are evaluated. However, in a broader approach, the suitability of the mesh can be decided based on the skewness, smoothness, and aspect ratio.

Skewness

This parameter is defined as the "difference" between the shape of the cell and the shape of an equilateral cell of equivalent volume. Highly skewness cells can decrease accuracy and destabilize the solution. The skewness of a grid is an indicator of the mesh quality and suitability. Large skewness compromises the accuracy of the interpolated regions. The more important methods for determining the skewness of a grid are based on:

- **Equilateral volume:** this method is only applicable to triangles and tetrahedron and this is also the default method;

- **Deviation from normalized equilateral angle:** this method applies to all cell and face shapes and is mostly used for prisms and pyramids.

A skewness of 0 is the best possible one and a skewness of one is almost never preferred. Thus low orthogonal quality or high skewness values are not recommended. Generally, a minimum orthogonal quality > 0.1 or maximum skewness < 0.95 must be kept, although for hex and quad cells, skewness should not exceed 0.85 to obtain a fairly accurate solution. However, these values may be different depending on the flow and the location of the cell. Moreover, if the mesh contains degenerate cells, negative cell volumes will be reported.

Smoothness

Rapid changes in cell volume between adjacent cells translate into larger, truncation, errors. The smoothness of the mesh can be improved by refining the mesh based on the change in cell volume or the gradient of cell volume.

Aspect ratio

This is a measure of the stretching of the cell. It is also the ratio of longest to the shortest side in a cell. Ideally, it should be equal to 1 in order to ensure best results. For multidimensional flow, it should be near to one. Also local variations in cell size should be minimal, i.e. adjacent cell sizes should not vary by more than 20% and having a large aspect ratio can result in an interpolation error of unacceptable magnitude. However and for high anisotropic flows, extreme aspect ratios may yield accurate results with fewer cells.

Since you are discretely defining a continuous domain, the degree to which the salient features of the flow (such as shear layers, separated regions, shock waves, boundary layers, and mixing zones) are resolved, depends on the density and distribution of nodes in the mesh. In many cases, poor resolution in critical regions can dramatically alter the flow characteristics. For example, the prediction of separation due to an adverse pressure gradient depends heavily on the resolution of the boundary layer upstream of the point of separation.

The resolution of the boundary layer (i.e., mesh spacing near walls) also plays a significant role in the accuracy of the computed wall shear stress and heat transfer coefficient. And this is particularly true in laminar flows.

A proper resolution of the mesh for turbulent flows is also very important. Due to the strong interaction of the mean flow velocity and turbulence, the numerical results for turbulent flows tend to be more susceptible to mesh dependency than those for laminar flows. In the near-wall region, different mesh resolutions are required depending on the near-wall model being used.

In general, no flow passage should be represented by less than 5 cells. Most cases will require many more cells to adequately resolve the passage. In regions of large gradients, as in shear layers or mixing zones, the mesh should be fine enough to minimize the change in the flow variables from cell to cell. Unfortunately, it is very difficult to determine the locations of important flow features in advance. Moreover, the mesh resolution, in most complicated 3D flow fields, will be constrained by

CPU time and computer resource limitations (i.e., memory and disk space). Although accuracy increases with larger meshes, the CPU and memory requirements to compute the solution and postprocess the results also increase. Solution-adaptive mesh refinement can be used to increase and/or decrease mesh density based on the evolving flow field, and thus provides the potential for more economical use of grid points (and hence reduced time and resource requirements).

Mesh quality recommendations

Several items can be checked and tests can performed in order to better understand the behavior of a mesh. Some of them are explained below.

Rate of convergence

The greater the rate of convergence the better the mesh quality. This means that the correct solution is achieved faster. An inferior mesh quality may leave out certain important phenomena such as the boundary layer that occurs in fluid flow. In such cases the solution may not converge.

The creation of structured or block-structured meshes intended for complex geometries can be time consuming or impossible to converge. This is a major motivation for using unstructured meshes, employing triangular/tetra angular cells.

Solution precision

An improved mesh quality provides a more precise solution. The mesh can be refined at certain areas of the geometry where the gradients are high, increasing the fidelity of solutions in those regions. Thus, the mesh quality is dictated by the required precision and several meshes should be tested before prior to define the final mesh.

CPU time span

CPU time span is a necessary yet undesirable factor. For a highly refined mesh, where the number of cells per unit area is maximum, the CPU time required will be relatively large. Time will generally be proportional to the number of elements. Thus, the definition of an adequate mesh must include this parameter by trying to reduce the number of cells maintaining the results quality.

Grid independence

This is an important test to be performed prior to start using the case definition. A mesh can be designed with much more resolution than the detail needed but, afterwards, that mesh must be coarsened while the results are kept. Once the computations are done and the desired property of fluid does not vary with respect to different mesh elements, the mesh is detailed enough to achieve a good solution without compromising the CPU time span.

Initial solution independence

Additionally, an independence test with regard to the initial solution must also be performed. In that test, different initial solutions, usually both underestimation and overestimation solutions, should be tested to check if the achieved solution is identical.

In addition to the direct tests already mentioned (skewness, smoothness, aspect ratio, etc), the abovementioned tests are essential tools to know how good will the mesh behave.

3. Turbulence

A turbulent flow is a type of fluid (gas or liquid) flow in which the fluid undergoes irregular fluctuations or mixing, in contrast to laminar flow, in which the fluid moves in smooth paths or layers. In turbulent flow the speed of the fluid at a point is continuously undergoing changes in both magnitude and direction.

To model turbulence it is necessary to concern with an unsteady, irregular motion in which transported quantities (mass, momentum, scalar properties) fluctuate in time and space. It is also necessary to pay attention to fluid properties and velocity random variations. Energy transfer is performed from larger eddies to smaller eddies and in smallest eddies turbulent energy is converted to internal energy through viscous dissipation.

Turbulence is the 3-dimensional unsteady random motion observed in fluids at moderate to high Reynolds numbers. As technical flows are typically based on fluids of low viscosity, almost all technical flows are turbulent.

While turbulence is, in principle, described by the Navier-Stokes equations, it is not feasible in most situations to resolve the wide range of scales in time and space by Direct Numerical Simulation (DNS) as the CPU requirements would by far exceed the available computing power for any foreseeable future. For this reason, averaging procedures have to be applied to the Navier-Stokes equations to filter out all, or at least, parts of the turbulent spectrum. The most widely applied averaging procedure is Reynolds-averaging (which, for all practical purposes is time-averaging) of the equations, resulting in the Reynolds-Averaged Navier-Stokes (RANS) equations. By this process, all turbulent structures are eliminated from the flow and a smooth variation of the averaged velocity and pressure fields can be obtained. However, the averaging process introduces additional unknown terms into the transport equations (Reynolds stresses and fluxes) that need to be provided by suitable turbulence models (turbulence closures). The quality of the simulation can depend crucially on the selected turbulence model and it is important to make the proper model choice as well as to provide a suitable numerical grid for the selected model. An alternative to RANS are Scale-Resolving Simulation (SRS) models. With SRS methods, at least a portion of the turbulent spectrum is resolved in at least a part of the flow domain. The most well-known method is Large Eddy Simulation (LES), but many new hybrid models, between RANS and LES, are appearing. As all SRS methods require time-resolved simulations with relatively small time steps, it is important to understand that these methods are substantially more computationally expensive than RANS simulations.

Models

The choice of turbulence model will depend on considerations such as the physics of the flow, the established practice for a specific class of problem, the level of accuracy required, the available computational resources, and the amount of time available for the simulation and so on. To make the most appropriate choice of model for your application, you need to understand the capabilities and limitations of the various options.

The computational effort and cost in terms of CPU time and memory of the individual models must also be part of the equation. While it is impossible to state categorically which model is best for a specific application, general guidelines are presented to help you choose the appropriate turbulence model for the flow you want to model.

The main classes of computational models approaches for modeling turbulent flows are:

- Reynolds-Averaged Navier-Stokes Models (RANS);
- Large Eddy Simulation (LES);
- Direct Numerical Simulation (DNS).

The first category, RANS, solves time-averaged N-S equations and they allow the use of any turbulent length scales. They are used for calculating industrial flows.

The second type of models, LES, solves spatially averaged N-S equations. Large eddies are directly resolved and eddies smaller than the mesh are modeled. This category is less computationally expensive than DNS but most expensive than RANS.

DNS models can simulate all turbulent flows because they can numerically solve the full N-S equations. However, not all CFD packages have this process implemented.

Even though, with the two first classes of models presents several possible combinations of computational models:

- Transition models- used to predict boundary layer development and calculate transition onset;
- Coupling models;
- Reynolds Stress Model (RSM);
- Scale-Adaptive Simulation (SAS) Model
- Reynolds-Averaged N-S Equations (RANS);
- Detached Eddy Simulation (DES);
- Near Wall Treatment for Wall Bounded Turbulent Flow

Reynolds Averaged Navier-Stokes (RANS) Turbulence Models

RANS models (Reynolds (Ensemble) averaging in the Theory Guide) offer the most economic approach for computing complex turbulent industrial flows. Typical examples of such models are the k-ε or the k-ω models in their different forms. These models simplify the problem to the solution

of two additional transport equations and introduce an eddy-viscosity (turbulent viscosity) to compute the Reynolds stresses. More complex RANS models are available that solve an individual equation for each of the six independent Reynolds stresses directly (Reynolds Stress Models – RSM) plus a scale equation (ε-equation or ω-equation). RANS models are suitable for many engineering applications and typically provide the level of accuracy required. Since none of the models is universal, you have to decide which model is the most suitable for a given applications.

Spalart-Allmaras (S-A) one-equation model

The Spalart-Allmaras model is a relatively simple one-equation model that solves a modeled transport equation for the kinematic eddy (turbulent) viscosity. The Spalart-Allmaras model was designed specifically for aeronautics and aerospace applications involving wall-bounded flows and has been shown to give good results for boundary layers subjected to adverse pressure gradients. It is also gaining popularity in turbomachinery applications. Do not use the model as a general purpose model, as it is not well calibrated for free shear flows (large errors for example in jet flows).

k-ε models

Two-equation models are historically the most widely used turbulence models in industrial CFD. They solve two transport equations and model the Reynolds stresses using the eddy viscosity approach. The standard *k*-ε model falls within this class of models and has become the workhorse of practical engineering flow calculations since the time it was proposed by Launder and Spalding [1972]. Robustness, economy, and reasonable accuracy for a wide range of turbulent flows explain its popularity in industrial flow and heat transfer simulations.

There are three differences in the *k*-ε models:

- The method for calculating turbulent viscosity;
- the Prandtl numbers that are present in *k* and ε;
- The generation and destruction of terms in ε-equation.

When nonzero gravity and temperature gradient are simultaneously present, these models account for the generation of *k* due to buoyancy and the corresponding contribution to the production of ε. In such conditions, the effects of buoyancy on the generation of *k* are always included.

In transport equation, turbulent kinetic energy for *k* tends to be augmented in unstable stratification. However, stable stratification buoyancy tends to suppress the turbulence.

Convective heat and mass transfer modeling uses an analogy to turbulent momentum transfer and energy equation may have additional terms depending on the underlying physical model.

The use of the Realizable *k*-ε model is recommended relative to other variants of the *k*-ε family. The *k*-ε model should be used in combination with either the Enhanced Wall Treatment (EWT- ε) or the Menter-Lechner near-wall treatment. For cases where the flow separates under adverse pressure gradients from smooth surfaces (airfoils, and so on), *k*-ε models are generally not recommended.

Standard k-ε (SKE) model (Launder and Spalding)

SKE model is the most used model for industrial applications. It is robust and accurate. It also contains sub models for compressibility, buoyancy, combustion, among other. The limitations of SKE are two:

- One term of ε equation cannot be calculated at the wall;
- The performance for flows with strong separation is poor.

Renormalization Group k-ε (RNG) model

In this model, equations are derived using the statistical technique called renormalization group theory and it yields more accurate results than SKE model.

- RNG has an additional term in the ε -equation that improves the accuracy for strain flows;
- Reynolds number (Re) effect on turbulence is induced enhancing accuracy for swirling flows;
- Differential viscosity to account for low Re effects;
- Analytically derived algebraic formula for turbulent Prandtl number.

This model performs better than SKE for more complex shear flows and flows with high strain rates, swirl and separation. Moreover, RNG provides an option to account for the effects of swirl or rotation by modifying the turbulent viscosity appropriately. The main difference between RNG and SKE is in the fourth term in ε-equation. RNG models yields a lower turbulence viscosity than SKE.

Realizable k-ε model

The term realizable means that the model satisfies certain mathematical constrains on the Re stresses, consistent with the physics of turbulent flows: positivity of normal stresses and Schwarz inequality for Re shear stresses.

This model contains an alternative formulation for the turbulent viscosity. It has a modified transport equation for the dissipation rate ε which has been derived from an exact equation for the transport of the mean square vorticity equation.

Limitations of the model:

- Produces non-physical turbulent viscosities in situations when the computation domain contains both rotating and stationary fluid zones. This is due to the fact of this model includes the effects of mean rotation in the definition of the turbulent viscosity;
- In the equation of transport, the forth term provides a better representation of the spectral energy transfer and the third term doesn't present a singularity as in previous models;
- Turbulent viscosity is modeled as a variable instead of a constant.

Benefits:

- It predicts more accurately the spreading rate of both planar and round jets;

- It also provides superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients, separation and recirculation.

k-ω models

The *ω*-equation offers several advantages relative to the *ε*-equation. The most prominent one is that the equation can be integrated without additional terms through the viscous sublayer. Furthermore, *k-ω* models are typically better at predicting adverse pressure gradient boundary layer flows and separation. The downside of the standard *ω*-equation is a relatively strong sensitivity of the solution depending on the freestream values of *k* and *ω* outside the shear layer. For this reason, the use of the standard *k-ω* model is not generally recommended.

The group of *k-ω* models includes the Standard *k-ω* (SKW), the Baseline *k-ω* (BSL) and the Shear-Stress Transport *k-ω* (SST) models. All of them present similar transport equations for *k* and *ω*. Moreover, the turbulence damping is available only in with *k-ω* models.

The *k-ω* turbulence models have gained popularity mainly because:

- The model equations do not contain terms which are undefined at the wall, which means that they can be integrated to the wall without using wall functions;
- They are accurate and robust for a wide range of boundary layer flows with pressure gradient.

Both the BSL and SST *k-ω* models have been designed to avoid the freestream sensitivity of SKW model, by combining elements of the *ω*-equation and the *ε*-equation. In addition, the SST model has been calibrated to accurately compute flow separation from smooth surfaces. Within the *k-ω* model family, it is therefore recommended to use either the BSL or SST model. These models are some of the most widely used models for aerodynamic flows (namely aerospace and turbo-machinery). They are typically somewhat more accurate in predicting the details of the wall boundary layer characteristics than the S-A model.

Standard k-ω (SKW) model (Wilcox)

This model is based on the Wilcox formulation and it incorporates modifications for low Re effects, compressibility and shear flow spreading. One of the weak points of the Wilcox model is the sensitivity of the solutions to values for *k* and *ω* outside the shear layer (freestream sensitivity).

The standard *k-ω* model is an empirical model based on model transport equations for the turbulence kinetic energy (*k*) and the specific dissipation rate (*ω*), which can also be thought of as the ratio of *ε* to *k*. As the *k-ω* model has been modified over the years, production terms have been added to both the *k* and *ω* equations, which have improved the accuracy of the model for predicting free shear flows. Moreover, an additional limitation of this model is that compressibility effects have not been calibrated for a sufficient number of experiments thus they are disabled by default.

Baseline k-ω (BSL) model (Mentor)

The main down side of the Wilcox model is its well-known strong sensitivity to free stream conditions. The BSL model designed by Mentor was developed to blend the robust and accurate formulation of the *k-ω* model in the near wall region within the free stream independence of the *k-ε* model in the far field. To achieve this, the *k-ε* model was converted into a *k-ω* formulation.

BSL model is similar to SKW model but includes some refinements:

- The SKW model and the transformed *k-ε* model are both multiplied by a blending function and both models are added together;
- BSL incorporates a damped cross diffusion derivative term in *ω*-equation;
- Model constants are different.

Shear Stress Transport (SST) k-ω model

SST model includes the refinements of the BSL model and accounts for the transport of the turbulence shear stress in the definition of the turbulent viscosity. The model is more accurate for a class of flows like adverse pressure gradient flows and airfoils transonic shock waves than both SKW and BSL models. As in the S-A model the concept of wall turbulent viscosity has been adopted.

- The SST *k-ω* model uses a blending function to gradually transition from the SKW near the wall to a high Re number version of the *k-ε* model in the outer region of the boundary layer;
- It also contains a modified turbulent viscosity formulation to account for the transport effects of the principal turbulent shear stress.

The k-kl-ω transition Model

This model is used to predict boundary layer development and calculate transition onset. This model can be used to effectively address the transition of the boundary layer from a laminar to a turbulent regime.

The *k-kl-ω* model is considered to be a three-equation eddy-viscosity type, which includes transport equations for turbulent kinetic energy (k_T), laminar kinetic energy (k_L) and the inverse turbulent time scale (ω).

Transition SST Model

The transition SST model (also known as the γ-Re_θ model) is based on the coupling of the SST *k-ω* transport equations with two other transport equations, one for the intermittency and one for the transition onset criteria, in terms of momentum-thickness Reynolds number. Langtry and Menter developed an empirical correlation to cover standard bypass transition as well as flows in low freestream turbulence environments.

In addition, a very powerful option has been included to allow the user to enter its own user-defined empirical correlation, which can then be used to control the transition onset momentum thickness Reynolds number equation.

Limitations for this model are:

- This model is only applicable to wall bounded flows and not to transition in free shear flows. It will predict free shear flows as fully turbulent;
- The Transition SST model is not Galilean invariant and should therefore not be applied to surfaces that move relative to the coordinate system for which the velocity field is computed (for such cases the intermittency model should be used instead);
- The Transition SST model is designed for flows with a defined nonzero free stream velocity (that is the classical boundary layer situation);
- The transition SST has not been calibrated in combination with other physical effects that affect the source term of the turbulence model, such as buoyancy and multiphase turbulence.

Intermittency Transition Model

The γ (intermittency) transition model is a further development based on the γ-Re_θ transition model (already referred to as the Transition SST model). The γ transition model solves only one transport equation for the turbulence intermittency γ, and avoids the need for the second Re_θ equation of the γ-Re_θ transition model. The γ transition model has the following advantages over the γ-Re_θ transition model:

- It reduces the computational effort (by solving one transport equation instead of two);
- It avoids the dependency of the Re_θ equation on the velocity U, which makes the γ transition model Galilean invariant. It can therefore be applied to surfaces that move relative to the coordinate system for which the velocity field is computed.
- The model has provisions for cross flow instability that are not available for the k-kl-ω or the γ-Re_θ on the transition model.
- The model formulation is simple and can be fine-tuned based on a small number of user parameters.
- Like the γ-Re_θ, the γ transition model is based strictly on local variables.

Model limitations are:

- The γ transition model is only applicable to wall-bounded flows. Like all other engineering transition models, the model is not applicable to transition in free shear flows. The model will predict free shear flows as fully turbulent;
- The γ transition model has only been calibrated for classical boundary layer flows. Application to other types of wall-bounded flows is possible, but might require a modification of the underlying correlations;
- The γ transition model has not been calibrated in combination with other physical effects that affect the source terms of the turbulence model, such as buoyancy or multiphase turbulence.

The V^2-f Model (V2F)

The V^2-f model (V2F) is similar to the standard k-ε model, but incorporates near-wall turbulence anisotropy and non-local pressure-strain effects. A limitation of the V2F model is that it cannot be used to solve Eulerian multiphase problems, whereas the k-ε model is typically used in such applications. The V2F model is a general low-Reynolds number turbulence model that is valid all the way up to solid walls, and therefore does not need to make use of wall functions. Although the model was originally developed for attached or mildly separated boundary layers, it can also simulate accurately flows dominated by separation.

The distinguishing feature of the V2F model is its use of the velocity scale, v^2, instead of the turbulent kinetic energy, k, for evaluating the eddy viscosity. $\overline{v^2}$ can be thought of as the velocity fluctuation normal to the streamlines.

Reynold Stress Model (RSM)

Reynolds Stress Model (RSM) include several effects that are not easily handled by eddy-viscosity models. The most important effect is the stabilization of turbulence due to strong rotation and streamline curvature (as observed for example, in cyclone flows). RSM on the other hand often demand a significant increase in computing time partly due to the additional equations but mostly due to reduced convergence. This additional effort is not always justified by increased accuracy. Their usage is therefore not generally recommended and should be restricted to flows for which their superiority has been established, especially flow with strong swirl and rotation. If wall boundary layers are important, the combination of RSM with the ω- or BSL-equation is more accurate than the combination with the ε-equation. The combination of RSM with BSL removes the free-stream sensitivity observed with the ω-equation in the same way as for two-equation models.

This model is the most elaborate type of RANS turbulence model available at LNEG due to its anisotropic approach of turbulence calculation. Such as most of the remaining models, it solves the transport equation for Re stress together with an equation for dissipation rate. However, unlike those models, that equations are solved for each dimension. Thus, in 2D flows five equations are used and in 3D flows seven equations are used.

The RSM model accounts for the effects of streamline curvature, swirl, rotation and rapid changes in strain rate in a more rigorous manner than the models with one or two equations.

However, fidelity prediction is limited by closure assumptions employed to model various terms in the transport equation terms. Pressure-strain and dissipation rate terms modeling are responsible to compromise the accuracy of this method.

Laminar-Turbulent Transition Models

The Transition SST model (also known as the γ-Re_θ model), the Intermittency Transition model (also known as the γ model) and the Transition k-kl-ω model for transition prediction are available. For many test cases, those three models produce similar results. Due to their combination with the SST model, the Transition SST model and the Intermittency Transition model are recommended over the Transition k-kl-ω model. Among those three models, only the Intermittency Transition model is capable of accounting for crossflow instability.

When using these models, note the following:

- These models are only applicable to wall-bounded flows. Like all other engineering transition models, they are not applicable to transition in free shear flows. They will predict free shear flows as fully turbulent;
- These models have not been calibrated in combination with other physical effects that affect the source terms of the turbulence model, such as:
    - Buoyancy;
    - Multiphase turbulence.
- No special calibration has been performed for the combination of the Transition SST and Intermittency Transition model with scale-resolving methods;
- Proper mesh refinement and specification of inlet turbulence levels are crucial for accurate transition prediction;
- In general, there is some additional effort required during the mesh generation phase because a low-Re mesh with sufficient streamwise resolution is needed to accurately resolve the transition region. Furthermore, in regions where laminar separation occurs, additional mesh refinement is necessary in order to properly capture the rapid transition due to the separation bubble;
- The decay of turbulence from the inlet to the leading edge of the device should always be estimated before running a solution as it can have a large effect on the predicted transition location. Physically correct values for the turbulence intensity should be achieved near the location of transition.

Wall Treatment for RANS Models

The k-ε family and RSM models are not valid in the near wall region, but S-A and k-ω models are valid providing that the mesh is sufficiently fine. To work near walls two approaches can be used:

- Wall Function Approach: for equilibrium and non-equilibrium turbulent boundary layers;
- Enhanced Wall Treatment Option: blended law-of-the-wall and a two-layer zonal model.

It is recommended that you use a y^+-insensitive wall treatment for all models for which it is available (Spalart-Allmaras, ε-equation and ω-equation). It provides the most consistent wall shear stress and wall heat transfer predictions with the least sensitivity to y^+ values.

When Wall Functions are used, it is necessary to avoid fine grids near wall spacing. It is recommended that $y^+>30$ is used in the entire domain. The application of Wall Functions is, however, not generally recommended as they do not allow a systematic refinement of the near wall grid. Wall Functions are especially damaging for flows at low to medium Reynolds numbers (Re$\sim 10^4$-10^6), as the assumption of an extended logarithmic layer is not valid in these cases.

Grid Resolution for RANS Models

Grid generation has a strong impact on model accuracy. There are many considerations that have to be followed when generating high quality CFD grids. From a turbulence modeling standpoint, the most important one is that the relevant shear layers should be covered by at least ~10 cells normal to the layer. Below this resolution, the model will not be able to provide its calibrated performance. Especially for free shear flows, whose location are not known during grid generation, this is a requirement that is hard to achieve. Nevertheless, for lower resolution, the model performance can degrade.

For wall bounded flows, a structured mesh in wall-normal direction is highly recommended. The structured portion of the mesh should cover the entire boundary layer and extend beyond the boundary layer thickness to avoid restricting the growth of the boundary layer. Advanced turbulence models for wall boundary layers like the Spalart-Allmaras model and the SST model will only provide improved results to other models if a minimum of 10 or more structured (hex or prism) cells are located inside the boundary layer. In addition, one should ensure that the prism layer covers the wall boundary layer entirely. Note that these are not specific requirements for these models, but are general requirements for wall boundary layer simulations.

Scale-Resolving Simulation (SRS) Models

The alternative to RANS models are models that resolve at least a portion of the turbulence for at least a portion of the flow domain. Such models are generally termed “Scale-Resolving”.

Large Eddy Simulation (LES) model

The most widely known SRS modeling concept is the Large Eddy Simulation (LES) model. It is based on the approach of resolving large turbulent structures in space and time down to the grid limit everywhere in the flow. However, while widely used in the academic community, LES had very limited impact on industrial simulations. The reason lies in the excessively high resolution requirements for wall boundary layers. Near the wall, the largest scales in the turbulent spectrum are nevertheless geometrically very small and require a very fine grid and a small time step. In addition, unlike RANS, the grid cannot only be refined in the wall normal direction, but also must resolve turbulence in the wall parallel plane. This can only be achieved for flows at very low Reynolds number and on very small geometric scales (the extent of the LES domain cannot be much larger than 10-100 times the boundary layer thickness parallel to the wall). For this reason the use of LES is only recommended for flows where wall boundary layers are not relevant and need not be resolved or for flows where the boundary layers are laminar due to the low Reynolds number.

Hybrid RANS-LES Models

In order to avoid the high resolution requirements of LES model, additional models were developed that combine certain elements of RANS and LES approaches in a way that allows for the simulation of high Reynolds number flows. With hybrid models, the attached wall boundary layers are typically covered by the RANS part of the model, while large detached regions are handled in ‘LES’ mode, meaning with a partial resolution of the turbulent spectrum in space and time. Hybrid models rely

on a strong enough flow instability to generate turbulent structures in the separated zone. This is typically the case for flows behind bluff bodies, where URANS (unstable-RANS) models predict single-mode periodic vortex shedding. Hybrid models allow these vortices to generate smaller eddies down to the available grid limit.

Scale-Adaptive Simulation (SAS) Model

SAS is an improved RANS formulation which allows the resolution of the turbulent spectrum in unstable flow conditions. The introduction of Von Karman length scale into the turbulent scale equation allows SAS models to dynamically adjust to resolved structures in a URANS simulation. More specifically, the inclusion of this term allows the model to adjust its length scale to already resolved scales in the flow and thereby provide a low enough eddy viscosity to allow the model to operate in 'LES' mode.

Detached Eddy Simulation (DES) model

The DES model achieves the switch between RANS and LES by a comparison of the turbulent length scale with the grid spacing. The model selects the minimum of both and thereby switches between RANS and LES. Once the model selects the grid spacing as the minimum, the model is operating in 'LES' mode.

The grid spacing enters explicitly into the DES model. This can affect the RANS solution in regions, where the grid is between RANS and LES resolution (so-called "gray zones" in DES) and/or where the flow instability is not strong enough to generate LES structures. Another issue to consider with DES is the problem of "grid-induced-separation" (GIS). It occurs if the grid for an attached wall boundary layer flow is refined to a point where the DES limiter becomes active and affects the RANS solution. However, in such situations, the flow instability is not strong enough to balance the reduced RANS content by the resolved turbulence. This will typically result in an artificial flow separation at the location of the grid refinement.

A blending function of the SST-DES model was proposed by Menter *et al.* to shield the boundary layers from the DES limiter. Later, alternative blending functions for the same purpose have been proposed by Spalart *et al.* [Daly and Harlow, 1970] resulting in the terminology Delayed-DES (DDES). The DDES model, as originally proposed for the Spalart-Allmaras model, provided limited protection against GIS for two-equation models such as BSL, SST, and k-ε. Therefore, the DDES function has been re-calibrated for the BSL, SST, and k-ε models and is now the recommended choice and the default setting when using these models.

Near-Wall treatments for wall bounded turbulent flows

Turbulent flows are significantly affected by the presence of walls. The mean velocity field is affected through the no-slip condition that has to be satisfied at the wall. However, the turbulence is also changed by the presence of the wall in non-trivial ways. Very close to the wall, viscous damping reduces the tangential velocity fluctuations, while kinematic blocking reduces the normal velocity fluctuations. Toward the outer part of the near-wall region, however, the turbulence is

rapidly augmented by the production of turbulence kinetic energy due to the large gradients in mean velocity.

The near-wall modeling significantly impacts the fidelity of numerical solutions, inasmuch as walls are the main source of mean vorticity and turbulence. After all, it is in the near-wall region that the solution variables have large gradients and the momentum and other scalar transports occur most vigorously. Therefore, accurate representation of the flow in the near-wall region determines successful predictions of wall-bounded turbulent flows.

Traditionally, there are two approaches to model the near-wall region. In one approach, the viscosity affected inner region (viscous sublayer and buffer layer) is not resolved. Instead, semi-empirical formulas called "wall functions" are used to bridge the viscosity-affected region between the wall and the fully turbulent region. The use of wall functions obviates the need to modify the turbulence models to account for the presence of the wall.

In another approach, the turbulence models are modified to enable the viscosity-affected region to be resolved with a mesh all the way to the wall, including the viscous sublayer. For the purposes of discussion, this will be termed the "near-wall modeling" approach. These two approaches are depicted schematically in Figure 2.

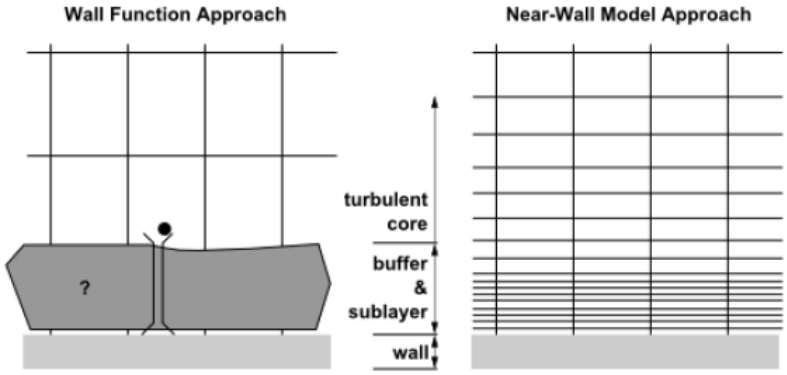

Figure 2: Available near-Wall Treatments.

The main shortcoming of all wall functions is that the numerical results deteriorate under refinement of the grid in the wall normal direction. y^+ values less than 15 will gradually result in unbounded errors in wall shear stress and wall heat transfer. While this was the industrial standard some years ago, steps had been taken to offer more advanced wall formulations, which allow a consistent mesh refinement without a deterioration of the results. Such y^+–independent formulations are the default for all ω-equation-based turbulence models. For the ε-equation-based models, the Menter-Lechner and Enhanced Wall Treatment (EWT) serve the same purpose. A y^+-insensitive wall treatment is also the default for the Spalart-Allmaras model and allows you to run this model independent of the near-wall y^+ resolution.

Model Hierarchy

As discussed, turbulence modeling is a balance between accuracy and cost. The recommendation is to use RANS models as much as possible and as long as they provide the accuracy required for the simulation. RANS models will remain the workhorse of turbulence modeling for many years to come. Within the RANS family, eddy-viscosity models are typically sufficient for most engineering flow simulations. The application of RSM is only recommended for flows that are known to systematically benefit from their usage and justify the increase in computing power.

In cases where steady RANS or URANS models cannot provide the accuracy or unsteady information required, it is recommended that you switch to the SAS approach. It is relatively forgiving in terms of the grid resolution and will not deteriorate the results in case of insufficient resolution in the unsteady zone. The SAS model will only provide scale-resolution if a strong flow instability is present. Visual inspection (using iso surfaces of the Q criterion) will quickly allow for the judgment whether the model provides sufficient unsteadiness and resolution relative to the grid spacing.

The most important models, their differences and applications are summarized in Table 1. The computational cost per iteration of the referred models increases from the top to the bottom of Table 1.

Table 1: Turbulence models summary.

Models	Description and Application
RANS - One Equation	
Spalart-Allmaras	Is a single transport equation model solving directly for a modified turbulent viscosity. It may include strain rate in k production term. Is well suited to aerospace applications involving wall bounded flows near wall mesh. Allows the use of coarse meshes. Economical for large meshes. Suitable for quasi-2D external/internal flows and boundary-layer flows. Applicable to airfoils, wings, airplanes, missiles.
RANS - Two Equation	
Standard k-ε	Is a two transport equations model solving for k and ε. Its coefficients are empirical derived. Presents options to account for viscous, heating, buoyancy, and compressibility. Is valid for fully developed flows. Is robust. Is widely used. Is suitable for initial iterations, initial screening of alternative designs and parameterized studies.
RNG k-ε	Its equations and coefficients are analytically derived. Improved the ability to model strained flows. Presents options for swirl and low Reynolds number flows modelling. Is applied to shear flows involving rapid strain moderate swirl, vortices and local transitional flow.
Realizable k-ε	Is a mathematical improvement to SKE in order to obtain a better performance. Has similar applications as RNG. Is more accurate and easier to converge.
Standard k-ω	Is a two transport equation model solving for k and the specific dissipation rate ω (ε/k). Has superior performance for wall bounded low Reynolds number flows. Can predict transition flows. Presents option for free shear and compressible flows. Is applicable to complex boundary layer flows under adverse pressure gradient and separation: aerodynamics and turbo-machinery.
Baseline k-ω	Combines the SKW near the wall and SKE away from the wall using a blending function. Model constants are different from SKE. Incorporates a damped cross diffusion term and limits turbulent viscosity.

SST *k-ω*	Same refinements as BSL. Also accounts for the transport of the turbulence shear stress in the definition of the turbulent viscosity. Dependency on wall distance, makes this model less suitable for fee sheer flows.
Reynolds Stress Model	Is solved directly using transport equations for highly swirling flows. Avoids isotropic eddy viscosity assumption. Requires more CPU time and memory. Suitable for complex 3D with strong streamline curvature, strong swirl, rotation like cyclones.
SRS - Models	Description and Application
Large Eddy Simulation (LES)	Is based on the approach of resolving large turbulent structures in space and time down to the grid limit everywhere in the flow. Momentum, mass energy are transported by large eddies. Is applicable to all combustion models. Has excessively high resolution requirements for wall boundary layers.
Detached Eddy Simulation (DES)	Can work between RANS and LES by a comparison of the turbulent length scale with the grid spacing. In some conditions, when the grid for an attached wall boundary layer flow is refined, DES can affect the RANS solution. In such cases, an artificial flow separation can result at the location of grid refinement. Is suitable for complex 3D geometries with strong streamline curvature, strong swirl, rotation like cyclones. Requires more CPU time and memory.

4. Radiation

The flow of thermal energy from matter occupying one region in space to matter occupying a different region in space is known as heat transfer. Heat transfer can occur by three main methods: conduction, convection, and radiation. Physical models involving conduction and/or convection only are the simplest, while buoyancy-driven flow or natural convection, and radiation models are more complex.

Natural Convection and Buoyancy-Driven Flows

When heat is added to a fluid and the fluid density varies with temperature, a flow can be induced due to the force of gravity acting on the density variations. Such buoyancy-driven flows are termed natural convection (or mixed-convection) flows and can be modeled.

The importance of buoyancy forces in a mixed convection flow can be measured by the ratio of the Grashof (Gr) and Reynolds (Re) numbers. When this ratio approaches or exceeds unity, strong buoyancy contributions to the flow should be expected. Conversely, if it is very small, buoyancy forces may be ignored in the simulation. In pure natural convection, the strength of the buoyancy-induced flow is measured by the Rayleigh number (Ra), whereas Rayleigh numbers less than 10^8 indicate a buoyancy-induced laminar flow, with transition to turbulence occurring over the range of $10^8 < Ra < 10^{10}$.

Radiation Models

There are six models available at LNEG that allow to include radiation, with or without a participating medium, in the heat transfer simulations. Heating or cooling of surfaces due to radiation and/or heat sources or sinks due to radiation within the fluid phase can be included in the model using one of the following radiation models:

- Discrete Transfer Radiation Model (DTRM);

- P-1 (P-1) Radiation model;
- Rosseland Radiation model;
- Surface-to-Surface (S2S) Radiation model;
- Discrete Ordinates (DO) Radiation model;
- Monte Carlo (MC) Radiation model.

Typical applications well suited for simulation using radiative heat transfer and in the scope of the subtask include the following:

- Radiative heat transfer in flows;
- Surface-to-surface radiation heating or cooling;
- Coupled radiation, convection and/or conduction heat transfer;

Radiative heat transfer should be included in the simulation when the radiant heat flux is large compared to the heat transfer rate due to convection or conduction. Typically, this will occur at high temperatures where the fourth-order dependence of the radiative heat flux on temperature implies that radiation will dominate. For all models, particular attention should be paid in order to effectively represent the filler material inside the thermal energy storage tank and the radiation scattering due to the filler material.

Discrete Transfer Radiation Model (DTRM)

The main assumption of the DTRM is that the radiation leaving the surface element in a certain range of solid angles can be approximated by a single ray (Figure 3), thus instead of solving radiation heat transfer for an entire area, that area is replaced by a set of single rays and the radiation equation is solved only for those. Considering that a solid geometry is used, spherical coordinates are also used.

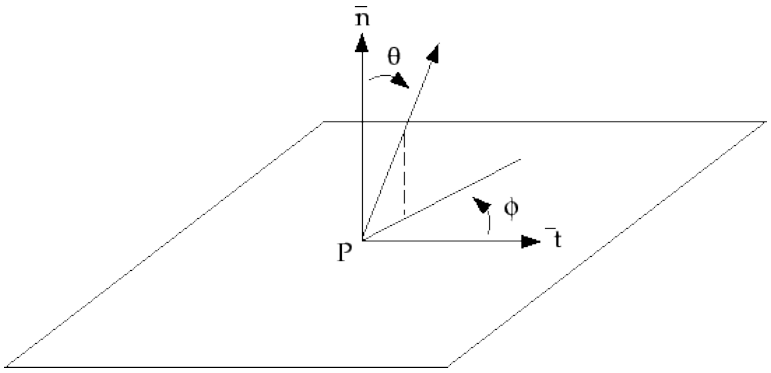

Figure 3: DTRM single ray approximation.

The ray paths are calculated and stored prior to the fluid flow calculation. At each radiating face, rays are fired at discrete values of the polar and azimuthal angles. Each ray is then traced to determine the control volumes it intercepts as well as its length within each control volume. This information is then stored in the radiation file.

There are three primary advantages of the DTRM: it is a relatively simple model, you can increase the accuracy by increasing the number of rays, and it applies to a wide range of optical thicknesses.

The user should also be aware of the following limitations when using the DTRM:

- It assumes that all surfaces are diffuse. This means that the reflection of incident radiation at the surface is isotropic with respect to the solid angle;
- The effect of scattering is not included;
- The implementation assumes gray radiation;
- Solving a problem with a large number of rays is CPU-intensive;
- It is not compatible with non-conformal interfaces or sliding meshes;
- It is not compatible with parallel processing (this limitation will probably invalidate the possibility of use this model).

P-1 radiation (P-1) model

The P-1 radiation model is the simplest case (four term) of the more general P-N model, which is based on the expansion of the radiation intensity into an orthogonal series of spherical harmonics [Cheng, 1964]. By default, only gray radiation is modeled. However, the modeling of non-gray radiation can be achieved using a gray-band model. Thus, particular wavelengths can be specified by start and end of the wavelength of the band. Because the cost of computation increases directly with the number of bands, the number of used bands should be minimized.

Included in the P-1 radiation model is the capability for modeling anisotropic scattering by means of a linear-anisotropic scattering phase function. A positive value for the linear-anisotropic phase function coefficient indicates that more radiant energy is scattered forward than backward, and a negative value means that more radiant energy is scattered backward than forward. A zero value defines isotropic scattering (that is, scattering that is equally likely in all directions).

The P-1 model has several advantages over the DTRM. For the P-1 model, the radiative transfer equation (RTE) is a diffusion equation, which is easy to solve with little CPU demand. The model includes the effect of scattering. For example, in combustion applications where the optical thickness is large, the P-1 model works reasonably well. In addition, the P-1 model can easily be applied to complicated geometries with curvilinear coordinates.

The following limitations should be considered when using the P-1 radiation model:

- The P-1 model assumes that all surfaces are diffuse. This means that the reflection of incident radiation at the surface is isotropic with respect to the solid angle;
- The implementation is restricted to either gray radiation or non-gray radiation using a gray-band model. The non-gray implementation assumes a constant absorption coefficient within each wavelength band. The non-gray implementation also assumes the spectral emissivity at walls to be constant within each band;
- There may be a loss of accuracy, depending on the complexity of the geometry, if the optical thickness is small;
- The P-1 model tends to over-predict radiative fluxes from localized heat sources or sinks.

Rosseland radiation model

The Rosseland or diffusion approximation for radiation is valid when the medium is optically thick. Radiative equilibrium is achieved and radiation acts purely diffusively with source terms due to emission. Example of an optically thick medium is melted glass.

The Rosseland or diffusion approximation for radiation is valid when the medium is optically thick and is recommended for use in problems where the optical thickness is greater than 3. It can be derived from the P-1 model equations, with some approximations. The Rosseland radiation model differs from the P-1 model because it assumes that the intensity is the black-body intensity at the gas temperature. The Rosseland model allows for anisotropic scattering, using the same phase function described for the P-1 model.

The Rosseland model has two advantages over the P-1 model. Since it does not solve an extra transport equation for the incident radiation (as the P-1 model does), the Rosseland model is faster than the P-1 model and requires less memory.

Note that the Rosseland model is not available when the density-based solver is being used; it is available only with the pressure-based solver. However, in this case this does not seem a problem.

The Discrete Ordinates (DO) radiation model

The discrete ordinates (DO) radiation model solves the radiative transfer equation (RTE) for a finite number of discrete solid angles, each associated with a vector direction $\vec{s}$ fixed in the global Cartesian system (x, y, z). The fineness of the angular discretization can be controlled, analogous to choosing the number of rays for the DTRM. Unlike the DTRM, however, the DO model does not perform ray tracing. Instead, the DO model transforms the radiative transfer equation (RTE) into a transport equation for radiation intensity in the spatial coordinates (x,y, z). The solution method is identical to that used for the fluid flow and energy equations. The DO model solves for as many transport equations as there are directions $\vec{s}$.

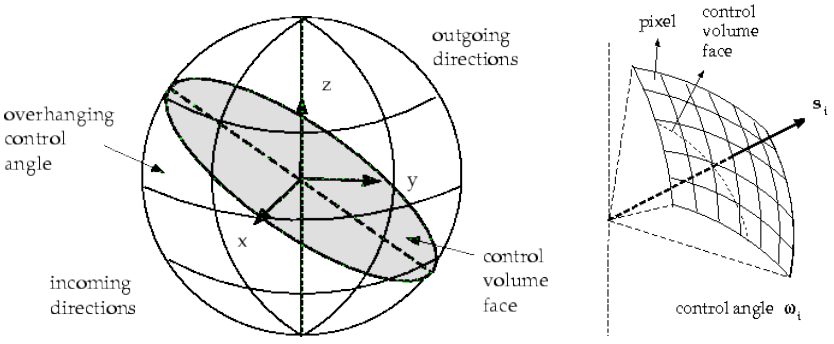

Figure 4: a) position of the cell face; b) grid with vector direction $\vec{s}$.

Two implementations of the DO model are available: uncoupled and (energy) coupled. The uncoupled implementation is sequential in nature and uses a conservative variant of the DO model

called the finite-volume scheme [Chui and Raithby, 1993] and its extension to unstructured meshes [Murthy and Mathur, 1998]. In the uncoupled case, the equations for the energy and radiation intensities are solved one by one, assuming prevailing values for other variables.

Alternatively, the coupling between energy and radiation intensities at a cell, which is also known as Coupled Ordinates METhod (COMET) [Mathur and Murthy, 1999], accelerates the convergence of the finite volume scheme for radiative heat transfer. This method results in significant improvement in the convergence for applications involving optical thicknesses greater than 10. This feature is advantageous when scattering is significant, resulting in strong coupling between directional radiation intensities.

DO admits a variety of scattering function phase, such as isotropic phase function, linear anisotropic phase function, Delta-Eddington phase function or even a user-defined phase function. The DO model allows to include the effects of a discrete second phase of particulates on radiation. For non-gray radiation, absorption, emission and scattering due to the particulate phase being included in each wavelength band for the radiation calculation. Particulate emission and absorption terms are also included in the energy equation.

There are some instances when COMET is not recommended or it is incompatible with certain models:

- COMET is not recommended for cases with weak coupling between energy and directional radiation intensities. This may result in slower convergence of the coupled approach compared to the sequential approach.
- COMET is not available when solving enthalpy equations instead of temperature equations.
- Specifically, COMET is not compatible with the non-premixed or partially premixed combustion models (in this situation this is not a limitation).

The DO model spans the entire range of optical thicknesses and allows you to solve problems ranging from surface-to-surface radiation to participating radiation in combustion problems. It also allows the solution of radiation at semi-transparent walls. Computational cost is moderate for typical angular discretization and memory requirements are modest. However, solving a problem with a fine angular discretization may be CPU-intensive.

The current implementation is restricted to either gray radiation or non-gray radiation using a gray-band model. The non-gray implementation is compatible with all the models available with which the gray implementation of the DO model can be used. Thus, it is possible to include scattering, anisotropy, semi-transparent media, and particulate effects. However, The DO model is not supported for use with granular (fluid-solid) Eulerian multiphase flows.

Surface-to-Surface (S2S) radiation model

The S2S radiation model can be used to account for the radiation exchange in an enclosure of gray-diffuse surfaces. The energy exchange between two surfaces depends in part on their size,

separation distance and orientation. These parameters are accounted by a geometric function called a "view factor".

The main assumption of the S2S model is that any absorption, emission or scattering of radiation can be ignored; therefore, only "surface-to-surface" radiation need be considered for analysis. Thus, this is a non-participating media method and it is based on view factor.

The surface-to-surface (S2S) radiation model is good for modeling the enclosure radiative transfer without participating media (for example, spacecraft heat rejection systems, solar collector systems, radiative space heaters and automotive underhood cooling systems). In such cases, the methods for participating radiation may not always be efficient. As compared to the DTRM and the DO radiation models, the S2S model has a much faster time per iteration, although the view factor calculation itself is CPU-intensive. This increased time for view factor calculation will be especially pronounced when the emitting/absorbing surfaces are the polygonal faces of polyhedral cells.

The S2S radiation model is computationally very expensive when you calculate the radiation and view factors for a large number of surfaces. To reduce the computational time as well as the storage requirement, the number of surfaces is reduced by creating surface "clusters". The surface clusters are made by starting from a face and adding its neighbors and their neighbors until a specified number of faces per surface cluster is collected.

By default, view factors are calculated using a face to face basis, in which clustering is used in a limited way only. The boundary faces act as surfaces for the view factor calculation and then a cluster view factor is obtained by taking the area-weighted average of the view factors of the faces within the cluster.

The following limitations should be considered when using the S2S radiation model:

- The S2S model assumes that all surfaces are diffuse;
- The implementation assumes gray radiation;
- The storage and memory requirements increase very rapidly as the number of surface faces increases;
- The S2S model cannot be used to model radiation problems with participating medium;
- The S2S model with the hemicube view factor method cannot be used if your model contains symmetry or periodic boundary conditions (depending on how the geometry will be defined, this may create limitations to use of this model);
- The S2S model does not support hanging nodes or hanging node adaption on radiating boundary zones.

Monte Carlo (MC) radiation model

The Monte Carlo radiation model simulates the underlying processes that govern the system of interest (that is, the physical interactions between photons and their environment). A photon is selected from a photon source and tracked through the system until its weight falls below some minimum, at which point it "dies". Each time the photon experiences an "event" (for example, a surface intersection, scattering or absorption), the physical quantities of interest are updated. This process generates a complete "history" of that photon in the system. Many photon histories need to be generated to get good estimates of the physical quantities of interest in a system. Photon sources

are selected (that is, "sampled") on the basis of emitted radiation, each band being treated independently for non-gray models.

For the radiative transfer equation (RTE), the Monte Carlo model assumes that the intensity is proportional to the differential angular flux of photons and treats the radiation field as a photon gas. Providing that the spectral (multiband) selection is done properly, the Monte Carlo tallying automatically integrates over the spectrum. Boundary conditions for the non-gray DO model are applied on a band basis. The treatment within a band is the same as that for the gray DO model.

The Monte Carlo radiation model generates photons in a stochastic (random) manner and will therefore produce speckled results if the target number of histories is relatively small. Increasing the target number of histories produces a smoother and more accurate solution, but at the expense of higher computation effort.

The MC model can solve problems ranging from optically thin (transparent) regions to optically thick (diffusion) regions, like combustion. It allows you to calculate quasi-exact solutions. While it is more accurate compared to other available models, it has a higher computational cost.

The following limitations can be found when using the MC radiation model:

- Has a higher computational cost;
- Among several other conditions[1], the following are currently not supported with the Monte Carlo model:
    - 2D cases;
    - Thin walls (as baffles);
    - Semi-transparent boundary condition on external walls;
    - Porous medium (this may invalidate the use of the model);
    - Discrete Phase Model (DPM) and multiphase models.

Comparison between radiation models

The DTRM, P-1, Rosseland, DO and MC radiation models require the absorption coefficient of the radiative Transfer Equation (RTE) as an input but the scattering coefficients can be constants. The absorption coefficient can be a function of local concentration of H_2O and CO_2, path length and total pressure (WSGGM).

The P-1 and DO radiation models are solved for the mixture material. Radiative properties like absorption coefficient, refractive index and scattering coefficient of the mixture are computed based on the volume fraction based averaging of the radiative properties of the individual phases. In simulations that use the porous media model with a radiation model the contribution of the radiative heat source in the energy calculation are scaled by the local porosity.

[1] For more details, please refer to "ANSYS Fluent Theory Guide", Release 18.2, August 2017, ANSYS, Inc, Canonsburg, PA, USA.

How to Choose a Radiation Model?

For certain problems, a particular radiation model may be more appropriate than the others. When deciding which radiation model to use, consider the following:

- Optical thickness: The optical thickness, aL, is a good indicator of which model to use in intended problem. Here, L is an appropriate length scale for the domain. For flow in a combustor, for example, L is the diameter of the combustion chamber. If $aL>>1$, your best alternatives are the P-1 and Rosseland models. The P-1 model should typically be used for optical thicknesses >1. For optical thickness >3, the Rosseland model is cheaper and more efficient. For high optical thickness cases, a second-order discretization scheme for the DO model is recommended. The DTRM, DO and MC models work across the full range of optical thicknesses but are substantially more expensive to use. Consequently, you should use the "thick-limit" models, P-1 and Rosseland, if the problem allows it. For optically thin problems ($aL<1$), only the DTRM, DO and MC models are appropriate;
- Scattering and emissivity: the P-1, Rosseland and DO models account for scattering, while the DTRM neglects it. Since the Rosseland model uses a temperature slip condition at walls, it is insensitive to wall emissivity;
- Particulate effects: only the P-1 and DO models account for exchange of radiation between gas and particulates;
- Non-gray radiation: only the P-1, DO and MC models allow you to compute non-gray radiation using a gray-band model.

In Table 2, a summary of the advantages and limitations of the radiation models is presented.

Table 2: Summary of Radiation Models.

Parameter	Advantages and limitations
Optical Thickness	aL>> DO; aL>3: Rosseland; aL>1: P-1; DTRM, DO and MC models are suitable for all optical-thickness but they are substantially more expensive to use. aL>1: Only DTRM, DO and MC models are suitable.
Scattering and emissivity	P-1, Rosseland and DO models account for scattering.
Particulate Effects	Only P-1 and DO models account for exchange on radiation between gas and particulates.
No-Gray Radiation	P-1, DO and MC models allow to compute non-gray radiation using a gray-band model.

Optical properties for radiation models

Depending on the chosen radiation model several optical properties may be needed, as described in Section "Comparison between radiation models". Those properties are defined in Table 3 and when they are needed they are needed in a pack. Table 4 describes the need of the pack of optical properties in the radiation models by material (fluid or solid).

Table 3: Optical properties package for radiation models.

Property	Description
Absorption Coefficient [1/m]	To define the absorption coefficient, you can specify a constant value, a temperature-dependent function, a composition-dependent function, or a user-defined function. The absorbing and emitting parts of the radiative transfer equation (RTE) are a function of the absorption coefficient. The absorbing or emitting effects depend on the chosen radiation model. If there are only absorption effects, then Lambert's Law of absorption applies. Along with the scattering coefficient, it describes the change in radiation intensity per unit length along the path through the fluid medium.
Scattering Coefficient [1/m]	The scattering coefficient is, by default, set to zero, and it is assumed to be isotropic. The user can specify a constant value, a temperature-dependent function, or a user-defined function. The user can also specify a non-isotropic phase function. Along with the absorption coefficient, it describes the change in radiation intensity per unit length along the path through the fluid medium. You may want to increase the scattering coefficient in systems where particulate matter may be present in the flow.
Scattering Phase Function	Scattering is assumed to be isotropic, by default, but the user can also specify a linear-anisotropic scattering function. If the used radiation model is DO model, Delta-Eddington and user-defined scattering functions are also available.
Refractive Index	The refractive index is the ratio of speed of light in the medium to the speed of light in vacuum. **It is by default set to 1**. The user can specify a constant value in the field next to Refractive Index.

Table 4: Pack of optical properties for the radiation models.

Material	Radiation models					
	DTRM[a]	P-1	Rosseland	DO	S2S	MC
Fluid	Y[b]	Y	Y	Y	N	Y
Solid	N	N	N	Y	N	

[a] The DTRM model is not compatible with parallel processing. [b] In the DTRM model only the Absorption Coefficient is required.

5. Concluding remarks

From the assessment hereby presented, some remarks will point the initial definitions for the modelling work to be developed in the scope of subtask 5.1 of WP5. These remarks will not be mandatory and, at any time, will limit future developments of the models. In line, with the present document, these remarks will address the mesh structure, the turbulence model and radiation model.

Mesh structure

Previous experience would lead us to an unstructured mesh according to more complex geometries. Moreover, the modelling of chemistry reactivity, usually considered, would be greatly improved with the use of an unstructured mesh due to the presence of turbulence in shear walls.

However, the expected geometry for the thermal energy storage tank to be built at EMSP (Évora Molten Salts Platform) may, indeed, be very suitable to a structured mesh. Thus, a first attempt in order to determine Reynolds (Re), Grashof (Gr) and Raleigh (Ra) numbers can be made using a structured mesh. If the wall effect is relevant enough for thermal diffusion due to near wall eddies or if the numerical convergence reveals itself hard to achieve, an unstructured solution will be attempted.

Moreover, the computational costs will also be addressed. However, the structure of the mesh can be highly dependent on the developed flow. Therefore, the type of mesh and the turbulence model will evolve side by side in order to choose the most interesting combination to study the proposed problem.

Turbulence model

Due to some limitations discussed previously in this document, the turbulence model must be defined only after both Re, Gr and Ra numbers are known. The knowledge of those numbers will allow us to better understand what type of flow will generally be developed inside the tank and, more specifically, near the walls. However, although the ease of use presented by the Spalart-Allmaras model, the versatility presented by the SST k-ω seems to represent a better choice for an initial attempt. Afterwards, the convergence response and the computational expense of both mesh and turbulence model will be assessed in order to define what can be the least expensive solutions without compromising the results.

Radiation model

With regard to the radiation model, several other problems must be addressed. The optical thickness is one of the most interesting parameters to consider in order to choose the radiation model. Although, several meters are an appropriate length scale for the domain, radiation will certainly find it hard reach surfaces across a medium with more than 60% (v/v) of opaque solid material. Thus, the most suitable radiation models for that length scale (e.g. P-1 or Rosseland) may very well yield inadequate results if the optical thickness were to be addressed as the mean free path. Therefore, if the appropriate length scale is reduced to a length of few centimeters, eventually other models should be considered (e.g. DTRM, DO or MC).

However, the DTRM is not compatible with parallel processing and DO model needs the optical properties package.

In conclusion, if a model capable of work across a full range of optical thicknesses must be used for a first approach (e.g. DTRM, DO or MC), it must be done accounting for the limitations of the models. The computational costs can also be addressed, but the DO model is a good candidate, providing that the packed bed is represented by porous material instead of multiphase material and that some partner provide the optical properties.

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